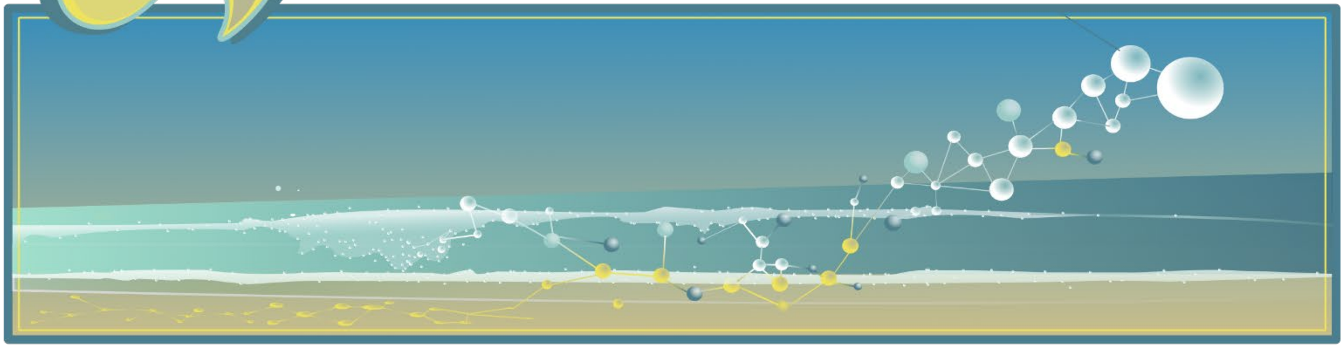
Soft Matter Around the World in Three Years

ISMC 2024

The 8th International Soft Matter Conference

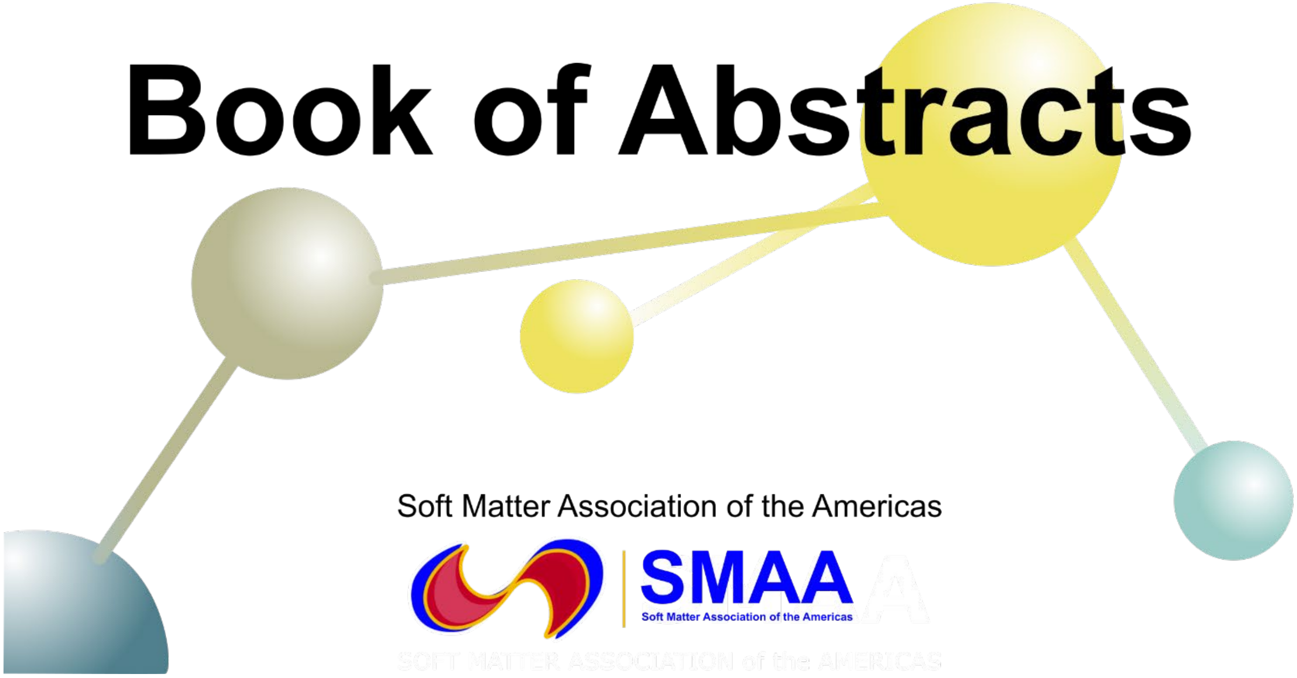


Blurring Boundaries Between Fields

Connecting to reshape the future of soft matter

July 29 – August 2, 2024
Raleigh, North Carolina

Book of Abstracts



Soft Matter Association of the Americas

SMAA
Soft Matter Association of the Americas

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Welcome from Organizers

On behalf of the Local Organizing Committee, I welcome all participants to the 8th International Soft Matter Conference (ISMC2024).

This conference is organized jointly by the Soft Matter Association of the Americas (SMAA – see the history of ISMC and SMAA on pages 31-33) and by the Triangle Universities – Duke University (Duke), North Carolina State University (NCSU), and the University of North Carolina at Chapel Hill (UNC). It is supported by the International Union of Pure and Applied Physics (IUPAP), the National Science Foundation, and many other organizations (see the complete list of sponsors on page 34). This is the first ISMC on the American continent, and as such, it concludes the first cycle of the Soft Matter around the World in Three Years series of ISMCs (see details on page 31).

The conference aims to bring together researchers from physics, chemistry, biology, chemical engineering, and materials science interested in various soft matter systems. We hope the conference will promote and intensify interdisciplinary collaborations and advance connections between academia and industry around soft matter technologies.

The conference features seven plenary talks, fifty-two invited keynote lectures, eighty-eight contributed oral presentations, and over two hundred and seventy posters. The rest of this booklet gives all the essential information needed to navigate your way through ISMC2024.

On behalf of all the organizers, I thank you for participating in ISMC2024 and wish you an enjoyable and fruitful conference.
Welcome to North Carolina!

Michael Rubinstein

Michael Rubinstein
Chair of the ISMC2024 Organizing Committee
Chair of the IUPAP Soft Matter WG-15
President of the Soft Matter Association of the Americas

On behalf of the ISMC2024 Local Organizing Committee:
Ronit Freeman, co-chair
Jan Genzer, co-chair
Christoph Schmidt
Patrick Charbonneau
Karen Daniels
Moumita Das
Lilian Hsiao
Daphne Klotsa
Stefan Zauscher

Committees

Local Organizing Committee

Michael Rubinstein (Duke), chair
Ronit Freeman (UNC), co-chair
Jan Genzer (NCSU), co-chair

Patrick Charbonneau (Duke)
Karen Daniels (NCSU)
Moumita Das (Rochester Institute of Technology)
Lilian Hsiao (NCSU)
Daphne Klotsa (UNC)
Christoph Schmidt (Duke)
Stefan Zauscher (Duke)

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Emanuela Zaccarelli (Sapienza University of Rome)

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Dimitris Vlassopoulos (FORTH, Crete)
Arjun Yodh (University of Pennsylvania)
Julia Yeomans (University of Oxford)
Slobodan Zummer (University of Ljubljana)

General Information

Venue and Parking

The conference will be held at the Raleigh Convention Center (RCC), 500 South Salisbury Street, Raleigh, NC 27601 (see floor maps of the RCC on pages 9-10).

Transportation & Directions

- **By air:** If you are flying through Raleigh-Durham International Airport (RDU), taxis, ridesharing, and car rentals are available at both terminals. It is an 18-minute drive to and from the RCC.
  By bus, Google and gotriangle.org provide information on local routes and paying fares. The GoRaleigh Station is a convenient 3 1/2 blocks walk from the RCC. The free downtown R-LINE bus circulates to major food and retail areas every 15 minutes during the evenings and stops at the main entrance of the RCC.
- **By train:** Two Amtrak trains serve downtown Raleigh daily at Raleigh Union Station (RGH): the Carolinian and the Piedmont. More information is available **here**.
- **By car:** The RCC is adjacent to the Red Hat Amphitheater.
    - **From the west:** I-40 east; take Exit 298B South Saunders Street.
    - **From the east:** 64/264 to I-440 East I-40 West; take Exit 298B South Saunders Street.
    - **From the south:** US-1 North to I-40 east; take Exit 298B South Saunders Street.

From the north: US-1 South into the city; left on Lenoir Street.

Parking

- **Map of parking decks in Downtown Raleigh**. The closest public parking decks to the RCC are at:
    - Lenoir Street between Salisbury Street and Fayetteville Street;
    - Lenoir Street between Salisbury Street and McDowell Street;
    - South Street between Salisbury Street and McDowell Street;
    - Davie Street between McDowell Street and Dawson Street;
    - Cabarrus Street between McDowell Street and Dawson Street;
    - Salisbury Street between Cabarrus Street and Davie Street
- **Accessible parking spaces** are available on the first level of each garage; visit the City of Raleigh **Accessibility** page for more information.

Please note that the RCC does not control the parking rates or maintenance of these garages. For concerns with a parking facility or more information, contact McLaurin Parking directly.

Registration desk

The registration desk is located in the main lobby of the RCC (see floor map on page 10). Its operating hours are

Monday, July 29	5:00 pm – 8:00 pm
Tuesday, July 30	8:00 am – 8:00 pm
Wednesday, July 31	8:30 am – 7:00 pm
Thursday, August 1	8:30 am – 8:00 pm
Friday, August 2	8:30 am – 1:00 pm

Internet

The RCC provides free Wi-Fi internet access to all conference delegates.
Public networks: **Legacy Devices** and **Raleigh Convention Center**. No password is needed.

Conference Attendee App

The **EVENT APP** can be downloaded and installed on mobile devices and contains most of the conference information. The program (Agenda) can be customized (My Agenda) with times, locations, titles, abstracts, and invited speakers' information. The app also provides a way to communicate with other attendees and organizers. To install the conference Attendee App follow the three steps below:

Step 1: Download the app.

Apple: Google: Others (HTML):

Step 2: Enter event code: **ismc24** and click **Submit** button.

Step 3: Sign in using your Events Air registration credentials.

Use of Mobile Devices During Lectures

During lectures, please turn your mobile phone ringers off. There are some power outlets throughout the RCC for charging your mobile devices and laptops.

No Smoking Policy

The RCC is a smoke free facility. Smoking is prohibited in all areas within the facility without exception.

Lost & Found

Personal belongings left in the conference rooms or other locations within the RCC will be collected by the ISMC2024 or the RCC staff. Contact an RCC security guard or call the security team at 919-302-8238 or 919-996-8911. The conference staff can also be reached at ISMC24@soft-matter.com .

ATM Locations

There is a PNC Bank ATM on the main level of the RCC and a CashPoints ATM on the Mezzanine level.

Safety & Security

As in any large city, we advise you to be vigilant when going out late at night. Please always pay attention to your surroundings and belongings. Should you have any questions, please do not hesitate to ask for information at the registration desks of hotels or of the conference.

Access to the conference center is restricted to people with a valid conference badge. Please wear your conference badge at all times on the RCC premises. When leaving the conference, please deposit your badge in the collection box near the registration desk. Please do not dispose of your badge in your hotel room or any public places.

COVID Safety Protocol

We kindly ask that all participants take a rapid antigen test before traveling and refrain from traveling if you test positive. If you start feeling ill during the conference, we will ask that you test yourself. **If you test positive at any point during the conference, we ask that you self-isolate to avoid spreading the virus to other participants**. N95 masks will be available at the conference information desk.

Medical Care & Emergencies

- **Emergency:** dial 911 free from any phone
- Please report any accidents to the RCC Security Team at 919-996-8911 or 919-302-8238
- **Urgent Care:** FastMed, 107 W Hargett Street (8-minute walk) 984-255-2107
- **Pharmacy:** Glenwood South Pharmacy & Market, 401 Glenwood Avenue (30 min walk)
- **On-site First Aid:** contact an RCC security guard

Child Care

(not endorsed by ISMC)

There are two childcare options in the downtown Raleigh area: Platinum Childcare and Care.com (vetted local sitters). Baby changing stations are available in every restroom of the RCC.

Mamava Lactation Pods

Two Mamava lactation pods are available on the Main and Mezzanine levels, accessed via the Mamava app.

Restaurants

(not endorsed by ISMC)

Food

Beasley's Chicken & Honey – Known for its southern cuisine and famous chicken and waffles
Gonza Tacos y Tequila – Some of the Triangle's best Mexican food
La Santa – Another good Mexican restaurant
Taverna Agora – Greek cuisine with an atmosphere to match
Poole's Diner – A modern take on the traditional American diner
Mulino Italian – Italian restaurant with a patio perfect for an after-conference dinner
The Station – Upper-quality bar food…plus they have a nice brunch
Sam Jones – Wood-fired, 100% authentic North Carolina BBQ
The Pit – BBQ and southern cuisine – you can even buy a bottle of their sauce to take home with you
Boulted Bread – Fresh baked croissants, pastries, and other breads. It was named the 'best bakery' by at least one committee chair!
Sitti – Authentic Lebanese cuisine with sidewalk dining

Drink

Jubala – Coffee shop with nice breakfast options like waffles and biscuits
Little Native Coffee Co. – Coffee shop with light breakfast and indoor/outdoor seating
Beer Garden – Over 350 beers on tap and also serves food
Willard – Rooftop lounge and bar
Dram & Draught – Neighborhood bar feel, whiskey savvy
Boxcar – Lively atmosphere with an adult arcade
Big Easy – New Orleans-style bar, serves Cajun food
Trolley Pub – Tour downtown Raleigh while you have drinks on this boozy wagon
Watts & Ward – Underground bar with a speakeasy vibe
Whiskey Kitchen – A converted garage that maintains that industrial atmosphere – over 300 whiskeys
The Green Light – Small, hidden speakeasy-style bar

Tourist Information

See more information at https://soft-matter.com/ismc2024/ismc-area/.
Visit Raleigh
North Carolina Museum of Natural Science
Marbles Kids' Museum
Haunted Raleigh Walking Tour
NC Museum of Art

August 2nd will be First Friday in Downtown Raleigh. You will find art walks and a lively atmosphere.

Code of Conduct

Registered attendees agree to abide by the IUPAP Code of Conduct.

Free Circulation of Scientists: The principle of the Universality of Science is fundamental to scientific progress. This principle embodies freedom of movement, association, expression, and communication for scientists, as well as equitable access to data, information, and research materials. In pursuing its objectives with respect to the rights and responsibilities of scientists, we actively uphold this principle, and in doing so, we oppose any discrimination. Participation at this conference is open to all nationalities, religions, genders, political views, ages or any other factors. We explicitly encourage varied and diverse participation.

Harassment at Conferences: It is the policy of the IUPAP that all participants in Union activities will enjoy an environment that encourages the free expression and exchange of scientific ideas and is free from all forms of discrimination, harassment, and retaliation. The conference organizers have named advisors who will consult with those who have suffered from harassment and suggest ways of redressing their problems, as well as an advisor who will counsel those accused of harassment. The conference organizers may, after due consideration, take such action they deem appropriate.

Reporting: For incidents involving discrimination, harassment, sexual harassment or retaliation, please use the NCSU Online Reporting Form System: go.ncsu.edu/oiedreportform. Be sure to include **ISMC-24** somewhere within the narrative of your report to ensure that the designated advisors are notified. This reporting process can be either anonymous or non-anonymous. Anonymous reporting may limit the actions taken by the advisors. For all other incidents and reporting, please contact the named advisors (Local Organizing Committee members) Karen Daniels (kdaniel@ncsu.edu, 919-513-7921) and/or Patrick Charbonneau (patrick.charbonneau@duke.edu, 919-613-6261). Using this method is not necessarily anonymous.

Preconference Event: Young Investigator Workshop on July 27-28, 2024 on the NCSU campus (see https://smaa.eventsair.com/cmspreview/ismc-yiw-2024/#young-investigator-workshop)

Information for Session Chairs

Session chairs should arrive to the session room 15 minutes before the beginning of their session to meet speakers and ensure that they work with the A/V staff to connect their laptop or transfer their presentation to the provided laptop. Session chairs introduce the speakers. They will be provided with timers to monitor the presentation time, alerting speakers when 5 minutes of presentation time remains. Sessions chairs should stop the lecture when time is up and moderate the discussion after the presentation. At the end of discussion, Session chairs then assist the next presenter to get set up and introduce the next speaker.

Information for Presenters

Information for Plenary Speakers

All plenary talks will take place in Ballroom B (see RCC floor map on page 10). Presentations are **35 minutes** long, followed by 10 minutes of questions. The session Chair will notify the speaker when 5 minutes of presentation time remains.

Please meet the A/V staff in Ballroom B 25-30 minutes before your lecture to connect your laptop or to connect a memory stick with your talk to the laptop provided, check your presentation, and attach the wireless microphone.

Connection to the projection equipment is via an HDMI or USB-C port connector; we ask that presenters *bring their own adapters* if needed to make these connections.

Clickers/laser pens (if required) will be provided. These devices connect via a USB-A port connector; please bring suitable adaptors if needed.

Information for Keynote and Contributed Talks Speakers

All talks will take place on Main (300) Level (Rooms 301 – 306 – see RCC floor map on page 10).

Keynote talks are **25 minutes** long followed by 5 minutes for questions and changeover. **Contributed** talks are **12 minutes** long with 3 minutes for questions and changeover. The session chair will indicate when 5 minutes presentation time remains and stand up when 1 minute remains.

Speakers should go to the assigned lecture room during the catering break (coffee/tea or second half of lunch) before their session to check that their presentation displays correctly from their laptops or download their talk onto the laptop provided by A/V tech.

Connection to the projection equipment is via HDMI or USB-C connector; we ask that presenters *bring their own adapters* if needed to make these connections.

The laptop of a contributed talk speaker will be disconnected during questions to allow the next speaker to connect.

For presenters without their own laptops there will be laptops provided in each room onto which PDF and PowerPoint files can be loaded. In this case, presenters are asked to please bring a USB-A compatible pen- or hard-drive at the beginning of the catering break before their session to upload their presentation.

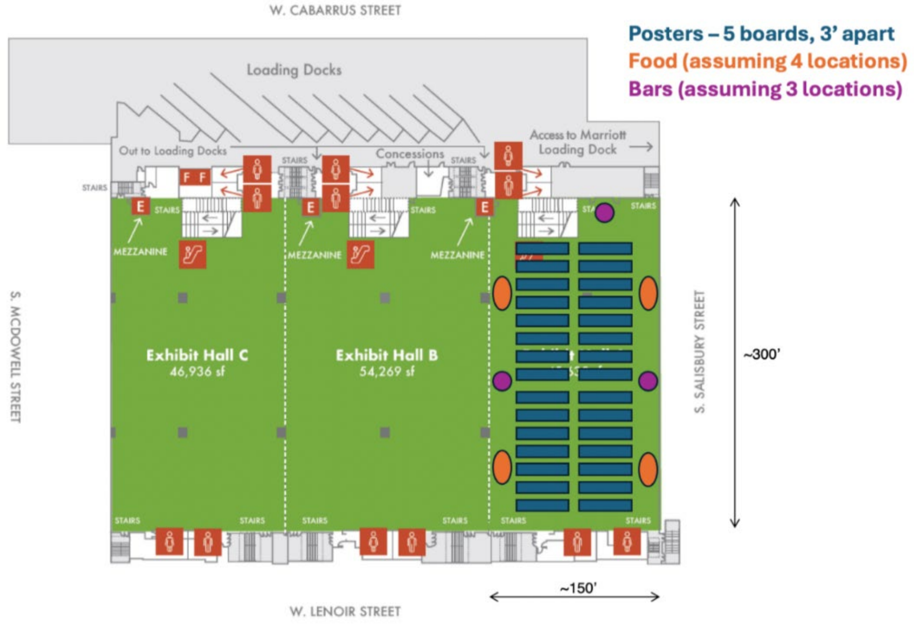
Clickers/laser pens (if required) will be provided. These devises will connect via a USB-A connector; please bring suitable adaptors if needed.

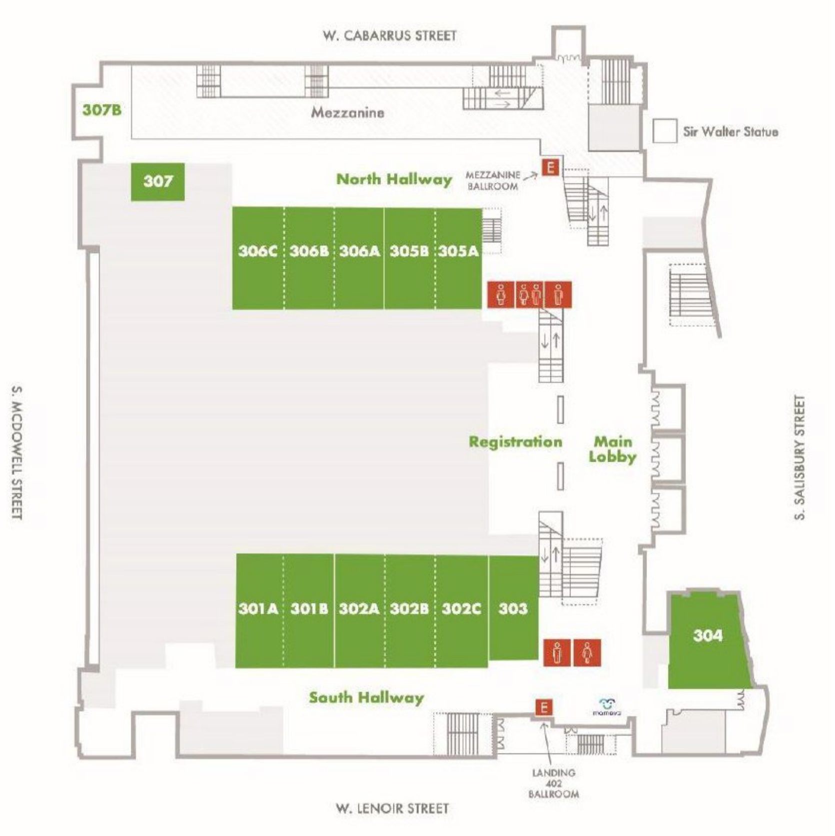
Information for Poster Presenters

There will be two poster sessions: Session 1 for odd numbered posters from 6:00-8:00 PM on Tuesday, July 30 and Session 2 for even numbered posters from 6:00-8:00 PM on Thursday, August 1. Numbered poster boards are in Exhibit Hall A (see map below). You can put your poster up as early as the afternoon of Monday, July 29, and take it down as late as the morning of Friday, August 2. Any posters not taken down by Friday afternoon will be removed and discarded.

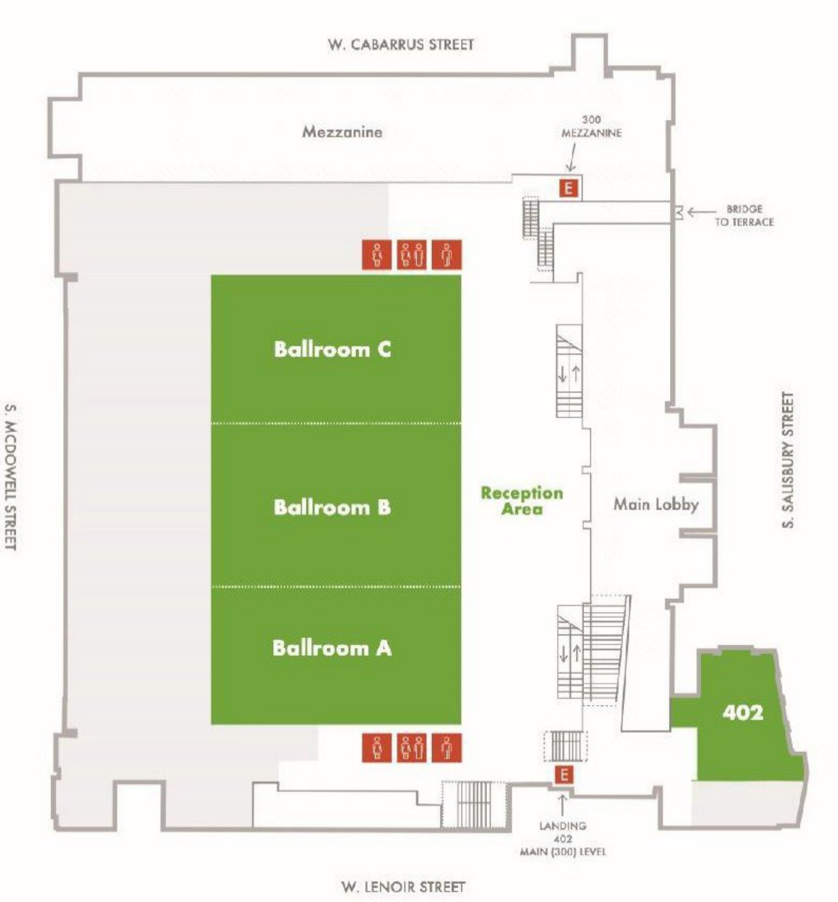
Means to attach posters to the boards will be provided. Poster boards accommodate poster sizes up to 8' (horizontal) by 4' (vertical).

Exhibit Hall (100) Level floor plan. Poster sessions are in Exhibit Hall A.





- 🚺 Women
- 🚹 Men
- 🚻 All-gender/Family
- E Elevator
- ▨ Open to Below
- ⬜ Back of House



Monday, July 29 Satellite Event – Duke Soft Matter Day – Gross Hall, Duke University

Reserve a free bus between ISMC hotels and Duke by registering for the Duke Soft Matter Day event

Time	Activity		
9:00 – 9:30 am	Breakfast		
9:30 – 9:45 am	Welcome Address		
9:45 – 10:25 am	Plenary Talk I (30 min +10 min discussion) **Fyl Pincus-** "***A Personal View of the Evolution of Soft Condensed Matter Physics***"		
10:25 – 11:05 am	Plenary Talk II (30 min + 10 min discussion) **Jian Ping Gong-** "***Mechanochemistry in Double Network Materials***"		
11:05 – 11:35 am	Poster Session & Coffee Break		
11:35 – 12:15 pm	Plenary Talk III (30 min + 10 min discussion) **Andrea J. Liu-** "***Many More is Different***"		
12:25 – 1:10 pm (45 minutes session)	Lunch & Roundtable Discussion with Duke Faculty (frontiers of soft matter research-theme 1)	Lunch & Poster Session (from Duke Soft Matter Groups)	Lab Tours (Duke Soft Matter Groups)
1:20 – 2:05 pm (45 minutes session)	Roundtable Discussion with Duke Faculty (frontiers of soft matter research-theme 2)	Poster Session (from Duke Soft Matter Groups)	Lab Tours (Duke Soft Matter Groups)
2:15 – 2:55 pm	Plenary Talk IV (30 min + 10 min discussion) **Dave Weitz -** "***Soft Matter Physics for the Rheology of a Cell***"		
2:55 – 3:25 pm	Poster Session & Coffee Break		
3:25 – 4:05 pm	Plenary Talk V (30 min + 10 min discussion) **Eugenia Kumacheva-** ***"Nanoparticle-derived cholesteric liquid crystals: assembly under confinement"***		

ISMC 2024 Program

The conference program uses sorting categories and is color-coded accordingly:

Conference Sorting Categories

A	Active
B	Biological
C	Colloidal
F	Fluid Dynamics & Rheology
G	Glasses, Granular & Jamming
I	Interfaces, Surfaces & Membranes
L	Liquid Crystals
M	Measurement & Characterization
N	Networks & Gels
P	Polymers
S	Self-Assembly

Monday, July 29, 2024

5:00 PM – 6:30 PM Registration (see Registration and area on the map on the previous page)

6:30 PM – 8:00 PM Welcome Reception (see Reception area on the map on the previous page)

Tuesday, July 30, 2024

7:30 AM – Registration Opens (see Registration area on the map on the previous page)

8:45 AM – Conference Opening Ceremony, Ballroom B
Opening Remarks by:
Dr. Penny Gordon-Larsen, Vice Chancellor for Research, University of North Carolina at Chapel Hill
Dr. Chris Clemens, Provost and Chief Academic Officer, University of North Carolina at Chapel Hill
Dr. Jennifer Lodge, Vice President for Research and Innovation, Duke University
Dr. Peter Fedkiw, Interim Associate Dean for Research and Infrastructure, College of Engineering at NC State University
Dr. Genevieve Garland, Senior Associate Vice Chancellor of Research, Development and Operations, NC State University
Senator Paul Newton, North Carolina State Senate

Ribbon Cutting
Conference Background and Week Review:
Michael Rubenstein, Distinguished Professor, Duke University
Aleksandar S. Vesic, Distinguished Professor, Duke University

9:15 AM – 10:00 AM - Plenary Session F, Chair: Fyl Pincus, Ballroom B
Howard A. Stone “Physicochemical hydrodynamics and soft matter: From thin films to molecular biology to swimming cells”

10:00 AM – 10:30 AM - Coffee Break

Session	A1 (Room 306 BC)	B1 (Room 305 AB)	P1 (Room 302 BC)	G1 (Room 301 AB)
Chair	Fred MacKintosh	Paul Janmey	Timothy Fornes	Srikanth Sastry
10:30 AM	**A1.1: Steve Granick** A skeptic's guide to active matter	**B1.1: Dennis Discher** Rigidity percolation predicts tissue viscoelasticity scaling with fibrillar collagen based on collagenase kinetics imaged by SHG	**P1.1: Sanat Kumar** Mechanism of micro and nanoplastics	**G1.1: Zahra Fakhraai** Controlling Glass Equilibration Using Soft Substrates
10:45 AM		**B1.2: Kinjal Dasbiswas** Modeling active contractility in fibrous living matter		
11:00 AM	**A1.2: Carles Calero** Self-propulsion at the nanoscale	**B1.3: Gijsje Koenderink** Living soft matter: bridging cell-free and live-cell perspectives	**P1.2: Daniel Rau** Multi-material additive manufacturing of polymeric composites with seamless soft-hard interface integration from molecular bonding	**G1.2: Francesco Zamponi** Creating equilibrium glassy states via random particle bonding
11:15 AM	**A1.3: Suzanne Ahmed** Tunability and switchability of nanomotor modes of motion utilizing biocompatible actuation methods		**P1.3: Alina Kirillova** 3D Printing of polymeric and composite porous scaffolds for biomedical applications	

11:30 AM	**A1.4: Clemens Bechinger** Brownian particles in non-equilibrium baths	**B1.4: Sam Safran** Novel mesoscale properties of protein condensates: Non-equilibrium activity and conformational freedom	**P1.4: Mark Ediger** Surface-directed assembly of structured glasses	**G1.3: Cacey Bester** Force signatures of creep in a photoelastic granular medium
11:45 AM				**G1.4: Kai Huang** Role of gravity on granular drag: From impacting on to digging into sand
12:00 PM	Sessions end			

12:00 PM - Lunch

12:15 PM – 1:00 PM - Panel Discussion 1, Ballroom B

2:15 PM – 3:00 PM - Plenary Session B, Chair: Patricia Bassereau, Ballroom B
Kinneret Keren "Topological defects and their role in Hydra morphogenesis"

3:00 PM – 3:30 PM Coffee Break

Session	I1 (Room 306 BC)	B2 (Room 305 AB)	C1 (Room 302 BC)	N1 (Room 301 AB)
Chair	Beverly Asoo Stonas	José R Alvarado	Jacinta Conrad	Aniket Bhattacharya
3:30 PM	**I1.1: Eric Dufresne** Controlling interfacial tension without surfactants in biomolecular condensates	**B2.1: Brent Hoffman** Coupling during collective cell migration	**C1.1: Jasna Brujic** Colloidal protein analogs	**N1.1: Eric Weeks** Highly polydisperse colloidal gels
3:45 PM		**B2.2: Alexander Alexeev** Collective behavior of platelets in fibrin fiber clots		**N1.2: Liheng Cai** A universal strategy for decoupling stiffness and extensibility of polymer networks
4:00 PM	**I1.2: Yohko Yano** Investigating viscoelastic behavior of lipid monolayers in spontaneous oscillation of surface tension induced by the Marangoni effect	**B2.3: Lakshminarayanan Mahadevan** Endless forms most beautiful: geometry, physics and biology	**C1.2: Prerna Sharma** Folding of colloidal membranes into non-Euclidian geometries	**N1.3: Kohzo Ito** Slide-ring materials for circular economy
4:15 PM	**I1.3: William Ducker** Porous thin films facilitate rapid evaporation of water droplets			
4:30 PM	**I1.4: Jacob Klein** Lipid bilayers under trans-membrane fields: cell-inspired, massive electro-modulation of friction	**B2.4: Sharon Lubkin** Cell packing in the notochord	**C1.3: Amir Pahlavan** Diffusiophoretic transport of colloids in disordered media	**N1.4: Olga Kuksenok** Characterizing dynamic heterogeneities and properties of degrading polymer networks
4:45 PM		**B2.5: Julio Belmonte** Connectivity and Contraction in Cytoskeletal Networks	**C1.4: Jeffrey Richards** Engineering the electrical response of conductive suspensions	**N1.5: C. Nadir Kaplan** Rapid, non-linear diffusiophoretic swelling of chemically responsive hydrogels
5:00 PM	**I1.5: Di Jin** Thin films under an electric field	**B2.6: Toshiyuki Nakagaki** Adaptable network of veins to environmental complexity in an huge amoeboid organism of	**C1.5: Ning Wu** Assembly of particles under orthogonally applied electric and magnetic field	**N1.6: Costantino Creton** Ionically conducting elastomers: balancing strength, reversible elasticity and conductivity

5:15 PM	**I1.6: Jacopo Vialetto** Deposition of complex colloidal assemblies from drop evaporation	Physarum plasmodium	**C1.6: Gaurav Arya** Machine-assisted design of effective potentials for colloidal self-assembly	
5:30 PM	Sessions end			

6:00 PM – 8:00 PM - Poster Session 1, Exhibit Hall A

Wednesday, July 31, 2024

9:15 AM – 10:00 AM – Plenary Session A, Chair: Jean-François Joanny, Ballroom B
Ramin Golestanian "Non-reciprocal active matter across the scales"

10:00 AM – 10:30 AM - Coffee Break

Session	A2 (Room 306 BC)	L1 (Room 305 AB)	F1 (Room 302 BC)	S1 (Room 301 AB)
Chair	Orlin Velev	Timothy Bunning	Charles Schroeder	Dean DeLongchamp
10:30 AM	**A2.1: Ludovic Berthier** Collective motion in very dense active matter	**L1.1: Chinedum Osuji** Polymer self-assembly and liquid demixing in the presence of liquid crystals	**F1.1: Véronique Trappe** Memory of shear flow in soft jammed materials	**S1.1: Madhavi Krishnan** A charge dependent long-ranged force drives tailored assembly of matter in solution
10:45 AM			**F1.2: Vanessa Ward** Shear Banding as a cause of Non-Monotonic Stress Relaxation	
11:00 AM	**A2.2: Menachem Stern** Physical networks become what they learn	**L1.2: Slobodan Žumer** Topological soft matter: Some examples from photonics to active and bio-systems	**F1.3: Itai Cohen** Viscosity Metamaterials	**S1.2: Erika Eiser** Using multivalency and superselectivity of DNA-coated colloids for whole genome detection
11:15 AM	**A2.3: Shengkai Li** Memory-induced spontaneous symmetry breaking			
11:30 AM	**A2.4: Julia Yeomans** Active nematics: A new approach to mechanobiology?	**L1.3: Xinyu Wang** Moiré effect enables versatile design of topological defects in nematic liquid crystals	**F1.4: Ralph Colby** Determination of molecular weights using a polydisperse Rouse model for semidilute unentangled polyelectrolyte and neutral polymer solutions	**S1.3: Thi Vo** Rational design of nanoparticle surface patterning for directed self-assembly
11:45 AM		**L1.4: Kushal Bagchi** Functional soft materials from the directed self-assembly of liquid crystals		**S1.4: Andraž Gnidovec** Towards controlled self-assembly of curved surfaces
12:00 PM	Sessions end			

12:00 PM - Lunch

12:15 PM – 1:00 PM - Panel Discussion 2, Ballroom B

2:15 PM – 3:00 PM – Plenary Session L, Chair: Seth Fraden, Ballroom B
Shu Yang "Responsive liquid crystalline elastomeric droplets and particles"

3:00 PM – 3:30 PM Coffee Break

Session	I2 (Room 306 BC)	B3 (Room 305 AB)	P2 (Room 302 BC)	S2 (Room 301 AB)
Chair	Ryan Fuierer	James Harden	Matthew Becker	Ramón Castañeda-Priego
3:30 PM	**I2.1: Vivek Narsimhan** Pearling, buckling, and wrinkling instabilities of multicomponent vesicle threads	**B3.1: Oded Farago** Multiscale lattice modeling and simulations of heterogeneous membranes	**P2.1: Matthew Tirrell** Molecular arrangement in polyelectrolyte complex coarcervates	**S2.1: Greg Grason** Misfits unite: Understanding & engineering self-limitation in geometrically frustrated assembly
3:45 PM	**I2.2: Dean DeLongchamp** Polarized resonant soft X-ray scattering measurements in polymer-grafted nanoparticles	**B3.2: Valeria Milam** Competition-based selection of universal DNA ligands for antibody fragments		
4:00 PM	**I2.3: Yendry Corrales Urena** Functionalized carbon nanocones performance in water harvesting	**B3.3: Ankur Jain** Sequence programmable nucleic acid condensates	**P2.2: Jacinta Conrad** Phage probes couple to DNA relaxation dynamics across scales and regimes	**S2.2: Dwaipayan Chakrabarti** Programming self-assembly of colloidal gyroids for advanced materials
4:15 PM	**I2.3.1: Penger Tong** AFM force clamping and extension spectroscopy studies of velvet worm slime proteins at different pH and buffer conditions	**B3.4: Atanu Chatterjee** Adapt to bend: An cooperative transport of soft rods	**P2.3: Thomas Schroeder** Triggering inorganic crystal deposition from polymer-induced liquid precursors	**S2.3: Edward Van Keuren** Multicomponent liquid-core nanocapsules synthesized with flash nanoprecipitation
4:30 PM	**I2.4: Abdelhamid Maali** Direct measurement of the hydro-capillary lift force acting on sphere moving along liquid interfaces	**B3.5: Cesar Rodriguez Emmenegger** Phagocytic synthetic cells: non-living predators to fight bacteria	**P2.4: Zhen-Gang Wang** Origin of the entropic driving force in polyelectrolyte complex coacervation	**S2.4: Xiaoming Mao** Frustrated assemblies as incompatible graphs
4:45 PM	**I2.5: David Cheung** Effect of surface chemistry on conformation and aggregation of amyloid peptides	**B3.6: Jay Tang** Gastric mucin Promotes the spread of growing bacterial swarm on agar surface		
5:00 PM	**I2.6: Ko Okumura** A hydrodynamic analog of critical phenomena: an uncountably infinite number of universality classes	**B3.7: Andela Šarić** Shape-shifting soft matter across evolution *"2023 Soft Matter Lectureship Award"*	**P2.5: Panayotis Benetatos** Stretching bistable linear polymers and loops	**S2.5: Yulia Shmidov** Self-Assembly of Recombinant Elastin-like Polypeptide
5:15 PM			**P2.6: Geoffrey Geise** Microwave dielectric relaxation spectroscopy: A technique to inform ion transport in hydrated polymer membranes	**S2.6: Maggie Daly** Design of Peptide-DNA Architectures to Build Functional Artificial Cells
5:30 PM	Sessions end			

7:00 PM – 9:00 PM - Conference Banquet, Ballroom A

Thursday, August 1, 2024

9:15 AM – 10:00 AM – Plenary Session N, Chair: Jian Ping Gong, Ballroom B
Zhigang Suo "Mechanical behavior of a tanglemer – a polymer network in which entanglements greatly outnumber crosslinks"

10:00 AM – 10:30 AM Coffee Break

Session	A3 (Room 306 BC)	L2 (Room 305 AB)	P3 (Room 302 BC)	S3 (Room 301 AB)
Chair	Daphne Klotsa	Edward Samulski	Thomas Halsey	Leah Johnson
10:30 AM	**A3.1: Cecile Cottin-Bizonne** Active colloids climbing up a wall	**L2.1: Christopher Quinones** Interparticle friction in sheared, dense suspensions of rod-like particles: Simulations	**P3.1: Gary Grest** Dynamics of ring polymers	**S3.1: Oleg Gang** Programming self-assembly and transformations of nanoscale systems
10:45 AM		**L2.2: Thomas Parton** Chiral doping of a colloidal liquid crystal phase in cellulose nanocrystal suspensions		
11:00 AM	**A3.2: Hartmut Löwen** Active matter: self-propelled colloids and beyond	**L2.3: Ivan Smalyukh** Knotted chiral meta matter	**P3.2: Ting Ge** Elastomer mechanics of cross-linked ring-linear polymer blends	**S3.2: Timothy Lodge** Equilibration of block copolymer micelles: How difficult can it be?
11:15 AM			**P3.3: Myoeum Kim** Dynamics of polymers with controlled distribution and density of associative groups	
11:30 AM	**A3.3: Orlin Velev** New mechanisms of active particle propulsion powered by temporally asymmetric AC fields	**L2.4: Timothy Atherton** Catching the wave: particle transport by a moving phase boundary	**P3.4: Kurt Kremer** Playing with entanglements to structure polymer materials	**S3.3: Kateri DuBay** Dissipative self-assembly within an oscillating energy landscape
11:45 AM	**A3.4: Nitesh Arora** Light-driven transformations in entangled active matter			**S3.4: Rae Robertson-Anderson** Timed material self-assembly controlled by circadian clock proteins
12:00 PM	Sessions end			

12:00 PM - Lunch

12:15 PM – 1:00 PM - Panel Discussion 3, Ballroom B

2:15 PM – 3:00 PM - Plenary Session C, Chair: Hajime Tanaka, Ballroom B
Emanuela Del Gado “Soft particulate networks and their hidden hierarchical nature”

3:00 PM – 3:30 PM Coffee Break

Session	A4 (Room 306 BC)	B4 (Room 305 AB)	F2 (Room 302 BC)	G2 (Room 301 AB)
Chair	James Harden	Rae Anderson	Bavand Keshavarz	Daniel Blair
3:30 PM	**A4.1: Alexander Grosberg** Active hydrodynamics in the nucleus of a living cell	**B4.1: Megan Valentine** New approaches to designing and deploying hydrogels for force sensing	**F2.1: Yoav Tsori** Electrolubrication in flowing liquid mixtures	**G2.1: Connie Roth** Impact of chain connectivity and covalent bonding on the local glass transition temperature of polymers

3:45 PM		and control	**F2.2: Saad Khan** Nanodiamond-stabilized Pickering emulsions: Microstructure and rheology	**G2.2: Gregory McKenna** Anomalous behavior of ultrastable glasses and the implications for the glass “transition”
4:00 PM	**A4.2: Rony Granek** Active fractal networks with stochastic force monopoles and force dipoles unravel subdiffusion of chromosomal loci	**B4.2: Peter Olmstead** Diffusion in a multiscale model for the Stratum Corneum	**F2.3: Dimitris Vlassopoulos** Rheological challenges with polymeric gels	**G2.3: Annie Colin** Flow of non Brownian suspensions
4:15 PM	**A4.3: Ram Adar** Environment-stored memory in active matter: a framework for extra-cellular matrix remodeling	**B4.3: Xianting Lei** De-novo ATP independent contractile protein network		
4:30 PM	**A4.4: Rodrigo Soto** Kinetic theory for active Brownian particles	**B4.4: Ioana Illie** Computational engineering of responsive meta-particles	**F2.4: Victor Steinberg** Amplification of vorticity fluctuations and stochastic resonance in inertia-less viscoelastic channel flow	**G2.4: Sarika Maitra Bhattacharyya** Exploring the structural contribution to dynamics in supercooled liquids
4:45 PM		**B4.5: William Polacheck** Cell-derived matrix hydrogels with tunable mechanics for donor-derived microphysiological systems	**F2.5: Sara Hashmi** Complex fluids in confined flows	
5:00 PM	**A4.5: Stewart Mallory** Phase behavior and transport of active colloids under extreme confinement	**B4.6: Jérémie Palacci** Bacteria as blacksmiths	**F2.6: Anette Hosoi** Bio-inspired filtration: Fluid mechanics of the Manta Ray	**G2.5: Shima Parsa** Emergence of preferential flow paths in transport of emulsions in porous media
5:15 PM	**A4.6: Paarth Gulati** Asymmetry in active-passive phase separation			**G2.6: Vinutha H. A.** Stress relaxation in soft jammed materials
5:30 PM	Sessions end			

6:00 PM – 8:00 PM - Poster Session 2, Exhibit Hall A

Friday, August 2, 2024

9:15 AM – 10:00 AM - Plenary Session M, Chair: Eugenia Kumacheva, Ballroom B
Roberto Cerbino “Multiscale dynamics in inert and living soft matter”

10:00 AM – 10:30 AM - Coffee Break

Session	A5 (Room 306 BC)	B5 (Room 305 AB)	C2 (Room 302 BC)	N2 (Room 301 AB)
Chair	Andrea Liu	Liheng Cai	Preeta Datta	Stephen L. Craig
10:30 AM	**A5.1: Sriram Ramaswamy** Bulk condensation by an active interface	**B5.1: David Hill** Neutrophil Extracellular Traps (NETs) in Muco-Obstructive Pulmonary Disease.	**C2.1: Paul Chaikin** Random to ordered packings: From candies to monster crystals from space	**N2.1: Barbara Ruzicka** Dynamical and structural behaviour of PNIPAM based microgels

10:45 AM		**B5.2:**		**N2.2: Krassimir Velikov** Cellulose microfibrils: Properties and application in complex fluids and soft materials
11:00 AM	**A5.2: Luca Giomi** Phase transitions in confluent epithelia	**B5.3: Meera Ramaswamy** Morphodynamics of bacterial communities proliferating in three dimensions	**C2.2: Nicolas Fares** Confined Brownian motion of soft colloid	**N2.3: Monica Olvera de la Cruz** Controlling the structure and function of confined electrolytes
11:15 AM		**B5.3: Danielle German** Bacterial dynamics at the swarm front	**C2.3: Steven van Kesteren** Light-controlled colloidal crystallization	
11:30 AM	**A5.3: Gwynn Elfring** The hydrodynamics of active matter in inhomogeneous environments	**B5.4: Rebecca Schulman** Programmed spatiotemporal dynamics and pattern recognition in soft materials with synthetic biochemical signaling networks	**C2.4: Delia Milliron** Interactions and assemblies of colloidal nanocrystals	**N2.4: Michael Dickey** Ultra tough ionogels
11:45 AM	**A5.4: Mickaël Bourgoin** Magnetic Janssen effect			**N2.5: Avisek Das** Correlated orientational disorder in crystalline assemblies of hard convex polyhedral
12:00 PM	Sessions end			

12:15 PM – 1:00 PM – Ballroom B Business Meeting of Soft Matter Association of the Americas and ISMC 2024 Closing Ceremony

List of Posters

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
	Active Matter
1	**Amir Abbasi** Non-equilibrium Thermodynamics of Phase Separations in Scalar Active Matter
3	**Sujin Bemplasseri Babu** Rutherford like scattering of squirmer from a semi-circular wall configuration.
5	**John Berezney** Active soft composites

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
	Active Matter
2	**Amir Abbasi** Non-Markovian Modeling of Nonequilibrium Fluctuations and Dissipation in Active Viscoelastic Biomatter
4	**Guilherme Giardini** The Fluctuating Nature of Mesenchymal Cell Movement: Beyond Velocity Definitions
6	**Kameryn Hinton** Designing Cell-Inspired Microswimmers

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
7	**Bhuvnesh Bharti** Field-driven Assembly of Active Colloids
9	**Bipul Biswas** Electrohydrodynamic flows make semiflexible colloidal filaments active
11	**Sizhe Cheng** Trypanosoma swims with a unidirectionally rotating body and a bidirectionally rotating flagellum
13	**Luke Davis** Smooth control of active matter
15	**Matthew Deutsch** Agent-based simulations of confined active nematic filaments
17	**Riley Dickson** Elasticity of healthy airway mucus promotes directional transport of Pseudomonas aeruginosa
19	**Kazuaki Furukawa** 2x2 Rotation bit system composed of active matter: pattern and synchronization of self-propelled rotation
21	**Ravi Gautam** Activity-enhanced colloidal self-assembly: insights from simulations
23	**Adil Ghaznavi** Yielding in active granular matter is different than in sheared granular matter
25	**Guilherme Giardini** Emergence of Collective Behavior: An Evolutionary Approach to Vicsek-like Particles with Neural Networks
27	**Zhe Gou** A numerical framework for phoretic particles
29	**Itay Griniasty** Bifurcation instructed design of multistate machines
31	**Yuke Han** Shape-shifting gel-based micro-ribbons patterned by e-beam lithography

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
8	**Arnold Mathijssen** Transport and delivery by active materials in complex flow
10	**Michael Norton** Modeling Exogenously and Endogenously Controlled Bioinspired Materials
12	**Jayson Paulose** Activity beyond self-propulsion: parametric melting of a Lennard-Jones crystal via a dynamic pair potential
14	**Soni Prajapati** Effect of background flow on motility-induced phase separation
16	**Praneet Prakash** Spatio-temporal dynamics of nutrient exchanges in microbial active matter
18	**K. R. Prathyusha** Tangling induced phase separation in active polymers
20	**Harishwar Raman** Pair Interactions of active SiO2-Pt Janus Colloids
22	**Sattvic Ray** Fiber networks assembled and driven by an active fluid
24	**Shang-Yik Reigh** Diffusiophoretically induced interactions between chemically active and inert particles
26	**Rae Robertson-Anderson** Emergent micro-mechanics of active cytoskeleton composites
28	**Bappaditya Roy** Learning hydrodynamic equations from the collective behavior of active Brownian particles
30	**Isabel Ruffin** Dynamics of Active and Passive Microtubules in Entangled Actin Networks
32	**Amir Shee** Emergent Mesoscale Correlations in Active Solids with Noisy Chiral Dynamics

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
33	**Haruki Hayano** Distinct rheological behaviors between pusher and puller suspensions
35	**Zhi-Feng Huang** Emergence of active patterns from single-species nonreciprocity
37	**Tali Khain** The wake of a sphere in a chiral fluid
39	**Ella King** Emergent Activity in Wave-Mediated Interactions
41	**Itamar Kolvin** Bending and stretching of active fibrous membranes
43	**Min Kyung Lee** Active-assisted Assembly of Colloidal Crystal
45	**Wan Jung Lin** Collective interactions of soft vesicles containing self-propelling granular rods
47	**Rupesh Mahore** Topological non orientability in non reciprocal soft-robotic metamaterial.
49	**Amir Pahlavan** Chemotactic response of bacteria to ephemeral nutrient plumes
Biological Matter	
51	**Ram M. Adar** Theory of cellular volume regulation in response to shocks and deformations
53	**Sadjad Arzash** Mechanics of confluent biological tissues as a learning problem
55	**Subhadip Biswas** Illuminating the dynamics of biomolecular condensates with alphabet-free exploration of stickers-spacers energy landscapes

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
34	**Ahis Shrestha** Self-propulsion of active particles through surface charge asymmetry
36	**Artur Soriani** Universal heat profiles and thermodynamic control of active field theories
38	**Tzer Han Tan** Odd dynamics in living chiral crystal
40	**Albane Thery** Enhanced bacterial contamination in complex fluids
42	**Nayana Venkatareddy** Phase separation kinetics in Two Temperature Induced Phase Separation(2-TIPS)
44	**Wei Wang** Electronically actuated artificial cilia for microfluidic manipulations
46	**Zhiyuan Zhao** Odd Viscosity-Induced Phase Separation of Counter-Driven Rotors
48	**Shuang Zhou** Softening and Enhanced Transport of Colloidal Chains in a Bacterial Bath
50	**Tingtao Zhou** Active doping controls the mode of failure in dense colloidal gels
Biological Matter	
52	**Brian Chan** Activity-driven chromatin organization during interphase: compaction, segregation, and entanglement suppression
54	**Subhadip Biswas** Molecular Drivers of Aging in Biomolecular Condensates: Desolvation, Rigidification, and Sticker Lifetimes
56	**Owen Blanchard** Active wetting and dewetting dynamics of zebrafish embryonic explants

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	Presenter & Poster Title
57	**Orelle Bulgin** The Effects of Nano-plastics on Developmental Stages in Zebrafish & Nano-plastics as MRI Contrast Agents
59	**Aniket Bhattacharya** Fine structures and missense mutations in intrinsically disordered proteins using Coarse-grained models and machi ne learning
61	**Priya Chiriyankandath** Exploring ALPHA-FOLD Predicted Structures of Nudix Proteins to Investigate Binding Site Dynamics Through Implicit Solvent
63	**Maria Ciko** Simulation Studies to Predict Protein-Peptide Binding Affinities via MELD accelerated Molecular Dynamics
65	**Zixuan Deng** Light-fueled self-sustained cilia
67	**Nuzhat Faiza** Substrate stiffness regulates collective colony expansion of the social bacterium Myxococcus xanthus
69	**Jim Fan** Frustrated Phagocytosis of Beads by Macrophages on Traction Force Q-gels
71	**Marco Aurelio Galvani Cunha** Remodeling and rigidity in the actin cortex
73	**Sounok Ghosh** The effects of substrates on biofilm growth
75	**Sebastian Gonzalez La Corte** Bacterial growth in complex fluids
77	**Amit Kumar** Size and shape fluctuations of mesoscale domains in non-equilibrium liquid-liquid phase separation
79	**Dongheon Lee** Unraveling Quantitative Relationships Between Intracellular Phase Separation and Gene Expression Through Single-cell Analysis
81	**Zhiyue Lu** Designing Life-Like Responses to Temporal Patterns in Artificial Materials: A Theoretical Framework

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	Presenter & Poster Title
58	**Micaila Curtis** Enhancing bone tissue regeneration through mechanical, chemical, and biological regulation of bone extracellular matrix using cal-
60	**Rajsekhar Das** Control of morphologies and dynamics of three-dimensional non-confluent tissues
62	**Dennis E Discher** Fat physics: fat is more rigid and disruptive to cells than you think
64	**Carolyn Feigeles** Condensate Induced Bundling of Biopolymer Networks
66	**Sarthak Gupta** Emergent Dynamics in Biopolymer Networks: Investigating the Interplay of Elasticity, Connectivity, and Activity
68	**David Hathcock** Signatures of energy dissipation in bacterial chemotaxis signaling pathways
70	**David Hill** Neutrophil Extracellular Traps (NETs) in Muco-Obstructive Pulmonary Disease.
72	**Sayantani Kayal** Mechanical imbalance as a cue for cell competition driving epithelial defense against cancerpo
74	**Taylor Kranbuhl** MELD Accelerated MD: A tool to study DNA-Protein Interactions
76	**Sunny Kumar** Kinks Enable Ultrafast Aerial Jumping in Nematodes and Soft Robots
78	**Soumik Mitra** A computational study of the shear response and fracture resistance of the cytoskeleton of the single-celled organism Stentor
80	**Farshid Mohammad-Rafiee** Exploring Ribosomal Dynamics: A Theoretical Model for Translation and Frame-Shifting Phenomena
82	**Nandish Mudegowdru Nagappa** Sustainable Nanoformulations of Anthracyclines

Poster Session 1 **(Tue. July 30,** 6:00-8:00 PM, Exhibit Hall A**)**	
Poster Board #	**Presenter & Poster Title**
83	**Katarina Matic** Cells Embedded in Cytoskeleton Composites for Living Materials
85	**Piyali Mukherjee** Coarse-Grained Molecular Dynamics Simulations of Elastin-Like Polypeptides
87	**Turash Haque Pial** Investigating the Self-assembly and Growth of Multicomponent Soft Nanoparticles Using Kinetic Monte Carlo
89	**Kyle Riker** Dynamic Display of ECM Ligands Controls Machinery of the Cytoskeleton from the Outside-In
91	**Haicen Yue** Revisiting Interface Behaviors of Voronoi and Vertex Models
93	**Pu Zhang** Spatial Distribution and Density of Fibroblasts Determine Angiogenic Response of Endothelial Cells
95	**Hongbo Zhao** Dissecting the Complexities of Phase Separation in Living and Synthetic Systems
97	**Shufeng Zhao** Bacterial surface motility modulated by picky eating habits
99	**Jinchang Zhu** Digital Assembly of Spherical Viscoelastic Bio-ink Particles (DASP): a conceptually new bioprinting technology
Colloidal Systems	
101	**Christian Balderas** Mie scattering theory applied to light scattering of large nonhomogeneous colloidal spheres
103	**Florian Benedetti** Data Driven Inference of Colloidal Interactions
105	**Lihy Buchbinder** Experimental Study of 2D Colloidal Glass

Poster Session 2 **(Thur. August 1,** 6:00-8:00 PM, Exhibit Hall A**)**	
Poster Board #	**Presenter & Poster Title**
84	**Meera Ramaswamy** Morphodynamics of bacterial communities proliferating in three dimensions
86	**Sangjin Ryu** A microfluidic study on the perfusion of a new substance and the removal of an old substance in a dragonfly forewing
88	**Renita Saldanha** Probing effects of vimentin on cell cytoskeleton dynamics through Differential Dynamic Microscopy (DDM)
90	**Corey Stevens** Dual-Functional Nanoparticles Show Potential for Enhanced Drug Delivery Through Simultaneous Mucus Transport and Cell Targeting
92	**Sijie Sun** Vimentin Intermediate Filaments as Worm-Like Micelles
94	**Babak Vajdi Hokmabad** Entrainment by biogenic bubbles enables long-range microbial dispersal in yield-stress environments
96	**Kaarthik Varma** Near-critical Protein mixtures
98	**Sam Wilken** Synthetic chromatin: transcriptional regulation of a model phase-separating liquid
100	**Hongbo Zhao** Condensate-mediated chromatin organization through elastocapillary interactions
Colloidal Systems	
102	**Ramón Castañeda-Priego** Effective interactions between colloids: an approach based on the contraction of the bare forces.
104	**Nicholas Cuccia** Colloids with a Twist: Controlling Filament Helicity and Length to Tune Macroscopic Rheology
106	**Darshana Malusare** Aerosol-assisted particle deposition for solvent-free fabrication of MOF-polymer composites

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
107	**Devika Gireesan Sudha** Motion of chemically powered Janus colloids in an anisotropic fluid.
109	**Mohit Gupta** Hydrophobic Forces in Foam and Emulsion Films
111	**Sofia Morozova** The effect of the glass transition temperature on the phase state of a colloidal system of oppositely charged latex particles
113	**Zizhao (Will) Wang** Precision measurement of homogeneous crystal nucleation of hard-sphere colloids
115	**Daniel Weidig** Dynamical long-time coupling in binary suspensions of highly charged colloidal particles
	Fluid Dynamics & Rheology
119	**Anna Barth** Universal scaling of shear thickening suspensions under acoustic perturbation
121	**Laura Adams** New Insights into Generating Monodispersed Drops with Glass Capillary Microfluidic Devices
123	**Rafał Błaszkiewicz** Microscale hydrodynamic flows created by beating cilia
125	**Chinmay Katke** Variational formulation of physics-informed neural networks (vfPINN)
127	**Viviana Londono-Calderon** Microactuators for Efficient Fluid Manipulation in Low Reynolds Environments
129	**Shravan Pradeep** Unifying yielding mechanics in multiphase soft particulate matter systems

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
108	**Sylvio May** Collision-mediated Transfer Kinetics of Cargo Items Among Mobile Nanocarriers
110	**Antonio Ortiz Ambriz** Bidirectional currents in confined driven colloids
112	**Isaac Spivack** Theory of Entropy Driven Self-Assembly of Hard Particles
114	**Joe Tracy** Reversible Assembly of Iron Oxide Nanoparticles on Gold Nanorods for Magnetic Alignment and Plasmonic Control
116	Dr. Steven Van Kesteren Light-controlled colloidal crystallization
118	**Matthew Walker** Mpemba effect in terms of mean first passage times
	Fluid Dynamics & Rheology
120	**Abhirup Basu** Dissipative Active Motion of Colloidal Particles Rotating in Non-Newtonian Fluids
122	**Albert Countryman** Using Vector Charge Electromagnetism to Examine Emergence of Gel Rigidity
124	**Lucas Hildebrand Pires da Cunha** The role of Hydrodynamic Interactions on the rheology of colloidal rods
126	**Samay Hulikal** Angular Thresholds in Breaking Capillary Bridges
128	**Mohamed Khattab** Chemical species transport near sharp corners
130	**Xiaoxiao Ma** Understanding fluid dynamics for all-aqueous printing of a viscoelastic droplet in yield-stress fluids

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
131	**Rae Robertson-Anderson** Topological DNA blends exhibit resonant deformation fields and strain propagation dynamics tuned by steric constraints
133	**Yihong Shi** Mutual information as a measure of mixing efficiency in viscous fluids
135	**Christina Tang** Low-cost optical plate for imaging shear sensitive liquid crystals
137	**Günther Turk** Fluctuating hydrodynamics of an autophoretic particle near a permeable interface
139	**Greg Voth** Quantifying chiral geometry with sedimenting helical ribbons
	Glasses, Granular & Jamming
141	**Aditya Advani** Can you hear a landslide coming (before it begins)?
143	**Haoyu Li** Metallic Glass Have More Rugged Potential Energy Landscape
145	**Jeffrey Olafsen** Coefficient of restitution of two colliding particles in experiment and simulation
147	**Owen Tower** Studies into the structural order of random pinning systems and their driven dynamics
149	**Dhanush Udayashankara Jamadgni** Solid Lubricants for Bio particles with Complex Shapes
151	**Hongyi Xiao** Locomotion of a scallop-like swimmer in granular media
153	**Chetan Yadav** Granular active matter on approaching glassiness

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
132	**Shravan Pradeep** Baseball gripping mechanics as a multiscale soft matter problem
134	**Yug Chandra Saraswat** Brittle-to-ductile rheology in composite hydrogels with a microfibrous network
136	**Navneet Singh** Dynamic thickening and dethickening of 3D dense suspensions of Quincke rotors
138	**Austin Walker** Rheology and 3D rotational dynamics of sheared dense colloidal suspensions
140	**Chenxian Xu** Growth and Coalescence of Nanoscopic Mesas in Stratifying Micellar Foam Films
	Glasses, Granular & Jamming
142	**Helen Ansell** Stokes-Einstein violations in models of dense cellular materials
144	**Carmen Lee** Relating the microscale to the macroscale in granular materials
146	**Maniya Maleki** Non-affine motion in a quasi-2-dimensional granular matter under simple shear
148	**Jeffrey Olafsen** The physics of sandcastles: Jammed granular columns with and without fluid.
150	**Baoshuang Shang** The transition from anelasticity to plasticity in amorphous solid: a molecular dynamics study
152	**Bret Tantorno** Glass Transition Behavior and Crystallization Kinetics of Celecoxib Carvedilol Co-Amorphous Formulations
154	**Michio Tateno** Compression-induced structural and mechanical transitions in disordered sticky-sphere systems

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
	Interfaces, Surfaces & Membranes
157	**Teagan Bate** Client competition regulates bulk and interface partitioning in biomolecular condensates
159	**Tak Shing Chan** Plateau-Rayleigh instability of a soft layer coated on a rigid cylinder
161	**Costantino Creton** Interfacial and Bulk Damage quantification of thin films on soft substrate
163	**Michael Dickey** Shaping a Soft Future with Liquid Metals
165	**Sebastian Hendrickx-Rodriguez** The Biomechanical Influence of Polysaccharides Found in Anti-Wrinkle Formulations on Human Skin
167	**Juha Koivisto** Strong and Functional Hierarchical Biofoam Structures
169	**Andrew Martin** Predicting Emergence of Nanoscale Order in Surfaces Oxides through Preferential Interactivity Parameter
171	**Jordan Shivers** Thermodynamics of morphological transitions in growing membranes
173	**Thomas Petersen** Modeling Electrolytes at Charged Mineral Interfaces Using Classical Density Functional Theory
175	**Zeb Rocklin** Fundamental principles of flexible solids
177	**Sangjin Ryu** Air bubbles entrapped during the coalescence of drops in a Hele-Shaw cell

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
156	**Stephen Thornton** Universal Scaling Solution for a Rigidity Transition: Renormalization Group Flows Near the Upper Critical Dimension
	Interfaces, Surfaces & Membranes
160	**Daniel Daniel** Exploding drops on lubricated surfaces
162	**Michał Góra** Nano-porous Surfaces and Associated Interfacial Forces
164	**Mohit Gupta** Hydrophobic Interactions in Unstable Wetting Films
166	**Robin McDonald** Enhancing Solar Panel Efficiency through Nanostructured Coatings
168	**Fan Meng** Exploring Nanostructured Biomimetic Surfaces: Measuring Hydrophobic Properties via Free Energy Barrier using Coarse-Grained Mo-
170	**Alana Pauls** Stereo-Structural Fine Tuning of Chromaticity
172	**Brahim El-khalil Remini** Study of the interface between liquid polymers and viscoelastic polymers in dynamic and static states.
174	**Ozgur Sahin** Hydration Forces, Hydration Solids, and The Hygroelastic Theory
176	**Gentian Muhaxheri** Bifurcations of inflating balloons and interacting hysterons
178	**Hooman Tafreshi** Physics of Multiphase Droplet Adhesion to a Fiber
180	**Yoav Tsori** Phase lines in mean-field models with nonuniform external forces

Poster Session 1 (Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)	
Poster Board #	**Presenter & Poster Title**
179	**Hooman Tafreshi** Multiphysics interactions between electret fibers and airborne particles and droplets
Liquid Crystals	
183	**Timothy Atherton** Catching the wave: particle transport by a moving phase boundary
185	**Asaf Dana** Collective action and entanglement of magnetically active liquid crystal elastomer ribbons
187	**Delace Jia** Flow-Induced Structures in Lyotropic Chromonic Liquid Crystals
Measurement & Characterization	
189	**(Amir)Hossein Salahshoor** Data-Driven Rheology: A Direct Link Between Complex Moduli and Predictions
Networks & Gels	
193	**Oreoluwa Alade** Modeling Phase Stability of Concentrated Suspensions of Compressible Microgels
195	**Tuhin Chakrabortty** Dynamics of Active Relaxing Networks
197	**George Degen** Mucin-derived adhesive hydrogels
199	**Nitsan Eliraz** Activating physical crosslinking in synthetic extracellular matrices by switch peptides

Poster Session 2 (Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)	
Poster Board #	**Presenter & Poster Title**
182	**Xu Wang** Experimental and Computational Investigation of nanoparticle ligand shell morphology
Liquid Crystals	
184	**Timothy Atherton** Morpho---A programmable environment for shape optimization and shapeshifting problems
186	**Alexia Chatzitheodorou** Shape Morphing of Twisted Nematic Elastomer Shells
Measurement & Characterization	
190	**Leroy Jia** Serial flow cytometry as a method to measure membrane elasticity
192	**Richard Sheridan** BOTTS: 500% Faster Viscoelastic Master Curves via Broadband Chirps
Networks & Gels	
194	**Mahesh Aryal** Modeling the Response of Compressible Microgels to Crowding by Nanoparticles
196	**Nate Brown** Organic Phosphate Degradation via Functionalized PA-6 Fabrics
198	**Yanxia Feng** Freezing hydrogels reveals a simple, power-law behavior of their osmotic pressure
200	**Yunxiang Gao** Pristine Carbon Nanotubes as Supramolecular Linkers to Crosslink Microgels into Macroscopic Hydrogel Composites for Versatile Ad-

Poster Session 1 **(Tue. July 30,** 6:00-8:00 PM, Exhibit Hall A**)**	
Poster Board #	**Presenter & Poster Title**
201	**Sidharth Gat** Measurement of vibrational modes in disordered metamaterials fabricated by laser powder bed fusion.
203	**Yunhua Guo** Controlling the complexation between polyanionic microgels and cationic peptides to create self-defensive antimicrobial surfaces
205	**Saad Khan** From gels to 3-D networks: Creating multifunctional hybrid polymer-metal oxide nanofiber based aerogels
207	**Alexander Marshall** Size dependent, stress driven transport in poroelastic media at the microscale
209	**Jonathan Michel** Developing Simulations to Guide Design of Biotic-Abiotic Machines
211	**Katherine Moody** Manufacturing Techniques of Disordered Metamaterials Using Laser and Electron Beam
213	**Mauro Mugnai** Network-Network Interactions in Multi-Component Gels
215	**Fu-Sheng Wang** Supramolecular Template of Entanglements and Their Spectroscopic Detection in Polymer Elastomers and Gels
217	**Xinyu Wang** Fracturing and Controlled Cracking Path in Topological Maxwell Lattice
219	**Fei Wang** Novel Volumetric mapping of 3D Nanomechanical Heterogeneities in Gelatin, Collagen, and Polypeptide Hydrogels and Films
Polymers	
221	**Sonam Zangpo Bhutia** Bound Layer in Hydrophilic Polymer Thin Films: Effect of Annealing
223	**Kateri DuBay** Modeling the emergence of collective nascent chain behavior and its implications for the sequences and aggregates of step-grown copol-

Poster Session 2 **(Thur. August 1,** 6:00-8:00 PM, Exhibit Hall A**)**	
Poster Board #	**Presenter & Poster Title**
202	**Tyler Hain** Programming rigidity transitions and multifunctionality in disordered underconstrained spring networks
204	**Harsha Koganti** Elastic microphase separation: the role of network parameters beyond elastic modulus
206	**Ricky Frank López-Santiago** Linear and nonlinear viscoelasticity in physical gels made with polycations, polyanions, and their mixtures; rheology and microrheol-
208	**Joan Montes De Oca** Water two liquids, anyway?
210	**Kengo Nishi** Peptide self-assembly orchestrates structure transition of in-vitro actin bundle networks
212	**Thomas Parton** Revealing the mechanism of kinetic arrest in suspensions of rod-like cellulose nanocrystals using angle-resolved optical spectros-
214	**Shu Wang** Nonlocal Intrinsic fracture energy of polymer networks
216	**Takaichi Watanabe** Toughening of poly(ionic liquid) gels with nanomaterials having different shapes
218	**Masahiro Yoshida** TEM study on hydrogel network formation via free-radical polymerization
220	**Boxue Zheng** Capillary-Induced Deformation and Solvent Transport in Hydrogels
Polymers	
222	**Mesbah Ahmad** Formation of ultrasoft, stretchable, and biodegradable films from plasticized agarose for sustainable electronics
224	**Tim Bernhard** Reproducing Viscoelastic Behaviours of End-linked Polymer Networks using Simulations

Poster Session 1 (Tue. July 30, 6:00-8:00 PM, Exhibit Hall A)	
Poster Board #	**Presenter & Poster Title**
225	**Hongshuang Guo** Halogen-bonded shape memory liquid crystal polymer
227	**Atte Kadoma** Hydrolytic Crack Growth and Embrittlement in Poly(ethylene terephthalate)
229	**Pooja Nanavare** Osmolyte-induced Conformational Stabilization of a Hydrophobic Polymer
231	**Emmanuel Oduro** Additive manufacturing of high-resolution architected copper by controlled shrinkage of highly swollen, infused bottlebrush hydrogel
233	**Jacob Peloquin** Overcoming premature fracture: Reduction of stress concentration effects in additively manufactured lattices using three-dimen-
235	**Sebastian Pineda Pineda** Charge Regulation Triggers Condensation of Short Oligopeptides to Polyelectrolytes.
237	**Sergei Rigin** Design of Composite Polymer Brushes for Adsorption of Contaminants from Water
239	**Martin Seifrid** The Data-Driven Organic Materials Lab
241	**Neha Tyagi** Quasi-active transport of tracer particles in flowing semidilute polymer solutions
Self-Assembly	
243	**Gaurav Arya** DNA assemblies with emergent functions
245	**Zoe Benton** Failure in the working curve: Determining interlayer adhesion in stereolithography printing via photorheology
247	**Safak Callioglu** Efficient Monte Carlo Framework for Simulating Self-Assembly of Faceted Nanoparticles

Poster Session 2 (Thur. August 1, 6:00-8:00 PM, Exhibit Hall A)	
Poster Board #	**Presenter & Poster Title**
226	**Pablo Cordero Alvarado** Combination therapy of microporous hydrogel scaffolds displaying supramolecular peptide assemblies to enhance wound healing
228	**Yixin Hu** Mechanochemically self-amplified HF release and polymer deconstruction
230	**Baiqiang Huang** Bottlebrush polyethylene glycol nanocarriers translocate across human airway epithelium via molecular architecture enhanced endocy-
232	**Tahmida Iqbal** Liquid-Liquid Phase Separation In Multicomponent Polymer System
234	**Silpa Mariya** The subdiffusive motion of sticky dendrimers in an associative polymer network
236	**Anicah Smith O'Brien** Understanding Polymer Biodegradation Under Different Environmental Conditions
238	**Logan Williams** The Crystallization and Rigid Fraction of PLLA
240	**Xiangyu Zhang** The Particle Geometry Effect on Polymer Chain Scaling Behaviors
Self-Assembly	
244	**Kireeti Akkunuri** Unraveling the conformational dynamics of 'clasping' polymer-grafted nanoparticles and their networks
246	**Nan Cheng** Geometrically frustrated self-assembly of hyperbolic crystals from icosahedral nanoparticles
248	**Naresh Dhanasekar** Enzyme-triggered peptide fibrillation in a synthetic droplet

Poster Session 1

(**Tue. July 30,** 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
249	**Daniel Duke** Dr. Gaurav Arya Illuminating the mechanism of DNA origami folding with a new mesoscopic model
251	**Yuan Gao** Reconfigurable self-assembly of peptide-peptoid hybrids
253	**Remya Ann Mathews Kalapurakal** Theory and Simulations of Light-Induced Self-Assembly in Colloids with Quantum Chemistry Derived
255	**Zexi Liang** Overcoming Kinetic Traps in Self-Assembly using Magnetic Decoupling
257	**Melody Lim** Magnetoelastic microscopic multistate machines
259	**Po-An Lin** Deep Inverse Design of Patchy Polygons for Mesoscale Assembly of 2D Superlattices
261	**Sanjib Majumder** Colloidal deposits with unique reflection symmetry to fractal patterns: effect of confinement
263	**Tero Mäkinen** Inducing hydrophobicity in biobased foams by the addition of lignin
265	**Rupam Saha** Synthetic modular building blocks for self-limited assembly
267	**Rony Waheibi** Self-assembly of bidisperse colloidal gels
269	**Ye Xu** Tunable alignment of highly-oriented silver nanowires through polymer-assisted evaporation processing for anisotropic electrical and
271	**Shihao Zang** Direct observation of non-classical crystallization pathways in binary colloidal systems

Poster Session 2

(**Thur. August 1,** 6:00-8:00 PM, Exhibit Hall A)

Poster Board #	**Presenter & Poster Title**
250	**Helena Freire Haddad** Enabling Asymmetrical Assembly of Supramolecular Peptide Nanofibers
252	**Taranpreet Kaur** Material properties of Condensates control Gene Expression
254	**Stephen Klawa** Uncovering Supramolecular Chirality Codes for the Design of Tunable Biomaterials
256	**Kat Lazar** Materials characterization of a self-assembling elastin-like polypeptide fusion protein as a platform for immunotherapies
258	**Jeremy Money** Harnessing Liquid Crystal Disclinations for Next-Generation Architected Materials
260	**Maks Pecnik Bambic** Optimal face-to-face coupling for fast self-folding kirigami
262	**Deleah Pettie** Peptide Nanomaterial Active Immunotherapy to counteract IL-22 Binding Protein for Intestinal Regeneration in Inflammatory Bowel Dis-
264	**Sourav Roy** Exploring Geometric Frustration in Self Assembly of Mechanical Metamaterial Using a Generalized Elasticity Theory
266	**Monirosadat (Sanaz) Sadati** Programming Bio-inspired Nanoscale Chiral Self-Assembly in 3D Printed Composites
268	**Nader Taheri-Qazvini** Multifunctional MXene-PAA microgel hybrids for high-performance conductive 3D printing inks and aerogels
270	**Michael Wang** Geometric frustration meets mechanical metamaterials
272	**Pinchu Xavier** Biophysical characterization of hard/soft nanoparticles for surface activity of pulmonary surfactants in the treatment of infant respira-
274	**Mengjie Zu** Designing athermal disordered solids with automatic differentiation

Poster Session 1

(Tue. July 30, 6:00-8:00 PM, Exhibit Hall A**)**

Poster Board #	**Presenter & Poster Title**
273	**Zhencheng Max Jiang N** Nonaffinity in colloidal gels
275	**Abishec Sundar Senthilvel** Modeling of Additive Compounds in Tire Materials

Poster Session 2

(Thur. August 1, 6:00-8:00 PM, Exhibit Hall A**)**

Poster Board #	**Presenter & Poster Title**
276	**April Espinoza** Chiral-based Hydrogel Scaffolds Bias Immune Mismatched Skin Transplantation Toward Engraftment Through Humoral Attenua-
278	**Ashif Akram** Competing addition processes give distinct growth regimes in the assembly of 1D filaments

History and Future of the ISMC

See details at https://soft-matter.com/ismc2024/ismc-about/

International Soft Matter Conferences (ISMC) started in Europe where the first six conferences were held every three years in a different European country:

- 1st ISMC, October 1-4, 2007, Aachen, Germany
- 2nd ISMC July 5-8, 2010, Granada, Spain
- 3rd ISMC, September 15-19, 2013, Rome, Italy
- 4th ISMC, September 12-16, 2016, Grenoble, France
- 5th ISMC, June 3-7, 2019, Edinburgh, United Kingdom
- 6th ISMC, September 19-23, 2022, Poznan, Poland was the first event of the International Soft Matter Conference Series: Around the World in Three Years, coordinated by the IUPAP Working Group 15.
- 7th ISMC, September 4-8, 2023, Osaka, Japan was the second conference in this series and the first one outside Europe.
- 8th ISMC, July 29-August 2, 2024, Raleigh, North Carolina, USA, completes the first cycle of this series with a first ISMC in the Americas.
- 9th ISMC is planned to be held September 29-October 3, 2025, at Minoa Palace Resort, Chania, Crete, Greece
- 10th ISMC is planned to be held May 25-29, 2026, at Burla Institute of Technology, Goa, India.

International Union of Pure & Applied Physics Working Group 15: Soft Matter

In October 2017, the 29th IUPAP General Assembly resolved to establish Working Group 15: Soft Matter with the following mission/mandate:

1. To organize/assist in organization of an International Conference "Soft Matter Around the World" which rotates every three years to each geographic region (Europe-Africa, the Americas, and Asia-Pacific).
2. To coordinate soft matter-related regional, national & local conferences, meetings & workshops.
3. To coordinate soft matter education, such as summer/winter schools and short courses and help organize them if a need appears.
4. To promote soft matter research through information exchange, publicity, prizes, publications, etc.
5. To strengthen the connection between academic and industrial soft matter research and development through outreach events, short courses, etc.

IUPAP WG-15 Members:

Michael Rubinstein (Chair); Seth Fraden (US); Daan Frenkel (United Kingdom); Gerhard Gompper (Germany)**;** Peter Harrowell (Australia)**;** Wonho Jhe (Korea)**;** Jean-François Joanny (France)**;** Eugenia Kumacheva (Canada)**;** Guruswamy Kumaraswamy (India); Andrea Liu (US); Hajime Tanaka (Japan); David Weitz (US); Ouyang Zhongcan (China)**;** Emanuela Zaccarelli (Italy)

Soft Matter Association of the Americas

The Soft Matter Association of the Americas (SMAA) was formed in 2023 with the support of the IUPAP Working Group 15: Soft Matter. Its objectives and tasks (to be discussed at the Business Meeting on August 2, 2024 at 12:15 PM) are (see www.soft-matter.com for more information):

- Exchange information between different soft matter professional organizations (events/activities/ideas);
- Facilitate the organization of regional soft matter workshops;
- Develop the soft matter workforce in the Americas, advertise job postings and other opportunities on the SMAA website;
- Facilitate collaborations between soft matter scientists and engineers in academia and industry.

The SMAA Board of Directors consists of Michael Rubinstein (President, Duke), Christoph Schmidt (Treasurer, Duke), Ronit Freeman (Secretary, UNC), and Jan Genzer (Vice President, NCSU).
The Advisory Board of SMAA consists of four Councils: (i) Professional Organizations Council; (ii) Regional Organization Council; (iii) Industrial Council; and (iv) Americas Council.

The roles of the **Professional Organizations Council** are

- Coordinate soft matter activities between different professional organizations and organize joint events
- Advertise events of a particular professional organization to members of other organizations
- Input from members of a particular professional organization on sessions/topics for the International Soft Matter Conference 2024 (ISMC2024)
- Advertise job postings and open positions for students, faculty and postdocs on the SMAA website (that is now being built – www.soft-matter.com)
- Solicit ideas from members of the professional organizations for other events at ISMC such as young investigator satellite meeting, and/or short courses, and free-standing events

  The members of the advisory board of the Professional Organizations Council are

  1. Pietro Cicuta (University of Cambridge) IUPAP C6
  2. Jacinta Conrad (University of Houston) – SOR
  3. Timothy Bunning (Wright-Patterson Air Force Base) – ACS - PMSE
  4. Lorena Tribe (The Pennsylvania State University) – ACS - COMP
  5. Mia Huang (Scripps Research) – ACS - CARB
  6. Charles Schroeder (University of Illinois Urbana-Champaign) – APS - DSOFT
  7. Mahesh Mahanthappa (University of Minnesota) – APS - DPOLY
  8. Moumita Das (Rochester Institute of Technology) – APS - DBIO
  9. Daphne Klotsa (UNC) – APS - GSNP
  10. Aniket Bhattacharya (University of Central Florida) – APS - DCOMP

The roles of the **Regional Organizations Council** are:

- Submit proposal to organize and host ISMC2027
- Information exchange between different organizations about their events and activities (help coordinate individual or hold joint events)
- Help set up soft matter workshops in different regions and exchange best practice experiences
- Advertise job postings and open positions for students, faculty and postdocs on the SMAA website
- Provide input to sessions/topics/round table discussions at ISMC and other events
- Facilitate collaborations between soft matter scientists and engineers in academia and industry
- Develop ideas for other events at ISMC or free-standing events

The members of the advisory board of the Regional Organizations Council are:

1. José R Alvarado (University of Texas at Austin) Texas Soft Matter

2. Rae Anderson (University of San Diego) Frontiers in Soft Matter & Macromolecular Networks
3. Daniel Blair (Georgetown University) Mid-Atlantic Soft Matter Workshops
4. Seth Fraden (Brandeis University) New England Complex Fluids
5. Stefan Zauscher (Duke) Triangle Soft Matter

The roles and benefits of the **Industrial Council** are:

- Access to soft matter societies, laboratories, groups, and other companies for updates on cutting-edge research and potential collaborative projects
- Participate in developing the soft matter workforce in the Americas and access to this workforce
- Provide input to the educational program – short courses oriented to particular industrial interest
- Provide input on sessions/topics/round table discussions at the International Soft Matter Conferences and other events
- Advertise job postings and open positions for students, faculty, and postdocs on the SMAA website
- Advertise the company and its products and discounts for booth/expo at the meeting
- Facilitate collaborations between soft matter scientists and engineers in academia and industry

The advisory board of the Industrial Council consists of:

1. Preeta Datta (Evonik)
2. Michael Dimitriou (Exponent)
3. Timothy Fornes (ParkerLord)
4. Ryan Fuierer (Asylum)
5. Leah Johnson (RIT)
6. Dean DeLongchamp (NIST)
7. Suman Sinha Ray (NASA)
8. Kurt Selle (BTEC)
9. Beverly Asoo Stonas (HP)
10. Davoud Zare (Fonterra)

The roles of the **Americas Council** are:

- Connect and network between groups in their country and other countries in the Americas or globally
- Advertise events in their members' countries to soft matter scientists in other countries
- Advertise job postings and open positions for students, faculty, and postdocs on the SMAA website
- Provide input from members of their organization on sessions/topics for the ISMC
- Solicit proposals to organize and host the next ISMC (ISMC2027)
- Develop ideas for other events at ISMC or free-standing
- Organize young investigator satellite meetings and/or short courses
- Facilitate collaborations between soft matter scientists and engineers in academia and industry

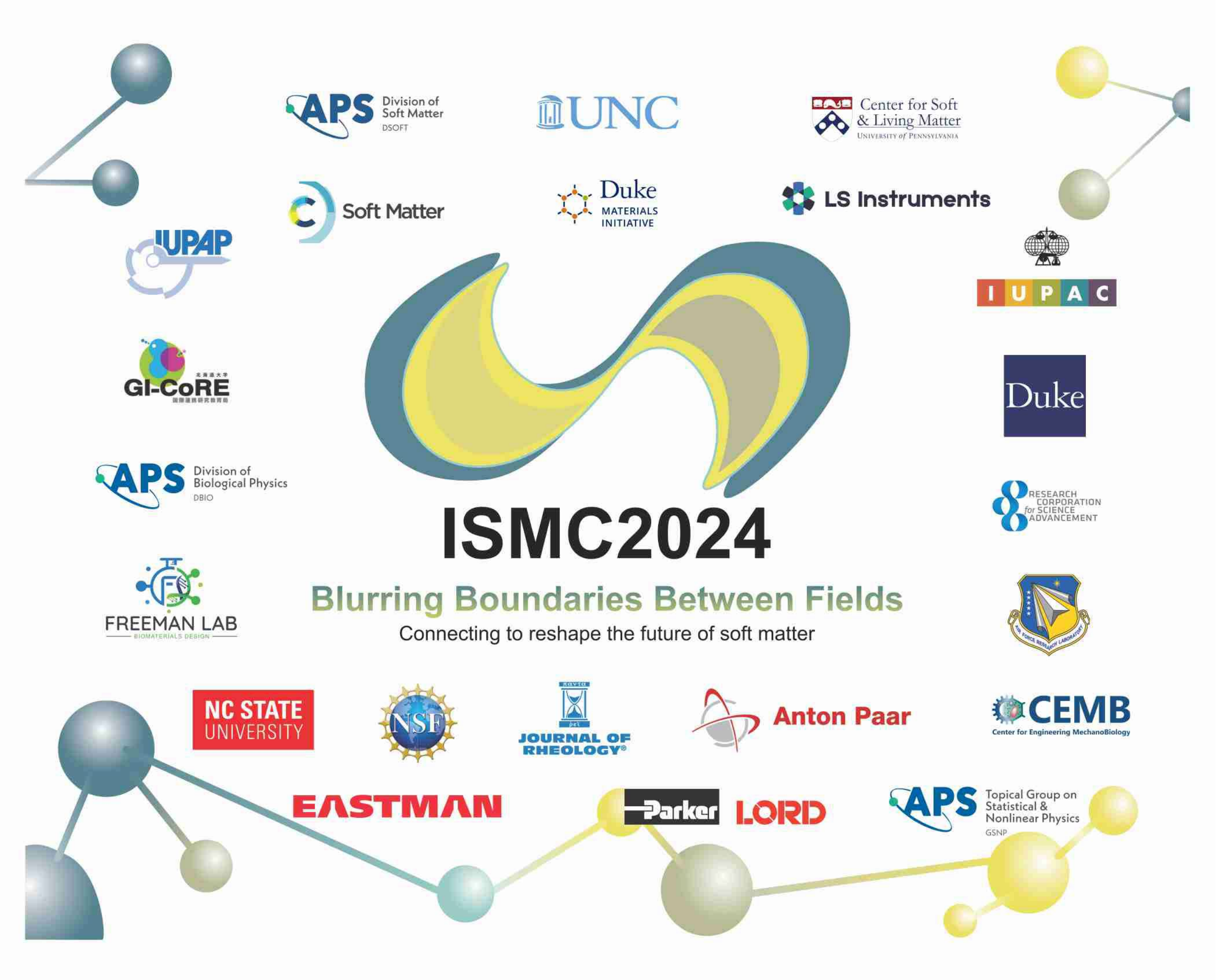
The advisory board of the Americas Council Consists of:

1. Ramón Castañeda-Priego (Universidad de Guanajuato) Red Mexicana de Materia Condensada Blanda
2. James Harden (University of Ottawa) Soft Matter Canada
3. Israel Omar Pérez López (Universidad Autónoma de Ciudad Juárez) MCNANO SMF
4. Verónica Marconi (Universidad Nacional de Córdoba) Asociación Física Argentina (AFA) División Materia Blanda

The SMAA may need to form the following Subcommittees:

- Structure and Rules Subcommittee (Bylaws: Executive Committee, rotation, elections, etc.)
- ISMC2027 proposal solicitation: development of proposal review protocol; next event site selection
- Idea solicitation for activities, e.g., short course or a series of short courses for industry or academia (educational material for SMAA website)
- SMAA website administrative support: content updates on Zoom weekly seminars, other events and activities, job listings etc.
- Local soft matter associations: coordinate activities and help start new local organizations.
- How to improve connectivity and exchange of ideas/people between different countries of the Americas
- How to best coordinate SMAA activities with professional societies

Thank you to our sponsors for making this event possible!



Program by sessions:

A1: Active Matter 1, Tuesday July 30, 10:30 AM – 12:00 PM
Room 306 BC, Chair: Fred McKintosh
B1: Biological Matter 1, Tuesday July 30, 10:30 AM – 12:00 PM
Room 305 AB, Chair: Paul Janmey
P1: Polymers 1, Tuesday July 30, 10:30 AM – 12:00 PM
Room 302 BC, Chair: Timothy Fornes
G1: Glasses, Granular & Jamming 1, Tuesday July 30, 10:30 AM – 12:00 PM
Room 301 AB, Chair: Srikanth Sastry
I1: Interfaces, Surfaces & Membranes 1, Tuesday July 30, 3:30 PM – 5:30 PM
Room 306 BC, Chair: Beverly Asoo Stonas
B2: Biological Matter 2, Tuesday July 30, Tuesday July 30, 3:30 PM – 5:30 PM
Room 305 AB, Chair: José R Alvarado
C1: Colloidal Systems 1, Tuesday July 30, Tuesday July 30, 3:30 PM – 5:30 PM
Room 302 BC, Chair: Jacinta Conrad
N1: Networks 1, Tuesday July 30, Tuesday July 30, 3:30 PM – 5:30 PM
Room 301 AB, Chair: Aniket Bhattacharya
A2: Active Matter 2, Wednesday July 31, 10:30 AM – 12:00 PM
Room 306 BC, Chair: Orlin Velev
L1: Liquid Crystals 1, Wednesday July 31, 10:30 AM – 12:00 PM
Room 305 AB, Chair: Timothy Bunning
F1: Fluid Dynamics & Rheology 1, Wednesday July 31, 10:30 AM – 12:00 PM
Room 302 BC, Chair: Charles Schroeder
S1: Self-Assembly 1, Wednesday July 31, 10:30 AM – 12:00 PM
Room 301 AB, Chair: Dean DeLongchamp
I2: Interfaces, Surfaces & Membranes 2, Wednesday July 31, 3:30 PM – 5:30 PM
Room 306 BC, Chair: Ryan Fuierer
B3: Biological Matter 3, Wednesday July 31, 3:30 PM – 5:30 PM
Room 305 AB, Chair: James Harden
P2: Polymers 2, Wednesday July 31, 3:30 PM – 5:30 PM
Room 302 BC, Chair: Matthew Becker
S2: Self-Assembly 2, Wednesday July 31, 3:30 PM – 5:30 PM
Room 301 AB, Chair: Ramón Castañeda-Priego
A3: Active Matter 3, Thursday August 1, 10:30 AM – 12:00 PM
Room 306 BC, Chair: Suman Sinha Ray
L2: Liquid Crystals 2, Thursday August 1, 10:30 AM – 12:00 PM
Room 305 AB, Chair: Edward Samulski
P3: Polymers 3, Thursday August 1, 10:30 AM – 12:00 PM
Room 302 BC, Chair: Thomas Halsey

S3: Self-Assembly 3, Thursday August 1, 10:30 AM – 12:00 PM
Room 301 AB, Chair: Leah Johnson
A4: Active Matter 4, Thursday August 1, 3:30 PM – 5:30 PM
Room 306 BC, Chair: James Harden
B4: Biological Matter 4, Thursday August 1, 3:30 PM – 5:30 PM
Room 305 AB, Chair: Rae Anderson
F2: Fluid Dynamics & Rheology 1, Thursday August 1, 3:30 PM – 5:30 PM
Room 302 BC, Chair: Bavand Keshavarz
G2: Glasses, Granular & Jamming 1, Thursday August 1, 3:30 PM – 5:30 PM
Room 301 AB, Chair: Daniel Blair
A5: Active Matter 5, Friday August 2, 10:30 AM – 12:00 PM
Room 306 BC, Chair: Andrea Liu
B5: Biological Matter 5, Friday August 2, 10:30 AM – 12:00 PM
Room 305 AB, Chair: Liheng Cai
C2: Colloidal Systems 2, Friday August 2, 10:30 AM – 12:00 PM
Room 302 BC, Chair: Preeta Datta
N2: Networks 2, Friday August 2, 10:30 AM – 12:00 PM
Room 301 AB, Chair: Stephen Craig

List of Plenary & Keynote Speakers

Bechinger, Clemens (A1.4)
Berthier, Ludovic (A2.1)
Brujic, Jasna (C1.1)
Cerbino, Roberto (Plenary Session M)
Chaikin, Paul (C2.1)
Cohen, Itai (F1.3)
Colby, Ralph (F1.4)
Colin, Annie (G2.3)
Cottin-Bizonne, Cécile (A3.1)
Creton, Costantino (N1.6)
Del Gado, Emanuela (Plenary Session C)
Dufresne, Eric (I1.1)
Ediger, Mark (P1.4)
Eiser, Erika (S1.2)
Fakhraai, Zahra (G1.1)
Gang, Oleg (S3.1)
Giomi, Luca (A5.2)
Golestanian, Ramin (Plenary Session A)
Granick, Steve (A1.1)
Grason, Greg (S2.1)
Grest, Gary (P3.1)
Grosberg, Alexander (A4.1)
Hosoi, Anette (F2.6)
Ito, Kohzo (N1.3)
Keren, Kinneret (Plenary Session B)
Klein, Jacob (I1.4)
Koenderink, Gijsje (B1.3)
Kremer, Kurt (P3.4)
Krishnan, Madhavi (S1.1)
Kumar, Sanat (P1.1)
Lavrentovich, Oleg (L2.4)
Lodge, Timothy (S3.2)
Löwen, Hartmut (A3.2)
Mahadevan, Lakshminarayanan (B2.3)
Maitra Bhattacharyya, Sarika (G2.4)
Mao, Xiaoming (S2.4)
Milliron, Delia (C2.4)
Nakagaki, Toshiyuki (B2.6)
Okumura, Ko (I2.6)
Olvera De La Cruz, Monica (N2.3)
Osuji, Chinedum (L1.1)
Palacci, Jérémie (B4.6)
Ramaswamy, Sriram (A5.1)
Safran, Sam (B1.4)
Šarić, Andela (B3.5)
Schulman, Rebecca (B5.4)
Sharma, Prerna (C1.2)
Smalyukh, Ivan (L2.3)
Soto, Rodrigo (A4.4)
Stone, Howard A (Plenary Session F)
Suo, Zhigang (Plenary Session N)
Tirrel, Matthew (P2.1)
Valentine, Megan (B4.1)
Vlassopoulos, Dimitris (F2.3)
Wang, Zhen-Gang (P2.4)
Yang, Shu (Plenary Session L)
Yeomans, Julia (A2.4)
Zamponi, Francesco (G1.2)
Zumer, Slobodan (L1.2)

Biography of Plenary & Keynote Speakers (ordered alphabetically)

Bechinger, Clemens (A1.4)

University of Konstanz

Bio: Clemens Bechinger's group is working on experimental research in colloidal systems, focusing on fundamental physical phenomena such as critical phenomena, stochastic thermodynamics, and collective behaviors of self-propelled particles. His recent work delves into understanding systems in nonequilibrium baths, revealing surprising effects arising from the time-delayed response of the bath to particle motion. Formerly at the University of Stuttgart and a Max-Planck-Fellow at MPI-IS, Clemens joined the University of Konstanz in 2017. He is a key member of the Cluster of Excellence on Collective Behavior and contributes to faculty-wide research on nonequilibrium fluctuations. Clemens has received prestigious awards, including the Schottky awards and two ERC Advanced grants, in recognition of his impactful research contributions.

Berthier, Ludovic (A2.1)

Université de Montpellier – CNRS

Bio: Ludovic Berthier is research director at CNRS in France. He received his Ph.D. in theoretical physics from Ecole Normale Supérieure in Lyon, France. He was a Marie Curie Postdoctoral Fellow at Oxford University before joining CNRS in 2002. In 2007, he was a visiting scientist at the University of Chicago and from 2019 to 2023 at the University of Cambridge. He works on the statistical mechanics of disordered materials, non-equilibrium systems and soft matter.

Brujic, Jasna (C1.1)

New York University

Bio: Jasna Brujic is a Professor of Physics at New York University. She is one of the core faculty in the Center for Soft Matter Research. Brujic is an experimental physicist, who received her Ph.D. for work on the statistical mechanics of granular matter at the Cavendish Laboratory of the University of Cambridge, UK. She then conducted post-doctoral research at Columbia University in the area of single molecule proteins. Since 2007, Brujic has led a research group at the interface between soft matter physics and biophysics. The group uses biomimetic emulsion systems to study jammed matter, cellular organization in tissues in 3D, protein-protein adhesion, and programmable self-assembly of materials with custom designs.

Cerbino, Roberto (Plenary Session M)

University of Vienna

Bio: Roberto Cerbino is a professor of Soft Matter Physics at the University of Vienna in Austria. Prior to his current position, he served at the Faculty of Medicine of the University of Milan. His work lies at the intersection of physics, biology, and material science, aiming to understand complex systems through innovative experimental approaches and techniques. Roberto is currently an associate editor of the journal Soft Matter.

Chaikin, Paul (C2.1)

New York University

Bio: Paul Michael Chaikin is an American physicist known particularly for many significant contributions to the field of soft condensed matter physics. Chaikin earned his B.S. in physics from California Institute of Technology in 1966, and his Ph.D. in physics from the University of Pennsylvania in 1971 working with Kondo superconductors. He joined the physics faculty at the University of California, Los Angeles in 1972 and studied thermopower, density waves, and high field phenomena mostly in organic superconductors. The lure of actually seeing the microscopics of a system led him to soft matter. He helped develop techniques to measure elasticity and motion and understand colloidal interactions. Hard and soft matter interests continued after joining the faculty at UPenn (1983), the staff at Exxon Research (1983) and the faculty at Princeton University (1988). His interests in geometry/topology led to his founding contributions to diblock copolymer nanolithography, and studies of defects, annealing, and pattern formation. He helped demonstrate and explain why ellipsoids pack more densely than spheres. In 2005 he helped found the Center for Soft Matter Research at New York University. His more recent research centers on artificial self-replication, self-assembly, active matter, DNA nanotechnology, topological defects on curved surfaces, and quantifying order far from equilibrium.

He is currently a Silver professor of physics at New York University.

Cohen, Itai (F1.3)

Cornell University

Bio: Professor Itai Cohen studies the physics of matter in motion. At Cornell, his research has focused on building microscopic robots, controlling the shear thickening behavior of microscopic and nanoscopic particles suspended in a fluid, exploring the mechanics of materials ranging from biological tissues to origami inspired metamaterials, discovering the aerodynamic and neuromuscular mechanisms used by insects during flapping flight, and determining how audiences at heavy metal concerts coordinate their movement. Understanding how emergent behaviors arise from the microscopic rules governing these systems remains one of the biggest challenges in Physics. Professor Cohen received his BS in Physics from the University of California at Los Angeles, and his PhD in Physics from the University of Chicago. Following his graduate studies, he was a Post-doctoral fellow in Physics and the Division of Engineering and Applied Science at Harvard University. In 2005 he joined Cornell and is currently a professor of Physics. Professor Cohen is an NSF Career grant recipient, he is a Fellow of the American Physical Society, and is the recipient of the Kappa Delta Ann Doner Vaughn Award for his work on cartilage mechanics. He has served as a Feinberg and Braginsky fellow (2012) and the Rosi and Max Varon Visiting Professor at the Weizmann Institute (2021) and the van der Waals Visiting Professor at the University of Amsterdam (2022). He has published over 110 research articles, given nearly 300 invited seminars, colloquia and conference presentations, and co-authored the book Finding Your Research Voice: Story Telling and Theater Skills for Bringing Your Presentation to Life. His lab has made the world's smallest origami bird, and holds the Guinness world record for the smallest walking robot. His work has been covered by various outlets ranging from the BBC, to Scientific American, NPR, and the NYTimes.

Colby, Ralph (F1.4)

Penn State University

Bio: Ralph Colby received his B.S. in Materials Science and Engineering from Cornell University in 1979. After working for two years at the General Electric Company in rheology research and process development, he attended graduate school at Northwestern University, where he received his M.S. and Ph.D. in Chemical Engineering in 1983 and 1985. Graduate research focused on rheology of linear polybutadiene melts and solutions, which included 15 months as a visiting scholar in the Exxon Research and Engineering Company, Corporate Research - Science Laboratories. He then worked for ten years at the Eastman Kodak Company in their Corporate Research Laboratories. In 1995, Dr. Colby was hired as Associate Professor of Materials Science and Engineering at the Pennsylvania State University and was promoted to Professor in 2000. He teaches a very demanding undergraduate course on Polymer Rheology and Processing and continues to use rheological experiments to probe the dynamics of polymers and other complex fluids. Dr. Colby has over 250 publications and published a textbook Polymer Physics in 2003. Current research topics include flow effects on polymer crystallization, associating aqueous poly(vinyl alcohol) solutions, polyelectrolyte solutions in polar solvents, native cellulose solutions in ionic liquids, thermotropic liquid crystalline phases of conjugated polymers, a flow-induced nematic phase of poly(ether ether ketone) and single-ion conducting ionomers with polar additives, such as zwitterions. He was the Editor of the Journal of Rheology 2011-2021 and was the recipient of the Society of Rheology's Bingham Medal in 2012.

Colin, Annie (G2.3)

ESPCI Paris

Bio: Annie Colin is the Director of the MIE, the Matériaux Innovants pour l'Energie at ESPI, Paris. She mostly deals with Mechanics, Rheology, Flow, Shear and Velocimetry. Her Mechanics research is multidisciplinary, incorporating elements of Microfluidics, Capillary action and Shear rate. Her Capillary action study incorporates themes from Microchannel and Nanotechnology.

She has researched Shear rate in several fields, including Shear, Shear velocity and Classical mechanics. Her biological study spans a wide range of topics, including Amorphous solid, Granular material, Soft matter, Thin layers and Fluid dynamics.

Cottin-Bizonne, Cécile (A3.1)

Université Lyon 1 - CNRS

Bio: Cécile Cottin-Bizonne is a CNRS researcher at the University of Lyon in France, in the team "Liquids and Interfaces" at ILM. Her research interests lie at the crossroads between soft condensed matter and fluid dynamics, with a special focus on interfacial transport and active matter. In particular, in active matter, she has developed different classes of model and complementary experimental systems ranging from active colloids to interfacial camphor swimmers. Her work primarily involves experimental methods, supplemented by simple and complementary modelling and simulation approaches.

Creton, Costantino (N1.6)

ESPCI Paris - PSL

Bio: Costantino Creton coordinates the research activities of the Soft Polymer Networks research group of the laboratory since 2009. He also holds since 2011 the position of scientific chairman of the Performance Polymers technology area of the Dutch Polymer Institute and has been appointed in 2016, Distinguished Professor at the Global Station for Soft Matter of Hokkaido University. Since may 2019 he is also the vice-president research of the ESPCI Paris-PSL.

He has published more than 220 articles in peer-reviewed journals, 13 book chapters and has given more than 120 invited and plenary lectures at international conferences. His research interests focus on the mechanical properties of polymers at interfaces and on deformation and fracture of soft polymer networks. More information can be found in the research pages and in the website of the laboratory. He has received several prizes and awards including the Prix Dédale of the French Adhesion Society in 2007, the Wake Medal from the UK Society of Adhesion and Adhesives in 2011 and the Adhesion Society's prize for Excellence in Adhesion Science in 2013. He was also elected in 2013 fellow of the American Physical Society and received an ERC Advanced Grant in 2016 to work on fracture of soft materials. More recently he has been awarded in 2021 the grand Prix Fondation Michelin - Académie des Sciences.

Del Gado, Emanuela (Plenary Session C)

Georgetown University

Bio: Emanuela Del Gado is a physics Professor and the Director of the Institute for Soft Matter Synthesis and Metrology at Georgetown University. She was a Marie Curie Fellow and the Swiss National Science Foundation Assistant Professor at ETH Zurich, and has held visiting position at MIT, ESPCI Paris, ENS Lyon, and University Paris Saclay. She was elected Fellow of the Royal Society of Chemistry in 2018, she is a Fellow of the American Physical Society (2020) and a Fellow of the Society of Rheology (2023). Her research is aimed at the spatiotemporal characterization of microscopic dynamical processes and the unraveling of microstructural underpinnings in the rheology of soft materials, with a focus on colloidal gels and other soft solids.

Dufresne, Eric (I1.1)

Cornell University

Bio: Eric R. Dufresne is a professor of Physics and Materials Science and Engineering at Cornell University. His research focuses on morphogenesis and mechanics in biological and synthetic soft materials. Before moving to Cornell in 2023, Eric was a graduate student at the University of Chicago, a post-doc at Harvard University, a professor at Yale University, and a professor at the Swiss Federal Institute of Technology in Zürich. Eric is a fellow of the American Physical Society and a member of the editorial board of Physical Review X.

Ediger, Mark (P1.4)

University of Wisconsin-Madison

Bio: Mark Ediger received his Ph.D. from Stanford University and is currently the Hyuk Yu Professor of Chemistry at UW-Madison. His research is focused on organic glasses, both polymeric and low-molecular-weight materials. Ediger is currently an Associate Editor for the Journal of Chemical Physics. He has served as Chair of two Gordon Conferences: Polymer Physics and Chemistry and Physics of Liquids. He received the American Physical Society's Dillon Medal in 1993 and also the Polymer Physics Prize in 2015, as well as the American Chemical Society Hildebrand Award for the Experimental and Theoretical Chemistry of Liquids in 2013.

Eiser, Erika (S1.2)

University of Trondheim

Bio: Erika Eiser sttudied Solid State Physics at the Universiy of Konstanz, Germany, and received her Masters Degree based on research she did on the interdiffusion in binary polymer melts using a particle accelerator, which she did at the Weizmann Institute of Science in Rehovot, Israel. In the same group (Prof.Jacob Klein) she also did her PhD research, studying the normal and lubrication forces between polymer bearing surfaces using the Surface Force Balance. After receiving her PhD degree in 1997, she became an EU-postdoctoral researcher at the University of Montpellier II and subsequently at the European Synchrotron Radiation Facility (beam line ID1) in Grenoble, France. There she researched the self-assembly of block copolymers and their flow behaviour in combined Small Angle X-ray Scattering (SAXS) and rheology measurements. Continuing her love for Soft Matter Physics and in particular self-assembling systems, she became Assistent Professor at the University of Amsterdam in the Netherlands in 2000. There she started two research directions, one on the aging behaviour of clay suspentions, which she studied with Dynamic Light Scattering (DLS) and Micro-Rheology, and the self-assembly of DNA-functionalized Colloids, which she studied with confocal microscopy. In 2008 she was offered a Seniour Lectureship and later Professorship at the Cavendish Laboratory at the University of Cambirdge, UK, where she continued both research lines and expanded her reaserch to also develop new micro-rheology and video-microscopy methods. In addition her group developed an approch that includes experiments, simulations and theory.

In 2021, she accepted a Professorship at the Physics Department of the NTNU and became PI at PoreLab, a Centre of Excellence. In the past 2 years she has built up an experimental Soft Matter lab to continue her DNA-research for diagnostic applications and to expand into research of environmentally sustainable ground and binary flow in nano-porous media.

Fakhraai, Zahra (G1.1)

University of Pennsylvania

Bio: Zahra Fakhraai is a Professor of Chemistry at the University of Pennsylvania, with a secondary appointment at the Department of Chemical and Biomolecular Engineering. She received her PhD degree in Physics from the University of Waterloo in 2007, where she studied the dynamics of polymers in thin films and at interfaces. After two postdoctoral fellowships at the University of Toronto (2008-09) and the University of Wisconsin-Madison (NSERC post-doctoral fellow, 2009-11) she joined the Department of Chemistry at the University of Pennsylvania. Her group at Penn combines experiments and modeling to explore structure, dynamics, and optical properties of glasses and soft materials at nanometer length scale and interfaces. Zahra is a member of the American Physical Society, American Chemical Society, and the American Association for the Advancement of Science. She is the recipient of the APS Padden Award (2007), NSF Career award (2014), Sloan fellowship in Chemistry (2015), the Journal of Physical Chemistry JPC-PHYS lectureship award (2017), APS Dillon Medal (2019), and ACS Rising Starts Award (2021). She is also active in broadening participation of historically marginalized groups in STEM and is serving as a faculty mentor for the Penn chapter for the Alliance for Diversity in Science & Engineering (ADSE). She has received the Dean's Award for Mentorship of Undergraduate Research (2021) and the Trustees Council of Penn Women Faculty Award for Undergraduate Advising (2024).

Gang, Oleg (S3.1)

Columbia University

Bio: Oleg Gang is a professor of Chemical Engineering and of Applied Physics and Materials Science at Columbia University and a group leader at the Center for Functional Nanomaterials at Brookhaven National Laboratory. His research explores molecular and nanoscale self-assembly phenomena, the bottom-up strategies for creating designed biomaterials and nanomaterials, and applying them to enable material functions. Gang is a Fellow of the American Physical Society and has received numerous accolades for his work.

Giomi, Luca (A5.2)

Leiden University

Bio: Luca Giomi's research aims at exploring the fuzzy interface between soft condensed matter and biological physics, using the universal language of geometry and mechanics and following the North Star of experimental evidence. After studying theoretical physics in Rome, he moved to Syracuse University, where he obtained his PhD under the supervision of Mark Bowick, with a thesis on the interplay between topological defects and spatial curvature in two-dimensional crystals. As a postdoc in the group of Mahadevan at Harvard, he worked on a variety of topics about the physical organisation of biological systems, before establishing his independent research group at Leiden University in 2014. His research endeavour resulted into a number of exciting discoveries, such as those related with the dynamics of defects and chaos in active matter, the geometry of bacterial monolayers and the origin of their transition to multilayered structures, the dynamics of cooperative sperm aggregates in competitive environments, the geometry and thermodynamics of lipid mixtures on curved topographies etc.

Golestanian, Ramin (Plenary Session A)

Max Planck Institute for Dynamics and Self-organization, Göttingen

Bio: Ramin Golestanian (born on 26 February 1971) obtained his BSc from Sharif University of Technology in Tehran, and his MSc and PhD from the Institute for Advanced Studies in Basic Sciences (IASBS) in Zanjan. His PhD work was conducted under the remote supervision of Mehran Kardar from MIT, and was followed by an independent postdoctoral research fellowship at the Kavli Institute for Theoretical Physics at the University of California at Santa Barbara. He has held academic positions at IASBS, the University of Sheffield, and Oxford University, and risen through the ranks until he became a Full Professor in 2007. He has a broad interest in various aspects of nonequilibrium statistical physics, soft matter, and biological physics. Golestanian is distinguished for his work on active matter, and in particular, for his role in developing microscopic swimmers and active colloids.

Granick, Steve (A1.1)

University of Massachusetts Amherst

Bio: Steve Granick is an American scientist and educator. In 2023 he joined the University of Massachusetts-Amherst as the Robert Barrett Endowed Chair of Polymer Science and Engineering, with joint appointment in the Chemistry, Physics, and Chemical Engineering Departments after serving as director of the Institute for Basic Science Center for Soft and Living Matter, an interdisciplinary blue-sky research center in Ulsan, South Korea that pursues basic science research. Until 2015 he was professor at the University of Illinois at Urbana-Champaign. He is a member of the American Academy of Arts and Sciences and the U.S. National Academy of Sciences.

Grason, Greg (S2.1)

University of Massachusetts Amherst

Bio: Greg Grason is a Professor and Graduate Program Director of Polymer Science and Engineering (PSE) at University of Massachusetts Amherst. He received a Ph.D. in Physics from the University of Pennsylvania in 2005. Following a postdoctoral position in the Physics and Astronomy department at UCLA, he joined the faculty of UMass in 2007. His research group investigates the role of geometric frustration in soft matter and polymeric assemblies through the combined lens of condensed matter theory, statistical physics and differential geometry. Recent efforts have focused on geometry and complex order in filamentous assemblies and membranes, hierarchical order in block copolymer assemblies, physics of frustrated, soft matter assemblies and programmable self-assembly. He was awarded a NSF CAREER Award in 2010, Sloan Fellowship in 2011, and Fellow of the American Physics Society in 2019. He is an Editorial board member of the New Journal of Physics and Giant, and was an elected member of the Executive Committee for the Division of Soft Matter of the American Physical Society (2016-2020).

Grest, Gary (P3.1)

Sandia National Laboratories

Bio: Gary S. Grest is an American computational physicist at Sandia National Laboratories. He was awarded a B.Sc in physics (1971), an M.S in physics (1973) and a Ph.D in physics (1974) by the Louisiana State University. His interest is the theory and simulation of nanoscale phenomena. Since

1998 he has been a member of the technical staff of Sandia Laboratories, since 2009 an adjunct professor in department of chemistry, Clemson University and since 2013 a Distinguished Sandia National Laboratories Professor in the department of chemical and biological engineering, University of New Mexico. He was elected a Fellow of the American Physical Society in 1989 "for contributions to the understanding of the kinetics of domain growth, amorphous glasses, disordered magnets, and polymer dynamics" He was elected to the National Academy of Engineering in 2008. He received the Aneesur Rahman Prize for Computational Physics from the American Physical Society in 2008 for his work in computational physicsand the American Physical Society Polymer Physics Prize in 2011

Grosberg, Alexander (A4.1)

New York University

Bio: Born and educated in Moscow, in the former Soviet Union, I received my PhD under the supervision of Ilya M.Lifshitz. Since 1992, I have worked in the US, and presently I am a Professor of Physics and Mathematics in New York University.

Hosoi, Anette (F2.6)

Massachusetts Institute of Technology

Bio: Anette “Peko” Hosoi is the Neil and Jane Pappalardo Professor of Mechanical Engineering, Professor of Mathematics, and a core faculty member of the Institute for Data, Systems and Society at MIT. Her research contributions lie at the junction of fluid dynamics, biomechanics, and bio-inspired design. More recently, she has turned her attention to problems that lie intersection of biomechanics, applied mathematics, and sports. She previously served as the Associate Dean of the MIT School of Engineering. Prof. Hosoi has received numerous awards including the American Physical Society Stanley Corrsin Award, the SIAM I. E. Block Community Lectureship, and the Jacob P. Den Hartog Distinguished Educator Award. She is a Fellow of the American Physical Society, a Radcliffe Institute Fellow, and a MacVicar Faculty Fellow.

Ito, Kohzo (N1.3)

University of Tokyo

Bio: Kohzo Ito is a University Professor at The University of Tokyo and a fellow at National Institute for Materials Science. He received his B.E, M. E. and Ph. D. degrees in applied physics from The University of Tokyo. In 1986, he joined the Research Institute of Polymers and Textiles. He was transferred back to Faculty of Engineering, the University of Tokyo in 1991 and promoted to full professor at Graduate School of Frontier Sciences, the University of Tokyo in 2003. He is now the president of the Society of Polymer Science, Japan, and is running big national projects as a program director (SIP) and project manager (Moonshot Program). He has been researching the polymer physics and supramolecular chemistry, and now is focusing on polyrotaxane using cyclodextrin, necklace-like supramolecule with topological characteristics. He invented slide-ring materials with movable cross-links by cross-linking polyrotaxane in 2000, and set up a venture company to urge the application of the slide-ring materials in 2005. He has been the author of over 300 publications including original research papers, reviews, and books, and about 70 patents. He received The Award of the Society of Polymer Science, Japan (2006). And he is currently an editor of Polymer, Elsevir.

Keren, Kinneret (Plenary Session B)

Technion – Israel Institute of Technology

Bio: Kinneret Keren is a professor of Physics at the Technion - Israel Institute of Technology. She earned her Ph.D. from the Technion, her M.Sc. in Physics from the Weizmann Institute of Science, and her B.Sc. in Physics and Mathematics from the Hebrew University in Jerusalem. Her research focuses on self-organization in biological systems, cell and tissue biomechanics, and synthetic biology. Prof. Keren has received several awards, including the European Biophysical Societies' Association Young Investigator Award, the Krill Prize for Excellence in Scientific Research, and was named one of the top 100 young innovators in science and technology by MIT’s Technology Review (TR100).

Klein, Jacob (I1.4)

Weizmann Institute of Science

Bio: Jacob Klein is the Herman Mark Professor of Soft Matter Physics at the Weizmann Institute in Israel. From 2000-2007 he was the Dr. Lee’s Professor of Chemistry at the University of Oxford and Head of its Physical and Theoretical Chemistry Department (2000-2005). His research interests have ranged from the dynamics and interfacial properties of polymers to the behaviour of confined fluids and biological lubrication. His honours include the High Polymer Physics Prize of the American Physical Society (1995), the 2011 Soft Matter and Biophysical Chemistry Award of the UK Royal Society of Chemistry, the 2012 Tribology Gold Medal, the 2015 David Turnbull Lectureship Award of the Materials Research Society, the 2017 Liquid Matter Prize of the European Physical Society, the 2019 Gold Medal of the Israel Chemical Society, the 2020 Rothschild Prize, the 2021 Irving Langmuir Award in Chemical Physics of the American Physical Society and the Overbeek Gold Medal of the European Colloid and Interface Society. In 2009 and 2017, he received ERC Advanced Grants. In 2013 he was elected to the European Academy and in 2016 he was elected to the Israel Academy of Science and Humanities.

Koenderink, Gijsje (B1.3)

Delft University of Technology

Bio: Gijsje Koenderink is Professor of Cellular Biophysics at Delft University of Technology, Medical Delta professor at the Erasmus Medical School, and co-director of the Kavli Institute for Nanoscience Delft, Netherlands. Her research focuses on the soft matter principles that underlie cell and tissue mechanics and on the implications of mechanical abnormalities for disease (cancer, fibrosis, osteoarthritis and thrombosis). Her team combines concepts and experimental methods from soft matter physics, biophysics, synthetic biology, and cell biology. She received various distinctions, including an NWO VIDI (2008), NWO VICI (2019), ERC Starting Grant (2013), the P-G. de Gennes Prize (2018), and the Dresden Physics Prize (2020). She was elected a member of the Royal Netherlands Academy of Sciences (KNAW) in 2024.

Kremer, Kurt (P3.4)

Max Planck Institute for Polymer Research

Bio: Kurt Kremer joined the Max-Planck Society in September of 1995 as the sixth director of the Max-Planck Institute for Polymer Research, heading the newly established theory group. After studying physics he received his PhD in 1983 from the University of Cologne under the supervision of Prof. Binder, working at the National Research Center KFA Jülich. He performed computer simulations for dynamic and static properties of polymers in bulk and near surfaces. After spending another year at Jülich he moved for a post-doctoral stay to Exxon Research and Engineering Corporation, Annandale, New Jersey, USA, working on polymers and on charge stabilized colloids in collaboration with Drs. Grest, Pincus, and others. Being back in Germany he obtained his Habilitation in 1988 at the University of Mainz. After that he returned to the solid state laboratory of the KFA Jülich as senior scientific staff. He spent several extended visits as visiting professor/scientist at Exxon Research (Dr. Grest), UC Santa Barbara (Materials Dept., Prof. Pincus), and University of Minnesota (Dept. Chem. Engineering and Materials Science, Profs. Davis, Bates, Tirell, and others). After a short stay at the central research department of the Bayer AG, Leverkusen, he moved to the Max Planck Institute for Polymer Research. HE received several awards and recognitions and is member of the German National Academy of Science, Leopoldina.

Krishnan, Madhavi (S1.1)

University of Oxford

Bio: Madhavi Krishnan is a British chemist who is Professor of Physical Chemistry at the University of Oxford. Krishnan invented an electrostatic fluidic trap which permits the spatial control and manipulation of nanoscale materials. These traps can permit the sensitive detection of biomarkers of disease, allowing for early diagnosis.

Kumar, Sanat (P1.1)

Columbia University

Bio: Prof. Kumar received his B. S. degree in 1981 from Indian Institute of Technology in Chennai and then a Sc. D. from MIT in 1987, both in Chemical Engineering. After working as a postdoc at IBM Almaden, he joined the faculty at Penn State University (1988 – 2002, Materials Science/Chemical Engineering) then Rensselaer Polytechnic Institute (2002-6, Chemical Engineering). In 2006, he joined the Chemical Engineering Department of Columbia University, and served as department chair in 2010-16. Prof. Kumar has worked on a variety of problems in a broad range of polymeric and complex fluids systems. His current interests lie in recycling polymers and the creation and mitigation of nanoplastics.

Lavrentovich, Oleg (L2.4)

Kent State University

Bio: Oleg D. Lavrentovich, Trustees research professor at Kent State University, Ohio, received his Ph.D. (1984) and Doctor of Science (1990) degrees in Physics and Mathematics from the Ukrainian Academy of Sciences. In 1992, he joined the Liquid Crystal Institute at Kent State and served as the director of the Institute from 2003 to 2011. His current research interests are focused on electro-optics of liquid crystals, topological defects, hybrid colloid-liquid crystal systems, ferroelectric nematics, liquid crystals as environment to control active matter. He is a Fellow of the American Physical Society, of the International Society for Optical Engineering (SPIE) and an Honored Member of the International Liquid Crystal Society. With Maurice Kleman, he co-authored a textbook Soft Matter Physics: An Introduction (Springer, 2003).

Lodge, Timothy (S3.2)

University of Minnesota Twin Cities

Bio: Tim Lodge graduated from Harvard B.A. cum laude in Applied Mathematics (1975). He completed his PhD in Chemistry at Wisconsin in 1980, and then spent 20 months as a National Research Council Postdoctoral Fellow at NIST. Since 1982, he has been on the Chemistry faculty at Minnesota and, in 1995, he also became a Professor of Chemical Engineering & Materials Science. In 2013, he was named a Regents Professor, the University’s highest academic rank. He has authored or co-authored over 520 papers in the field of polymer science, and advised or co-advised over 150 PhD students and postdoctoral fellows. His research interests center on the structure and dynamics of polymer liquids, including solutions, melts, blends, and block copolymers, with particular emphases on self-assembling systems using rheological, scattering and microscopy techniques.

Löwen, Hartmut (A3.2)

Heinrich Heine University Düsseldorf

Bio: 23.5.1963 born in Hamm/Westfalen, Germany 1982 - 1986 Study of physics, mathematics and chemistry at the University of Dortmund, Diplom in Physics, Vordiplom in Mathematics 1987 PhD in physics on "Phase transitions" in polaron systems, do they exist or not? at the University of Dortmund

1988 - 1990 and 1991 - 1995 Postdoc at the Ludwig-Maximilians-Universität München with Prof. Dr. Herbert Wagner
1990 - 1991 Postdoc at the Ecole Normale Supérieure de Lyon with Prof. Dr. Jean-Pierre Hansen
1993 Habilitation at the Ludwig-Maximilians-Universität München
1995 Call on a chair in Theoretical physics at the Heinrich-Heine-Universität Düsseldorf (HHU)
2001 - 2003 Schlumberger Visiting Professor at the University of Cambridge, UK, Center of Computational Chemistry
2005 Visiting Professor at the Universita di Roma La Sapienza, Italy
2002 - 2013 Coordinator of the German-Dutch Collaborative Research Center SFB TR6 of the Deutsche Forschungsgemeinschaft (DFG)
2007 - 2013 DFG-Vertrauensdozent at HHU
2010 Visiting Professor at the University of Oxford, UK
2011 - 2013 Coordinator of the German-Japanese bilateral cooperation Soft Matter in nonequilibrium funded by the DFG
2014 - 2021 member of the DFG Senate
since 2018 - Co-Editor of Europhysics Letters

Prizes and Awards

1994 Heisenberg-fellowship of the DFG
1994 Gerhard-Hess-Forschungspreis of the DFG
1999 Fellow of the Institute of Physics
2003 Gentner-Kastler-Prize (award from the Deutsche Physikalische Gesellschaft and the Société Francaise de Physique for exceptional contributions to physics) for the contributions to the physics of soft matter, in particular for the work on colloids
2010 recipient of the ERC Advanced Grant INTERCOCOS (with G. Morfill)

2016 selected as an Outstanding Referee for the Journal of Chemical Physics
2017 selected as an Outstanding Referee of the Physical Review journals
2018 selected as an Outstanding Referee for the New Journal of Physics
2023 SigmaPhi Prize for seminal contributions to Statistical Physics

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Mahadevan, Lakshminarayanan (B2.3)

Harvard University

Bio: Lakshminarayanan Mahadevan FRS is an Indian-American scientist. He is currently the Lola England de Valpine Professor of Applied Mathematics, Organismic and Evolutionary Biology and Physics at Harvard University. His work centers around understanding the

organization of matter in space and time (that is, how it is shaped and how it flows, particularly at the scale observable by the unaided senses, in both physical and biological systems). Mahadevan is a 2009 MacArthur Fellow.

Maitra Bhattacharyya, Sarika (G2.4)

National Chemical Laboratory, Pune

Bio: Sarika Bhattacharyya, a Professor at AcSIR and a Senior Principal Scientist at the National Chemical Laboratory, Pune, India, completed her undergraduate studies in Physics at the University of Calcutta, Kolkata. Following this, she pursued her PhD at the Indian Institute of Science (IISc), Bangalore, focusing on dynamics in liquids using mode coupling theory. Her work earned her the Sudborough medal for the best thesis by IISc. Subsequently, she served as a Research Associate at IISc before embarking on her postdoctoral studies at the California Institute of Technology, USA, where she worked on the theoretical modelling of water dynamics around a protein surface. Upon her return to India in 2004, she joined IISc, Bangalore as a Senior Research Associate, later becoming a DST young scientist fellow. Her research involved extending mode coupling theory to investigate dynamics in supercooled liquids. In 2010, she joined the National Chemical Laboratory as a scientist, leading a group focused on soft condensed matter physics, particularly emphasising on the study of Glass transition using theoretical and computational methods. With over 56 publications in prestigious journals and a book chapter to her credit, she was awarded the POWER fellowship in 2021 by the Science and Engineering Research Board, India. This fellowship recognised her work in employing theoretical and computer simulation investigations to develop a novel metric for liquid structure, known as the softness of a confining potential. Her research has significantly contributed to understanding the interplay among the structure and dynamics of supercooled glassy systems.

Mao, Xiaoming (S2.4)

University of Michigan

Bio: Xiaoming Mao completed her PhD at the University of Illinois at Urbana Champaign in 2008, and was a postdoctoral fellow at the University of Pennsylvania during 2008–2012. She joined the faculty of the University of Michigan in 2012. Xiaoming's research group studies a range of questions in fields ranging from soft matter to materials and biophysics, including rigidity and flow in disordered systems, topological mechanical metamaterials, self-assembly of complex and open structures at the nano and colloidal scales, and motility of cells in the extracellular matrix.Xiaoming Mao completed her PhD at the University of Illinois at Urbana Champaign in 2008, and was a postdoctoral fellow at the University of Pennsylvania during 2008–2012. She joined the faculty of the University of Michigan in 2012. Xiaoming's research group studies a range of questions in fields ranging from soft matter to materials and biophysics, including rigidity and flow in disordered systems, topological mechanical metamaterials, self-assembly of complex and open structures at the nano and colloidal scales, and motility of cells in the extracellular matrix.

Milliron, Delia (C2.4)

The University of Texas at Austin

Bio: Delia J. Milliron is the Ernest Cockrell, Sr. Chair in Engineering #1 and Department Chair of Chemical Engineering at the University of Texas at Austin. Dr. Milliron received her AB from Princeton University and her PhD from the University of California, Berkeley. She initially worked for IBM's research division, then joined the research staff at the Molecular Foundry, Lawrence Berkeley National Lab. At UT Austin Dr. Milliron develops nanocrystal-based materials in which abundant interfacial area and confined volume produce drastically different properties than those of homogeneous bulk materials. Such unconventional properties offer new opportunities for optoelectronics and clean energy technologies. Dr. Milliron has been recognized with awards including the DOE Early Career Research Program, the ACS Inorganic Nanoscience Award, Senior Membership in the National Academy of Inventors, the Hackerman Award from the Welch Foundation, the O'Donnell Award in Engineering from the Texas Academy of Medicine, Engineering, Science & Technology, the Nanoscale Science and Engineering Forum Award from the American Institute of Chemical Engineers, and the MRS Medal.

Nakagaki, Toshiyuki (B2.6)

Hokkaido University

Bio: T. Nakagaki is a Professor of Mathematical and Physical Ethology Laboratory, in Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science (RIES), Hokkaido University. He got Bachelor of pharmaceutical sciences, in 1987, Hokkaido University, Japan, and Master of pharmaceutical sciences, in 1989, Hokkaido University. He worked in Pfizer Inc for 5 years, and moved back to University and get PhD of BioPhysics in 1997 from Nagoya University, became an associate professor in Hokkaido University in 2000. He received IgNobel prize twice in 2008 and 2010.

Okumura, Ko (I2.6)

Ochanomizu University

Bio: During his graduate study, he performed research in various topics in theoretical physics, including quantum field theory (particle physics), supersymmetry, nonequilibrium statistical mechanics, electron systems etc, to produce 8 academic papers. After becoming research associate, he made a significant contribution to molecular vibration spectroscopy by bringing in field-theoretical techniques to the field of molecular science. Furthermore, he started working on the toughness of pearl (nacre) with a Novel prized physicist, de Gennes, in Paris. There, he was deeply impressed by the spirit of impressionistic physics, which allows us to extract simple physical essences from complex real-world phenomena. As a result, he shifted his field towards soft matter physics, exploring statistical physics viewpoints such as scaling in critical phenomena. His current interests include wetting and thin film dynamics, granular dynamics, fracture and toughness of sheet materials, and so forth.

Olvera De La Cruz, Monica (N2.3)

Northwestern University

Bio: Monica Olvera de la Cruz obtained her Ph.D. in Physics from Cambridge University, UK, in 1985. She joined Northwestern University in 1986, where she is the Lawyer Taylor Professor of Materials Science & Engineering, Professor of Chemistry, and by courtesy, Professor of Physics and Astronomy and Chemical & Biological Engineering. She is the Director of the Center for Computation and Theory of Soft Materials. From 1995-97 she was a Staff Scientist in the Commissariat a l'Energie Atomique, Saclay, France, where she also held visiting scientist positions in 1993 and 2003. She has developed theoretical models to determine the thermodynamics, statistics, and dynamics of soft materials including multicomponent solutions of heterogeneous synthetic and biological molecules, and molecular electrolytes. She is a member of the American Philosophical Society, the National Academy of Sciences (NAS), the American Academy of Arts and Sciences, and a Fellow of the American Physical Society (APS). She has served in the Advisory Committees of the Department of Energy Basic Energy Science Program (2012-21) and the NSF Mathematical and Physical Science Directorate (2005-09), as well as in various committees of the National Research Council (NRC) including the Board of Physics and Astronomy (2009-15), and served as chair (2010-12), vice-chair (2008-10) and member (1006-10 and 2021-Pre) of the NRC Condensed Matter and Materials Research Committee. She serves in the scientific advisory committee of the Max Planck

Institute for Polymer Research, and ESPCI (École supérieure de physique et de chimie industrielles de la Ville de Paris). She is a member of the PNAS editorial board, and the Board of Trustees of the Gordon Research Conferences (2019-27).

Osuji, Chinedum (L1.1)

University of Pennsylvania

Bio: Dr. Osuji is the Eduardo D. Glandt Presidential Professor, and Chair, in the Department of Chemical and Biomolecular Engineering, and a secondary member of the faculty in Materials Science and Engineering, at University of Pennsylvania. He is an Associate Editor for Macromolecules and a member of the Board of Directors of the Materials Research Society (2021-2014). He leads an experimental research group focused on structure and dynamics of soft materials and complex fluids. Topics of interest include structure-property relationships in ordered soft materials, directed self-assembly of block copolymers and molecular materials, and rheology of dense, disordered systems. Prof. Osuji received his undergraduate degree in Materials Science and Engineering from Cornell followed by his Ph.D, also in Materials Science and Engineering from MIT in 2003. From 2003-2005 he was a Senior Scientist at a startup company, Surface Logix Inc., before moving to Harvard as a Postdoctoral Associate in Applied Physics (2005-2007). He was on the faculty at Yale University in the Department of Chemical and Environmental Engineering from 2007-2018 before moving to the University of Pennsylvania. Prof. Osuji is a Fellow of the American Physical Society, and a recipient of a CAREER award from the National Science Foundation (2008). He received an Office of Naval Research's Young Investigator award and a 3M Nontenured Faculty award in 2012. He is the recipient of the Dillon Medal of the American Physical Society (2015), the Hendrick C. Van Ness Award (2019), and the Nano Research Young Investigator Award (2019). In 2022 he received the Prince Sultan Bin Abdulaziz International Prize for Water (PSIPW).

Palacci, Jérémie (B4.6)

Institute of Science and Technology Austria

Bio: Jeremie Palacci is currently Professor at IST Austria, leading the Materiali Molli group and interested in experiments of Soft Matter, with an active and responsive twist. Jeremie received his PhD from Université Lyon 1 in 2010 and did a postdoc at the Center for Soft Matter Research (CSMR) at NYU until 2014. In 2015, he became assistant professor in the department of Physics at UC San Diego, where he got promoted Associate Professor with tenure in 2020. Jeremie joined ISTA in 2021, where he was promoted to Professor in 2023.

Ramaswamy, Sriram (A5.1)

Indian Institute of Science

Bio: Honorary Professor and J C Bose National Fellow in the Department of Physics, Indian Institute of Science. Also: Distinguished Visiting Professor, IIT Bombay, and ICTS-Simons Visiting Professor, ICTS-TIFR. Interests: nonequilibrium, soft matter and biological physics. One of the founders of the field of active matter. Recognitions: Bhatnagar Prize 2000; Infosys Prize for Physical Sciences, 2011; elected a Fellow of the Royal Society in 2016.

Safran, Sam (B1.4)

Weizmann Institute of Science

Bio: Sam Safran received his Ph.D. in Physics from MIT, followed by a postdoc at Bell Laboratories. From 1980-1990 he served as a Senior Staff member in the Complex Fluids Physics group of Exxon Research and Engineering in New Jersey. Prof. Safran joined the faculty of the Weizmann Institute of Science in 1990 and is currently in the Department of Chemical and Biological Physics. He has served as Dean of the Graduate School and as Vice President of the Weizmann Institute. His current research interests in the theory of soft and biological matter focus on the physics of phase separation of proteins and of chromatin as well as the mechanobiological response of cells. Honors include the de Gennes Award of the European Physical Journal, the Beller Lectureship of the American Physical Society and the International Sackler Prize in Biophysics. He is the author of a graduate text on the physics of surfaces, interfaces and membranes, translated into Japanese and Chinese and was the founding Editor-in-chief of the educational journal, The Biophysicist, published by the Biophysical Society.

Šarić, Andela (B3.5)

Institute of Science and Technology Austria

Bio: Andela received her PhD from Columbia University in New York in 2013, after which she moved onto a postdoctoral fellowship at the University of Cambridge, where she was also a Research Fellow of Emmanuel College. She is currently a Junior Group Leader in the Department of Physics & Astronomy at UCL.

Andela uses computer simulations to study biological assembly. She is interested in how proteins assemble “on-demand” into nanoscale structures that generate the molecular machinery of life. She is also devoted to understanding uncontrolled protein aggregation in the context of neurodegenerative diseases.

Schulman, Rebecca (B5.4)

Johns Hopkins University

Bio: Rebecca Schulman is an assistant professor of chemical and biomolecular engineering with a secondary appointment in computer science at Johns Hopkins University. She arrived at Johns Hopkins after working as a Miller Research Fellow in physics (advisor, Jan Liphardt) at the University of California Berkeley. She received a doctoral degree from the California Institute of Technology in Computation and Neural Systems, where she studied with Erik Winfree, and undergraduate degrees in computer science and mathematics from the Massachusetts Institute of Technology.

Prof. Schulman is an interdisciplinary investigator. Her research focuses on the development of materials and nanostructures with the capacity for growth, transformation and response similar to those of biological materials. She uses fundamental ideas from chemical engineering, biology, chemistry, soft matter physics, computer science and mathematics together to design and construct these materials and combines theory, modeling and experiment in her work. Dr. Schulman's work lies at the interface of structural and dynamic DNA nanotechnology, materials science and synthetic biology.

Sharma, Prerna (C1.2)

Indian Institute of Science

Bio: Prof. Prerna Sharma completed Ph.D. in soft matter physics from TIFR, Mumbai, India in 2011 followed by post-doctoral work at Brandeis University. She has been a faculty member at the Dept. of Physics, Indian Institute of Science, Bangalore since 2014. She is an experimentalist with research interests in bio-colloids and active matter. She is a recipient of prestigious Welcome Trust-DBT India Alliance fellowship and Indian National Young Scientist Award.

Smalyukh, Ivan (L2.3)

University of Colorado Boulder

Bio: Ivan Smalyukh is a full professor at the Department of Physics at CU-Boulder, which he joined in 2007 (promoted from Assistant to Associate Professor in 2014 and from Associate to Full Professor in 2017). He is also a founding fellow of Renewable Sustainable Energy Institute (a joint institute of CU-Boulder and NREL) and Materials Science Engineering Program. He directs the Soft Matter Physics Research Group at CU-Boulder and, recently, also the International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2) with headquarters in Hiroshima University, Japan. Among many of his research interests is the energy efficiency of windows and building envelopes overall, where he develops highly thermally insulating and stimuli-responsive materials, as well as colloids and topological solitons and defects in soft matter. He published over 250 peer-refereed articles, including many in Nature and Science. He is an elected fellow of the American Physical Society, Optica & SPIE. He received many awards, including the Bessel and Glenn Brown Awards, NASA iTech award and Mid-Career Award of International Liquid Crystal Society, the PECASE Award from the Office of Science and Technology of the White House and the GSoft Award from the American Physical Society, Langmuir Lectureship from American Chemical Society, among many other.

Soto, Rodrigo (A4.4)

Universidad de Chile

Bio: Full professor at the Physics Department of Universidad de Chile, has worked in different topics of soft matter and non-equilibrium physics, including granular flows, fluctuation induced forces, bacterial suspensions, tissue mechanics, fluid mechanics, and active matter. In 2016, published the book "Kinetic Theory and Transport Phenomena" (Oxford University Press). Presently, he is director of the Millenium Nucleus Physics of Active Matter research project in Chile.

Stone, Howard A (Plenary Session F)

Princeton University

Bio: Howard Stone received the B.S. degree in Chemical Engineering from UC Davis in 1982 and the PhD in Chemical Engineering from Caltech in 1988. After a postdoctoral fellowship at the University of Cambridge, in 1989 Howard joined the faculty of the School of Engineering and Applied Sciences at Harvard University, where he eventually became the Vicky Joseph Professor of Engineering and Applied Mathematics. In July 2009 Howard moved to Princeton University where he is Donald R. Dixon '69 and Elizabeth W. Dixon Professor in Mechanical and Aerospace Engineering

Howard's research interests are in fluid dynamics and soft matter, especially as they arise in problems at the interface of engineering, biology, chemistry, and physics.

Suo, Zhigang (Plenary Session N)

Harvard University

Bio: Zhigang Suo is Allen E. and Marilyn M. Puckett Professor of Mechanics and Materials at Harvard University. He earned a bachelor's degree from Xi'an Jiaotong University in 1985, and a Ph.D. degree from Harvard University in 1989. Suo joined the faculty of the University of California at

Santa Barbara in 1989, Princeton University in 1997, and Harvard University in 2003. His research centers on the mechanical behavior of materials.

Tirrel, Matthew (P2.1)

University of Chicago

Bio: Matthew Tirrell is the D. Gale Johnson Distinguished Service Professor Emeritus of Molecular Engineering at the University of Chicago, and senior advisor and senior scientist at the Argonne National Laboratory. From 2011 to 2023 he was the Founding Dean of the Pritzker School of Molecular Engineering. He also served as Deputy Laboratory Director for Science at Argonne from 2015-2018 and from 2022-2023. From 2009-2011, he was Professor and Chair of Bioengineering at the University of California, Berkeley. Professor Tirrell was Dean of Engineering at the University of California, Santa Barbara from 1999-2009. From 1977-1999, he was on the faculty of Chemical Engineering and Materials Science at the University of Minnesota, where he served as Head from 1995-1999. Professor Tirrell is a member of the National Academy of Sciences, the National Academy of Engineering, the American Academy of Arts & Sciences and the Indian National Academy of Engineering. Tirrell's work is in self-assembly and interfacial phenomena in organic material systems. Molecular-level forces such as hydrophobic, electrostatic, hydrogen bonding and others are deployed to create complexes and micellar nanoparticles, interfacially active materials, and hydrogels. This work has uncovered new physics of phase transitions and leads to development of new materials, especially new self-assembled hydrogels. In the realm of micellar nanoparticles, we design and synthesize self-assembling molecules that can organize into multifunctional, multivalent objects with targeting, image contrast and therapeutic capabilities. Recent areas of concentration have been on complexes that target vulnerable atherosclerotic plaque, that disrupt intracellular protein-protein interactions and that package nucleic acids for targeted and efficient delivery.

Valentine, Megan (B4.1)

University of California Santa Barbara

Bio: Megan T. Valentine is a Professor of Mechanical Engineering and Co-Director of the California NanoSystems Institute at the University of California, Santa Barbara. Her interdisciplinary research group investigates many aspects of biological and bioinspired materials, with an emphasis on understanding how forces are generated and transmitted in living materials, how these forces control cellular outcomes, and how the extraordinary features of living systems can be captured in manmade materials. This highly interdisciplinary experimental work lies at the intersection of engineering, physics, and biology.

Vlassopoulos, Dimitris (F2.3)

FORTH and University of Crete

Bio: Studied Chemical Engineering, NTU Athens and Princeton University. Industrial experience (Mobil R&D). Researcher at FORTH and Professor at University of Crete, Department of Materials Science & Technology. Research focuses on the rheology of soft materials. The underlying theme is the molecular engineering of soft matter by devising strategies based on the design of model systems with adaptable molar mass, macromolecular architecture or tunable interactions and bridging polymers and colloids. Current topics include nonlinear rheometry, ring polymers, supramolecular assemblies, associating networks, jammed soft colloids, microrheology at extreme pressures. He has received the Weissenberg Award of the European Society of Rheology and the Bingham Medal of the Society of Rheology. Currently he is Editor-in-Chief of the Journal of Rheology.

Wang, Zhen-Gang (P2.4)

California Institute of Technology

Bio: Zhen-Gang Wang is the Dick and Barbara Dickinson Professor and Executive Officer of Chemical Engineering at the California Institute of Technology. He also serves as an associate editor for the ACS Journal Macromolecules. Wang's research is the theoretical and computational study of structure, phase behavior, interfacial properties, and dynamics of polymers and soft matter. His current activities revolve around three main themes: charged systems, including polyelectrolytes, salt-doped polymers, and electric double layers; nucleation or more generally barrier crossing in polymers and soft matter; and nonlinear rheology of polymer gels and entangled polymers.

Yang, Shu (Plenary Session L)

University of Pennsylvania

Bio: Shu Yang is a Joseph Bordogna Professor of Engineering and Applied Science, Chair of the Department of Materials Science & Engineering, and Professor of Chemical & Biomolecular Engineering at University of Pennsylvania (Penn). Her group is interested in synthesis, fabrication, and assembly of soft and composite materials; dynamic tuning of their sizes, shapes and assembled structures, and use of geometry to create highly flexible, super-conformable, shape changing and energy efficient materials. Yang received her B.S. degree from Fudan University, and Ph. D. degree from Cornell University. She worked at Bell Laboratories, Lucent Technologies as a Member of Technical Staff before joining Penn. She was recognized by American Chemical Society Langmuir lectureship, Inventor of the Year at Penn, George H. Heilmeier Faculty Award for Excellence in Research from Penn Engineering. She is a Fellow of AAAS, Materials Research Society (MRS), American Chemical Society (ACS), American Physical Society (APS), Royal Society of Chemistry (RSC), and National Academy of Inventors.

Yeomans, Julia (A2.4)

University of Oxford

Bio: Julia Yeomans is Professor of Physics at the University of Oxford. She obtained her MA and DPhil in Physics from Oxford and then spent two years as a post-doc at Cornell University. She returned to the UK, as a Lecturer at the University of Southampton, before joining the Rudolf Peierls Centre for Theoretical Physics. Julia applies techniques from theoretical and computational physics to problems in soft condensed matter and biophysics. Her current research interests include active matter and mechanobiology. She has been awarded the Lennard Jones prize of the Royal Society of Chemistry and the Sam Edwards prize of the Institute of Physics, and she is a Fellow of the Royal Society.

Zamponi, Francesco (G1.2)

Sapienza University of Rome

Bio: Francesco Zamponi is a Professor of Theoretical Physics at the Sapienza University of Rome. His background is the statistical mechanics of disordered systems, and his scientific interests include various kinds of glassy systems (soft and hard), and interdisciplinary applications to biological sequence data, neural networks, and agent-based models in macroeconomy. He has been a PI of the Simons Collaboration "Cracking the Glass Problem".

Žumer, Slobodan (L1.2)

University of Ljubljana and Jozef Stefan Institute

Bio: Slobodan Žumer started his career in physics with a BSc & PhD at the University of Ljubljana (UL) and a postdoc at Univ Brussels (1975-76). In 1984-86 & and 1992-93, he was a visiting scientist and professor at Liquid Crystal Institute, KSU, Kent, USA. Since 1986, he is a professor of physics (UL) and a scientific councilor (Jozef Stefan Institute). He was the president of the International Liquid Crystal Society (2008-12) and since 2014 its Honored Member and recipient of the Pierre Gilles de Gennes ILCS Prize. He is an APS Fellow, an APS Outstanding Referee, and a member of the European Academy of Sciences and Arts. He received the Zois Lifetime Achievements Award (theoretical soft matter physics) and the Freederiksz Medal of the Russian Liquid Crystal Society. His interests are modeling, simulations, and theory of topological soft matter including liquid crystals, polymers, nematic elastomers, composites, colloids, active systems, and their use in optics and photonics.

Abstracts of Plenary & Keynote Talks

Bechinger, Clemens (A1.4)

Title: Brownian particles in non-equilibrium baths

Abstract: The power of thermodynamics comes at the expense of certain assumptions and idealizations. An important premise is the concept of a thermal bath in contact with the system under investigation. Typically, such baths are treated as an infinite reservoir of heat that remain in equilibrium regardless of whether the considered system is in equilibrium or not. Such description, however, is only valid when the relaxation time of the bath is much faster than typical time scales of the system. Otherwise, a driven system excites the bath out of equilibrium and thus interacts with nonequilibrium fluctuations. Experiments with externally or self-propelled colloidal particles suspended in viscoelastic baths whose relaxation times are on the order of seconds have revealed surprising phenomena that have no counterpart in viscous liquids. In my talk, I will discuss recent experimental findings including particle oscillations within moving optical traps, a fastened hopping dynamics across potential barriers, the strongly enhanced rotational diffusion of self-propelled particles, but also the occurrence of a memory-induced Magnus forces.

Berthier, Ludovic (A2.1)

Title: Collective motion in very dense active matter

Abstract: When crowding effects become important, active matter systems can display unique phenomena that are the direct result from the competition between crowding and non-equilibrium active forces. I will show examples, and explain the associated physics, of such remarkable behaviors and phase transitions emerging in systems controlled by self-propulsion or non-reciprocal active forces interfering with glassy dynamics and jammed states of matter.

Brujic, Jasna (C1.1)

Title: Colloidal protein analogs

Abstract: Our group is inspired by Nature's strategy of folding biopolymers into specific protein and RNA structures to build a toy model of polymeric chains of droplets, i.e. "colloidomers", that are designed via DNA interactions to fold into well-defined architectures. Indeed, simple alternating chains (up to 14 droplets long) with only two droplet flavors (ABABAB…) are sufficient to uniquely encode a dozen "foldamers", constituting 1% of all possible rigid structures in 2D. Subsequently, these 2D foldamers can self-assemble into larger nets that, upon density-matching, are able to further fold into unique 3D geometries, for example viral capsids. These hierarchical protocols circumvent the vast phase space of the nominal folding landscape, in which a random cluster of 12 particles has tens of thousands or rigid folds to choose from. Once the colloidal protein analog is formed, it can then be further programmed by the polymerase-exonuclease-nickase (PEN) toolbox of enzymes that interact with droplet-droplet DNA bonds, to produce highly non-linear dynamical systems. These "mayonnaise robots" promise to offer a bright and functional future on the colloidal length scale.

Cerbino, Roberto (Plenary Session M)

Title: Multiscale dynamics in inert and living soft matter

Abstract: Soft matter encompasses a wide array of materials, characterized by their complex behavior and deformability, and presenting unique challenges and opportunities for scientific investigation. In this talk, I will explore how light, often in conjunction with other tools, can be employed to probe and understand the properties of soft matter across different spatiotemporal scales, ranging from microscopic fluctuations to large-scale emerging collective behavior, both in inert and living matter. After a short introduction covering the main approaches to quantify structure and dynamics in direct and reciprocal space, I will mainly focus on two recent applications. The first case, in the domain of living matter, examines cell tissue undergoing phase transitions similar to those observed in inert soft matter, which are used to accomplish specific biological functions in development and disease. I will describe how the combination of direct and reciprocal space tools allows the quantification of the structural and dynamical properties of the tissue in different phases, as well as the biological and biophysical consequences of phase transitions for cancer. The second case focuses on the design and use of advanced rheo-microscopy setups and analysis tools for the multiscale study of yielding in soft materials. I will show how the use of such setups and tools provides a comprehensive view of the intricate interactions between macroscopic mechanical behavior, mesoscopic deformation patterns, and microscopic dynamics during yielding, opening up new perspectives in modern rheological characterization of materials.

Chaikin, Paul (C2.1)

Title: Random to ordered packings: From candies to monster crystals from space

Abstract: The densest packing of spheres, although known for millennia to be a Face-Centered Cubic (FCC) crystal with volume fraction φFCC ~0.74, has only recently been proven mathematically (2014). An equally ancient problem is "Random Close Packing", RCP, the densest packing of spheres poured into a jar described in Biblical times (Luke 6:38, KJV) as, "pressed down, and shaken together, and running over". RCP has escaped a noncontroversial definition although many experiments and simulations agree to a value φRCP ~0.64. We have found that a simple model, "Random Organization", RO, exhibits a dynamical phase transition between absorbing, 'dead', and active states that appears to have RCP as its critical endpoint. Invented to understand a reversible to irreversible transition in sheared colloids, RO finds RCP with emergent properties such as, randomness, isotropy, isostaticity, hyperuniformity and jamming. To close the book on the crystalline phase, we grew a single crystal on the international space station which found that FCC is the equilibrium structure as compared to the hexagonal close packed and the many other structures with φmax =0.74…

Cohen, Itai (F1.3)

Title: Viscosity Metamaterials

Abstract: Metamaterials are composite structures whose properties arise from a mesoscale organization of their constituents. Provided this organization occurs on scales smaller than the characteristic lengths associated with their response, it is often possible to design such materials to have properties that are otherwise impossible to achieve with conventional materials. Here, I will introduce and demonstrate a new material class-- viscosity metamaterials. To create these metamaterials we rapidly drive large viscosity oscillations in a shear-thickened fluid using acoustic perturbations with kHz to MHz frequencies. Because the time scale for these oscillations can be orders of magnitude smaller than the timescales associated with the global material flow, we can construct metamaterials whose resulting viscosity is a composite of the thickened, high-viscosity and dethickened, low viscosity states. Such viscosity metamaterials can be used to engineer a variety of unique properties including flow rectification, as well as negative, infinite, or zero viscosities – responses that are inconceivable with conventional fluids. The high degree of control over the resulting viscosity, the ease with which they can be accessed, and the variety of exotic properties achievable by viscosity metamaterials make them attractive for uses in technologies for which control over fluid flows and their instabilities are critical, ranging from coatings to cloaking to 3D printing.

Colby, Ralph (F1.4)

Title: Determination of molecular weights using a polydisperse Rouse model for semidilute unentangled polyelectrolyte and neutral polymer solutions

Abstract: The polydisperse Rouse model applies to dynamics of polymer solutions in the semidilute unentangled concentration regime. For neutral polymers, this regime typically spans a factor of ten in concentration, just above the overlap concentration, while for polyelectrolytes with no salt, the semidilute unentangled concentration regime widens as chain length increases, and can easily cover two or three decades of concentration for long chains. We exploit these simple dynamics to provide new methods of determining molecular weight. The polydisperse Rouse model expects the number-average molecular weight M_n to be determined from a combination of self-diffusion coefficient D (from NMR diffusometry) and correlation length ξ (from X-ray scattering), as $M_n = \xi^2 RTc_m / (6\eta_s D)$ where R is the gas constant, T is absolute temperature, c_m is mass concentration and η_s is solvent viscosity. We find this relation works nicely, with no adjustable parameters, for various monodisperse cesium polystyrene sulfonate (CsPSS) samples, their binary blends and NaPSS literature data. The polydisperse Rouse model expects the weight-average degree of polymerization N_w to be determined from a combination of specific viscosity η_{sp} and correlation length ξ as $N_w = \eta_{sp}\xi^3 c$ where c is the number density of repeat units. For neutral monodisperse polystyrene in the good solvents toluene and tricresyl phosphate we find that $\eta_{sp}\xi^3 c$ has

a perfectly linear dependence on N_w but there is a prefactor that requires calibration to determine N_w. For polyelectrolytes we find $\eta_{sp}\xi^3 c \sim N_w^{1.1}$ resulting in $N_w = 3.66\left(\eta_{sp}\xi^3 c\right)^{0.91}$ for the CsPSS samples, their binary blends and NaPSS literature data. Finally, we are now in the process of applying these methods to a wide variety of polydisperse polyelectrolytes and neutral polymer solutions in good solvent.

Colin, Annie (G2.3), coauthors: Guillaume Ovarlez and Anais Gauthier.

Title: Flow of Non Brownian suspensions

Abstract: Despite their apparent simplicity, suspensions of hard spheres in a Newtonian fluid show complex non-Newtonian behaviors (shear thinning-shear thickening) and remain poorly understood. Throughout this presentation, we will show that a precise flow analysis based on local measurements of normal forces and concentration fields, coupled with a characterization of inter-particle forces, provides a quantitative understanding of the mechanisms involved.

We will show that there are two mechanisms responsible for shear thinning behavior: competition between particle pressure and repulsive forces in the case of lubricated contacts, and load-dependent variation in the coefficient of friction in the case of non-lubricated contacts.

Shear-thickening process is understood as a transition under flow of the nature of the contacts – from lubricated to frictional – between initial repellent particles. Most systems are now assumed to fit in with this scenario, which is questionable. We will show that this is not the case for cornstarch suspensions, the most widely studied system. We conclude by proposing formulation and process strategies for handling concentrated suspensions.

Cottin-Bizonne, Cécile (A3.1)

Title: Active colloids climbing up a wall

Abstract: Active matter systems, composed of self-propelled particles, display intriguing dynamic properties, which have attracted considerable attention in recent years. In this study, we focus on active interfaces by considering a sediment of self-propelled Janus colloids. At low densities, they behave like a perfect hot gas, however at intermediate densities, new collective phenomena emerge, such as cluster formation. This leads us to question whether wetting-type effects manifest in these active fluids. In this context, we investigate an analogy to the classical capillary rise effect within the realm of active matter. Specifically, we examine how a non-phase separated sediment of self-propelled Janus colloids behaves upon contact with a vertical wall.

Creton, Costantino (N1.6)

Title: Ionically conducting elastomers: balancing strength, reversible elasticity and conductivity

Abstract: Stretchable elastic materials with high strength and toughness adapted to multiple deformation cycles, and good ionic conductivity are highly desirable for wearable devices and stretchable batteries. Sadly, limited success has been reported to attain these properties simultaneously. Tough and stretchable ionically conducting elastomers have been reported but they rely on viscoelastic or viscoplastic behavior which is not suitable for fatigue resistance [1]. Here, we report a novel family of ionically conductive elastomers (ICEs) without compromise between mechanical properties (high stiffness, reversible elasticity, fracture resistance) and ionic conductivity, by combining the well-known multiple network elastomer (MNE) architecture imparting strength and fatigue resistance [2] with a recently developed method to synthesize ionically conductive and viscoelastic stretchable elastomers [3]. Interestingly, our ICEs with an MNE architecture exhibit an ionic conductivity of the order of 10^(-6) 〖S.cm〗^(-1) and stress at break of ~8 MPa, whereas the simple networks with similar monomer composition show two orders magnitude lower ionic conductivity (10^(-8) 〖S.cm〗^(-1)) and comparably low strength (<1.5 MPa) at 25 °C than their MNE architecture based counterparts. Additions of soluble salts or ionic liquids allow to explore the parameter space and attain conductivities as high as a mS/cm while retaining the desirable fatigue resistant elastomeric mechanical properties. We believe the MNE architecture with a suitable low Tg monomer combines the stiffness and fracture toughness given by sacrificial bond breakage and improves ionic conductivity through increased segmental mobility.

[1] Zhang, W. et al. ACS Macro Letters 8, 17-23 (2019).
[2] Sanoja, G. E. et al. Science Advances 7, eabg9410 (2021)
[3] Yiming, B. et al. Adv Mater 33, 2006111 (2021)

Del Gado, Emanuela (Plenary Session C)

Title: Soft particulate networks and their hidden hierarchical nature

Abstract: Colloidal particles or agglomerated proteins, polymers, and other particulates, often form gels, where they are organized into a porous matrix embedded in a continuous fluid phase, providing rigidity and control of the mechanical response even with a small amount of solid material. Particulate gels are great at optimizing mechanical functionalities without necessarily blocking transport or diffusion, have highly adaptive and tunable rheological response, are highly reconfigurable, and can flow, be stretched, squeezed, or fractured. The microscopic physics that controls such rich mechanical behavior is notoriously challenging and elusive. We have developed microscopic simulations and statistical mechanics-based analyses to investigate viscoelastic response, stress localization, reconfigurability, yielding, stiffening and failure in this class of materials. New physical understanding of the hierarchies of timescales and lengthscales embedded in the structural and mechanical disorder has emerged, with locally floppy and rigid domains interspersed with each other, and highlighting the importance of the network topology for hierarchical stress transmission and redistribution under load. While gaining insight into a range of experimental observations, these findings help build a new scientific basis for material design in areas from 3D printing to recycling, adaptive behavior and memory encoding.

Dufresne, Eric (I1.1)

Title: Controlling interfacial tension without surfactants in biomolecular condensate

Abstract: Biomolecular condensates form spontaneously in living cells. While we know a lot about the molecular mechanisms that cells use to regulate phase separation, we know little about the origin and impacts of condensate's physical properties.

Interfacial tension is an essential physical property that governs coarsening, adhesion, and wetting. In soft matter science, we usually mitigate the effects of interfacial tension with surfactants. However, there is little evidence for surfactant-based regulation of biomolecular condensates in living cells.

In this talk, I will describe how to leverage bulk thermodynamics for control of interfacial tension without surfactants. I will demonstrate how these effects can lead to dialytaxis, the tendency of droplets to swim to their dissolution. I will discuss potential implications of these findings for active matter and cell biology.

Ediger, Mark (P1.4)

Title: Surface-directed assembly of structured glasses

Abstract: In the last 10 years, physical vapor deposition (PVD) has been shown to produce glasses with remarkable properties, including high density and high kinetic stability. By some metrics, these are the most stable glasses on the planet. The properties of PVD glasses can be explained by the surface equilibration mechanism. Even though the substrate is held below the glass transition temperature T_g, the glass surface is highly mobile and this allows incoming molecules to sample many packing arrangements before being buried by further deposition. In this process, the sample can equilibrate well below the conventional T_g.

During PVD, equilibration occurs in an anisotropic environment (the free surface) and this creates the opportunity to form anisotropic glasses. This is important for organic electronics where oriented glasses of organic semiconductors can have higher charge mobility and more efficient emission. PVD can produce glasses with substantial dipolar order (P_1) and orientation order (P_2). Even for molecules with no liquid crystal phases, PVD can prepare glasses with substantial smectic order. And for discotic mesogens, PVD allows the assembly of macroscopically aligned columnar structures more than 150 K below the clearing temperature. The surface equilibration mechanism allows an understanding of all these examples, and deposition conditions allow control over the amount of anisotropy in the deposited glasses.

Eiser, Erika (S1.2), coauthors: Peicheng Xu, Ting Cao, Qihui Fan, Xiaochen Wang and Fangu Ye

Title: Using multivalency and superselectivity of DNA-coated colloids for whole genome detection

Abstract: Fast detection and identification of pathogenic bacteria is an important challenge in the fight against antibiotic resistance. Polymerase Chain Reaction (PCR) is used as reliable standard but takes at least one hour, and, importantly, can only be done in a high-tech environment, not available in less developed regions. Curk et al. [1] proposed an approach based on whole bacterial genome detection, which making PCR redundant. The theoretical basis of this approach exploits the fact that multivalent probes can recognize the DNA of specific pathogens by binding weakly to many identical nucleotide sequences along its whole genome, rather than strongly to a single, unique long sequence. Curk et al. [1] developed an algorithm to find which 20-nucleotide sequences appear most frequently along a genome. In my talk, I report experiments aimed at testing this theory: we coated colloids with short DNA-sequences that are complementary to the most frequently appearing nucleotide sequences in the genome of the target bacteria. We demonstrate that these multivalent probes can be tuned to cooperatively bind to specific bacterial DNA of the target pathogen and we show that our method can even distinguish between closely related pathogens [2].

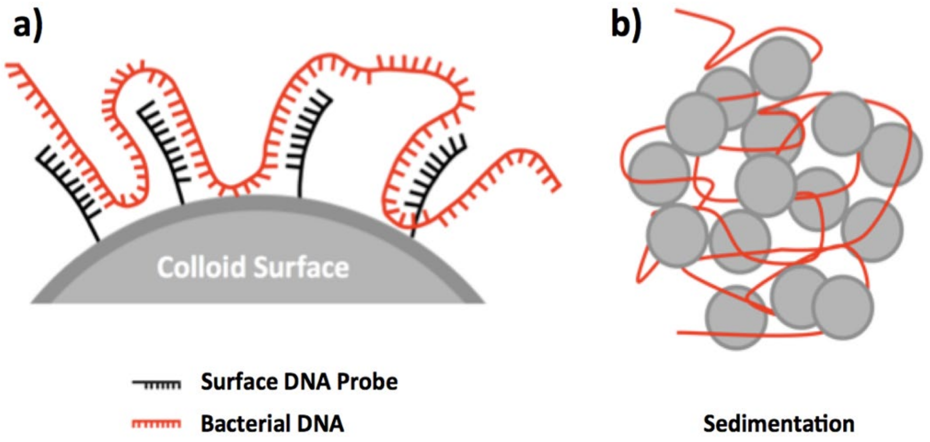

Figure 1. (a) Cartoon of a probe colloid coated with single-stranded, multivalent DNA probes that bind to complementary parts of a specific bacterial genomic DNA. (b) Cooperative binding of many DNA-coated particles to the genomic bacterial DNA of interest leads to observable aggregation. We can detect down to 5 genomes/ml.

[1] Curk et al. PNAS **117** (2020) 8719 - 8726.
[2] Xu et al., PNAS **120** (2023) e2305995120.

Fakhraai, Zahra (G1.1)

Title: Controlling Glass Equilibration Using Soft Substrates

Abstract: Glasses produced by physical vapor deposition (PVD) onto rigid temperature-controlled substrates have been shown to use the surface equilibration mechanism to access low-energy states in the energy landscape. PVD can thus produce glasses with high density (by up to 1.7%), improved kinetic stability, and structural anisotropy that can be controlled by variations of the deposition temperature and deposition rate. The most optimized stable glasses have been shown to have properties analogous to liquid-quenched glasses aged for ~1-100 million years, meaning that the surface equilibration rate is 6-8 decades faster than the bulk aging rate.

We demonstrate that when vapor deposition is performed on a soft substrate, such as PDMS rubber, the surface equilibrium rate is even dramatically enhanced, by an additional 6-8 decades, at distances 170 nm away from the soft substrate [1]. As a result, vapor-deposited films can be produced with densities up to 2.5% higher than those of liquid-quenched glasses within 2.5 h of deposition. Gaining similar properties by vapor deposition on rigid substrates, such as silicon, would require 10 million times slower deposition, taking well over ~3,000 years. By changing the modulus of the rubbery substrate through thermal curing, we can further control the vapor-deposited glass density and its optical anisotropy without changing the deposition conditions. As such, substrate modulus emerges as a new "external variable" to control glass mobility and therefore vapor-deposited glass properties.

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Gang, Oleg (S3.1)

Title: Programming self-assembly and transformations of nanoscale systems

Abstract: Integrating functional nanocomponents into complexly engineered architectures is required to enable novel functions for diverse emerging applications. The quest cannot be satisfied by current top-down fabrications. Conversely, self-assembly has uncovered the exciting richness of spontaneously forming structures, but bottom-up methods based on it typically do not provide designability, thus, translations to functions are limited. The talk will discuss our advances in developing DNA-programmable self-assembly for creating large-scale and finite-size nano-architectures from diverse inorganic and biomolecular nanocomponents with a prescribed organization. The exploration of assembly design principles and the experimental development of periodic and hierarchical organizations from inorganic nanoparticles and proteins across the scales using equilibrium and non-equilibrium assembly approaches will be presented. The established assembly approaches allow for the fabrication of functional nanomaterials with nano-optical, electrical, mechanical, and biochemical functions; examples of these efforts will be illustrated. Finally, the progress on establishing nanomaterials with prescribed transformation pathways will be discussed.

Giomi, Luca (A5.2)

Title: Phase transitions in confluent epithelia

Abstract: In spite of the absence of gaps and interstitial structures, confluent layers of epithelial cells are able to migrate collectively and remove excess cells by extrusion. While in common with foams and other passive confluent fluids, both these phenomena crucially rely on the active remodelling of the cellular network, via topological transformations known as T1 and T2 processes. Using a combination of active hydrodynamics and Renormalization Group methods, I will show that both collective migration and cell extrusion can be thought as continuum phase transitions, with the former being in the same universality class of the Kosterlitz-Thouless transition and the latter reminiscent of sublimation in solids.

Golestanian, Ramin (Plenary Session A)

Title: Non-reciprocal active matter across the scales

Abstract: Broken action-reaction symmetry has been recently explored in active matter in the context of nonequilibrium phoretic interactions between catalytically active colloids and enzymes [1], and hydrodynamic interactions [2,3], among others. It has been shown to lead formation of self-propelled active molecules that break time-reversal symmetry [4], oscillating active complexes that break time-translation symmetry [5], chiral bound-states [6], and active phase separation with specified stoichiometry [7,8,9]. Non-reciprocal interactions have been found to lead to rich physical phenomena involving various forms of spontaneous symmetry-breaking in other related nonequilibrium contexts [10]. Recent applications of non-reciprocal active matter have revealed exotic behaviour such as the appearance of effervescent travelling patterns [11] and shape-shifting multifarious self-organization [12], spontaneous escape of kinetic barriers [13], dynamical pattern formation in quorum-sensing active matter [14], as well as implications of the physics of non-reciprocal interactions on the origin of life [15,16,17].

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[3] D. J. Hickey, R. Golestanian, and A. Vilfan, PNAS 120, e2307279120 (2023)
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[5] R. Soto and R. Golestanian, PRE 91, 052304 (2015)
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[11] S. Saha and R. Golestanian, arXiv:2208.14985 (2022)
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[13] S. Osat, J. Metson, M. Kardar, and R. Golestanian, arXiv:2309.00562 (2023)
[14] Y. Duan, J. Agudo-Canalejo, R. Golestanian, and B. Mahault, PRL 131, 148301 (2023)
[15] V. Ouazan-Reboul, J. Agudo-Canalejo, and R. Golestanian, Nat. Commun. 14, 4496 (2023)

[16] V. Ouazan-Reboul, R. Golestanian, and J. Agudo-Canalejo, PRL 131, 128301 (2023)
[17] V. Ouazan-Reboul, R. Golestanian, and J. Agudo-Canalejo, NJP 25, 103013 (2023)

Granick, Steve (A1.1)

Title: A skeptic's guide to the enhanced diffusion problem of active matter

Abstract: Soft matter scientists agree enthusiastically about the importance of active matter, but about the details there is too little agreement. This talk will concern enzyme catalysis and other chemical reactions, for which some experimentalists report enhanced diffusion while others find no evidence for it. This talk reconciles many of the disagreements. The picture emerges that chemical reactions can function as active matter, executing mechanically asymmetric work.

Grason, Greg (S2.1)

Title: Misfits Unite: Understanding and engineering self-limitation in geometrically frustrated assembly

Abstract: Geometric frustration is most often associated with the disruption of long-range order and proliferation of defects in self-organizing systems. Soft and self-assembled materials, on the other hand, are composed of intrinsically flexible building blocks held together deformable and non-covalent forces. As such, soft assemblies systems are able to tolerate some measure of local misfit due to frustration, allowing imperfect order to extend over at least some finite range. This talk will focus on frameworks for exploiting geometrically-frustrated assemblies (GFAs) to realize size-controlled, self-limiting assembly. While concepts of GFA have been used to describe a broad range of soft matter structures (e.g. self-twisting protein bundles, chiral membranes, spherical colloidal shells), current challenges focus on exploit GFA principles to design and realize new classes of intentionally ill-fitting subunits that target assembly into finite-size structures, with tunable and well-defined dimensions much bigger than those building blocks. I will discuss emerging principles and ongoing efforts to engineer the intra-assembly stress propagation and thermodynamic self-limitation in assemblies through the shape, interaction and flexibility of those building blocks. First, I describe attempts to understand the statistical mechanics of GFA based on a minimal based model. Finite temperature simulation and classical aggregation models applied this generic model illuminate how competing thermodynamic states of GFA -- dispersion, self-limiting aggregation and bulk condensation -- are regulated by the relative importance of elastic costs of frustration, short-range cohesion and entropy. Second, I describe efforts to intentionally design self-limiting assembly from particle-scale properties of discretely ill-fitting subunits, motivated by a recent advance in shape-controlled DNA origami colloids. I will show how "programming" self-limiting size requires more than just control over the shape misfit between subunits, but also engineering the nature of intra-subunit stress gradients in frustrated assemblies.

Grest, Gary (P3.1), coauthors: Daniel L. Vigil, Ting Ge, Michael Rubinstein, and Thomas C. O’Connor

Title: Dynamics of Ring Polymers

Abstract: The topological constraints of no free ends force non-concatenated ring polymers in a melt to form compact loopy globular conformations. As a result, ring polymers have significantly different rheological properties from linear polymers due to differences in knotting and entanglements. When ring and linear polymers are blended, emergent rheological properties are observed as the blend can be more viscous than either of the individual components. This emergent behavior is due to the fact that ring-linear blends can form topological constraints via linear polymers threading of the ring polymers, which are long-lived. In this talk, I will present results from equilibrium and non-equilibrium molecular dynamics simulations of the dynamics, entanglement topology, and nonlinear extensional rheology of ring melts and ring/linear blends. For majority-linear blends, the relaxation rate of the topological constraints depends primarily on reptation of the linear polymer as the rings can relax only after the linear polymers reptate away, resulting in the diffusive time τ_d for rings of length N_R blended with linear chains of length N_L to scale as τ_d ~ NR2 NL3.4, compared with NR2.8 for a pure ring melt. The relaxation of the linear chains is essentially unchanged as the fraction of rings is varied. Under uniaxial extension, rings form topological links that connect multiple rings into supramolecular chains in both pure ring and in ring/linear blends. Once linked, these composite objects experience larger drag forces than individual rings, driving their strong elongation.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE’s National Nuclear Security Administration under Contract No. DE-NA-0003525.

Grosberg, Alexander (A4.1)

Title: Active hydrodynamics in the nucleus of a living cell

Abstract: The nucleus of a living cell is an arena of incessant activity (driven, as everything in biology, by ATP hydrolysis). In the talk, I plan to review experimental findings and possible theoretical explanations of the observed large scale non-thermal motions and fluctuations in the nucleus.

Hosoi, Anette (F2.6)

Title: Bio-inspired filtration: Fluid mechanics of the Manta Ray

Abstract: HVAC systems account for about 20% of U.S. energy consumption of which at least 7% is consumed by fans. Their energy efficiency strongly depends on their filters: reducing resistance can result in significant energy savings. We explore novel strategies for filtration inspired by the manta ray, which has evolved a system for filtering zooplankton that appears to be unlike any industrial filtration mechanism. Instead of a sieve strategy, the manta deploys microstructures, which are hypothesized to instigate eddies that push particles away from the filtration pores, resisting clogging, and enabling the filtration of particles much smaller than the pore size. We examine a series of problems that mimic various features of the filtration strategies employed by manta rays and compare our predictions with biological measurements and data from an experimental "table top" manta.

Ito, Kohzo (N1.3)

Title: Slide-ring materials for circular economy

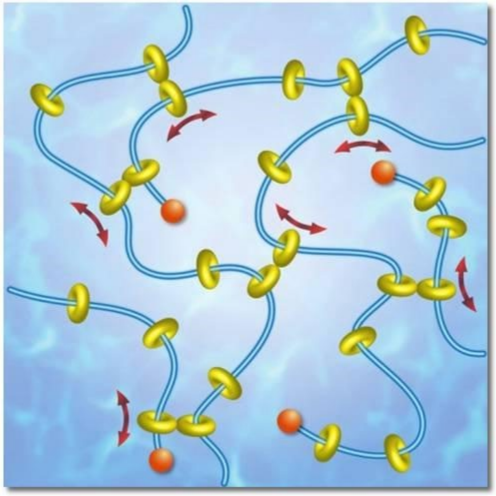

Figure 1. Schematic diagram of Slide-Ring materials

Abstract: We have developed a novel type of polymeric materials such as slide-ring (SR) materials and pseudo-polyrotaxane (PPR) nanosheet with cyclodextrins (CyDs) for sustainable engineering. In the SR materials, polymer chains are topologically interlocked by figure-of-eight cross-links.1) Hence, these cross-links can pass along the polymer chains freely to equalize the tension of the threading polymer chains similarly to pulleys. Recently, we have just reported the stretch induced crystallization of the SR gel, which leads to extremely high toughness and recoverability.2) The concept of the slide-ring gel is not limited to cross-linked gels but also includes elastomer, cross-linked polymeric materials without solvent. Accordingly, it can be applied to wide area such as paints, rubbers, soft actuator, resins and so on.3) The slide-ring materials were used as a key technology to create tough and sustainable polymers.4,5)

On the other hand, we have recently developed mass-producing, low-cost, and free-standing nanosheets using topological self-assembly of *β*-cyclodextrins (CDs) and poly(ethylene oxide)$_{75}$-*b*-poly(propylene oxide)$_{29}$-*b*-poly(ethylene oxide)$_{75}$ ($EO_{75}PO_{29}EO_{75}$) triblock copolymer, namely, pseudo-polyrotaxane (PPR) nanosheet by hierarchically ordered supramolecular self-assembly.6) The PPR nanosheets were obtained by just mixing triblock copolymer andβ-CD in water at room temperature. β-CDs threaded on poly(propylene glycol) segment of the triblock copolymer to form a monoclinic single crystal with a dimension of 10-20 nm thickness and a few micro meters size. The PPR nanosheet can be applied to a novel drag delivery system with cell adhesiveness and to a new common method to construct polymer brush layer on various kind of materials surfaces.7)

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Keren, Kinneret (Plenary Session B)

Title: Topological defects and their role in Hydra morphogenesis

Morphogenesis, the emergence of form and function in a developing organism, is one of the most remarkable examples of pattern formation in nature. We focus on the mechanical aspects of morphogenesis using Hydra, a small multicellular freshwater animal, as a model system. Hydra has a simple body plan and is famous for its ability to regenerate an entire animal from small tissue pieces, providing a flexible platform to explore how mechanical forces and feedback contribute to the establishment of the body plan during morphogenesis. We use live imaging to follow the nematic organization of the supracellular muscle fibers and tissue deformations in regenerating Hydra. We focus on topological defects in the nematic fiber organization, which emerge early in the regeneration process and identify the sites where morphological features develop in the regenerating animal. High-resolution imaging reveals that transient contractions of the supracellular fibers lead to mechanical strain focusing at defect sites. We suggest that these localized tissue deformations provide mechanical cues that are part of a mechanochemical feedback loop promoting the emergence of morphological features at defect sites.

Klein, Jacob (I1.4), coauthors: Yu Zhang and Di Jin

Title: Lipid bilayers under transmembrane fields: cell-inspired, massive electromodulation of interfacial energy dissipation

Abstract: Transient electric fields across cell bilayer membranes can lead to electroporation, as well as to cell fusion, effects crucial to cell viability, and their biological implications have been extensively studied. Little however is known about the effect of such fields on membranes in a materials context. Here we find that transmembrane electric fields similar to those in cells can lead to a massive, reversible modulation of the interfacial shear interactions between surfaces sliding across the lipid bilayer membranes – a 200-fold variation, up to 2 orders-of-magnitude greater than achieved to date. Atomistic simulations reveal that this arises from (fully reversible) electroporation of the interfacially-confined bilayers, and formation of bilayer bridges analogous to stalks preceding intermembrane fusion. The transverse fields on the lipid bilayers (which resemble such fields at cell membranes) force the slip plane on sliding to revert in part from the low-dissipation, hydrated lipid-headgroups plane to the intra-bilayer, high-dissipation acyl tail interface, while at the same time increasing the interfacial dissipation through reduced hydration at the slip-plane. Our results

demonstrate that lipid bilayers under transmembrane electric fields can have striking materials-modification properties.

Koenderink, Gijsje (B1.3)

Title: Living soft matter: bridging cell-free and live-cell perspectives

Abstract: Cells are the smallest living building blocks that we are made of, being themselves made of classical nonliving soft matter constituents such as polymers and membranes. Cells have unique material properties, combining high mechanical stability with the ability to actively reshape, self-repair and replicate. These unique features are governed by a fibrous protein scaffold known as the cytoskeleton. Fibrous networks inherently offer high mechanical stability at low volume fraction. However, it is still poorly understood how cytoskeletal networks can combine mechanical stability with the ability to dynamically adapt their structure and mechanics. We approach this question from two opposite directions: “top-down” research on isolated living cells and “bottom-up” research on simpler synthetic cells reconstituted from purified components. In this talk, I will show how these top-down and bottom-up experiments can be combined to identify the molecular basis of the cell’s material properties. Along the way I will mention connections to applications in bottom-up synthetic biology and in tissue (re)generation.

Kremer, Kurt (P3.4)

Title: Playing with entanglements to structure polymer materials

Abstract: Entanglements are known to dominate the rheological properties of long chain polymer melts and dense solutions. Their properties and consequences lead to the generally accepted and well established reptation/tube model, which is at the basis of our understanding of many properties and processes. However, beyond analysing their effects and understanding the very nature of entanglements, one also can take the approach to employ them to manipulate and structure materials, either by avoiding or explicitly using them. The talk will give a few such examples ranging from melts of non-entangled to very long, highly entangled polymer systems. By appropriately mapping chemical chain lengths onto idealized bead spring models one can (semi-) quantitatively compare simulation and experiment and predict new materials. Based on predictions from simulations we recently prepared stable nanoporous polymer films just by mechanical deformation. Furthermore, we applied a new data driven approach to determine the glass transition temperature of polymer melts in bulk and in (ultra) thin films.

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[2] H. P. Hsu, M. K. Singh, Y. Cang, H. Thérien-Aubin, M. Mezger, R. Berger, I. Leiberwirth, G. Fytas,and K Kremer, Adv. Sci. 10, 2207472 (2023).

[3] A. Banerjee, H. P. Hsu, K. Kremer, and O. Kukharenko, ACS Macro Lett. 12, 679 (2023).

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Krishnan, Madhavi (S1.1)

Title: A charge dependent long-ranged force drives tailored assembly of matter in solution

Abstract: The interaction between charged objects in solution is generally expected to recapitulate two central principles of electromagnetics: (1) like-charged objects repel, and (2) they do so regardless of the sign of their electrical charge. Here we demonstrate experimentally that the solvent plays a hitherto unforeseen but crucial role in interparticle interactions, and importantly, that interactions in the fluid phase can break charge-reversal symmetry. We show that in aqueous solution, negatively charged particles can attract at long range while positively charged particles repel. In solvents that exhibit an inversion of the net molecular dipole at an interface, such as alcohols, we find that the converse can be true: positively charged particles may attract whereas negatives repel. The observations hold across a wide variety of surface chemistries: from inorganic silica and polymeric particles to polyelectrolyte- and polypeptide-coated surfaces in aqueous solution. A theory of interparticle interactions that invokes solvent structuring at an interface captures the observations. Our study establishes a nanoscopic interfacial mechanism by which solvent molecules may give rise to a strong and long-ranged force in solution, with immediate ramifications for a range of particulate and molecular processes across length scales such as self-assembly, gelation and crystallization, biomolecular condensation, coacervation, and phase segregation.

Kumar, Sanat (P1.1)

Title: Mechanism of Micro and Nanoplastics Formation from Semicrystalline Polymers

Abstract: It is well-established that micro and nanoplastics (MNPLs) are released from polymers through environmentally triggered bond breaking. However, the mechanism by which this Å-level process leads to nm-m sized fragments is poorly enunciated. Through experimental studies on three distinct chemistries, we demonstrate that only polymers with a semicrystalline morphology produce MNPLs under quiescent conditions. In this morphology, comprised of alternate crystalline and amorphous domains, chain scission occurs faster in amorphous regions. Through theoretical arguments, we show that tie molecules and bridging entanglements (“connectors”), which provide structural integrity to the semicrystalline structure by connecting two adjacent crystals, are preferentially broken. We propose that the cleavage of a threshold amount of connectors (i.e., scission of as little as 1% of chain bonds), leads to the spontaneous release of MNPLs. The resulting fragments comprise highly polydisperse stacks of lamellae, with an individual lamella – tens of nanometers thick - being the building block. Degradation of the crystals occurs over much longer time scales, explaining the environmental persistence of MNPLs, even under non-quiescent conditions. Since ~70 % of

polymers are semicrystalline, engineering connectors may represent an effective strategy to reduce MNPL release rates.

Lavrentovich, Oleg (L2.4), coauthors: Kumari, Priyanka, Basnet, Bijaya, Thapa, Kamal, Paladugu, Sathyanarayana, Shiyanovskii, Sergij, Kurochkin, Olexandr, Buluy, Olexandr, Aryasova, Natalie Lavrentovich, Maxim O., and Nazarenko, Vassili

Title: Polarization patterns of ferroelectric nematics

Abstract: A ferroelectric nematic liquid crystal is formed by achiral molecules with large dipole moments. Its orientational order is universally described as unidirectionally polar, which raises the question of how the structure avoids a strong depolarization field and splay deformations which bring about a bound charge. We demonstrate a rich plethora of polarization patterns (1-3) that form in confined ferroelectric nematics not constrained by crystallographic axes. Domain walls adopt the shapes of conic sections, separating domains with uniform and circular polarization (2). When a flat ferroelectric nematic slab is anchored only at one bounding plate, its ground state is optically active, with left- and right-hand twists of polarization (3), Fig.1. Although the helicoidal deformations and defect walls separating domains of opposite handedness increase the elastic energy, the twists reduce the electrostatic energy and weaken when the material is doped with ions. An externally applied electric field unwinds the helices and produces complex three-dimensional structures. The study shows that the polar orientational order of molecules could trigger chirality in the soft matter with no chemically induced chiral centers.

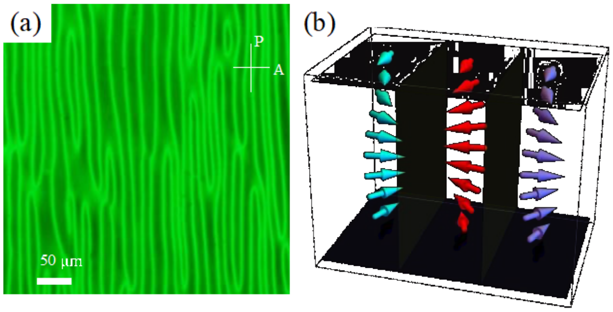

Figure 1 Ground state with left and right-twisted domains of polarization in a flat sample of a ferroelectric nematic.

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2. P. Kumar et al. Nature Communications 14, 748 (2023).
3. P. Kumari et al. Science 383, 1364-1368 (2024).

Lodge, Timothy (S3.2)

Title: Equilibration of Block Copolymer Micelles: How Difficult Can It Be?

Abstract: Block copolymers provide a remarkably versatile platform for achieving desired nanostructures by self-assembly, with dimensions ranging from a few nanometers up to microns. In particular, block copolymer micelles in selective solvents are of interest across a range of technologies, including drug delivery, imaging, catalysis, lubrication, and extraction. While block copolymers generally adopt the morphologies familiar in small molecule surfactants and lipids (*i.e.*, spherical micelles, worm-like micelles, and vesicles), one key difference is that polymeric micelles are typically not at equilibrium. The primary reason is the large number of repeat units in the insoluble block, N_{core}, which makes the thermodynamic penalty for extracting a single chain ("unimer exchange") substantial. As a consequence, the critical micelle concentration (CMC) is rarely accessed experimentally; however, in the proximity of a critical micelle temperature (CMT), equilibration is possible. We use time-resolved small angle neutron scattering (TR-SANS) to obtain a detailed picture of the mechanisms and time scales for chain exchange, for systems at or near equilibrium. The dependence of the rate of exchange on the key variables – concentration, temperature, N_{core}, N_{corona}, and chain architecture (diblock versus triblock) – will be discussed. Interestingly, almost none of the observed features are captured by available theory. Dissipative particle dynamics simulations provide a hint of the underlying physics. Then, when micelles are significantly larger or smaller than the equilibrium size, fragmentation and fusion mechanisms, respectively, can become operative. We will describe measurements using dynamic light scattering, small-angle X-ray scattering, and liquid-phase TEM to follow the fragmentation process in detail.

Löwen, Hartmut (A3.2)

Title: Active matter: self-propelled colloids and beyond

Abstract: While ordinary materials are typically composed of inert "passive" particles, active matter comprises objects or agents which possess an intrinsic propulsion. Examples are living systems like schools of fish, swarms of birds, pedestrians and swimming microbes but also artificial particles equipped with an internal motor such as robots and colloidal Janus particles. In this talk the statistical mechanics of synthetic artificial self-propelled colloidal particles [1] and possible phase transitions are discussed and the importance of inertia is highlighted [2]. Moreover breathing particles such as microgel particles in an time-oscillatory temperature field will be discussed. Such breathing stimuli can be exploited to anneal crystalline defects [3]. Finally two possible paths to next generation's active materials will be pointed out: i) functionalized microswimmers equipped with artificial intelligence [5], ii) ultracold atoms in optical fields opening the door to the new field of quantum active matter.

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[5] J. Grauer, F. J. Schwarzendahl, H. Löwen, B. Liebchen, Machine Learning Science and Technology 5, 015014 (2024).
[6] Y. J. Zheng, H. Löwen, arXiv:2305.16131

Mahadevan, Lakshminarayanan (B2.3)

Title: Endless forms most beautiful: geometry, physics and biology

Abstract: I will describe how simple geometrical ideas and physical principles associated with active growth and flow are beginning to help illuminate multicellular tissue morphogenesis in such instances as laying out the body plan, e.g. gastrulation, body elongation, and creating functional organs e.g. guts, brains, and beaks. Combining experiments and theory allows us to link molecular genetics to morphogenesis in a developing organism and construct evolutionary phase diagrams across organisms, sharpening the Darwinian question of how “endless forms most beautiful and most wonderful have been, and are being, evolved."

Maitra Bhattacharyya, Sarika (G2.4)

Title: Exploring the structural contribution to dynamics in supercooled liquids

Abstract: The behaviour of supercooled liquid differs significantly from that of the normal liquid. While the dynamics undergo significant changes, the structure only exhibits marginal change. The origin of dynamic heterogeneity (DH) in supercooled liquids is a subject of intense research. It is often theorised that, similar to crystals, structural defects exist in supercooled liquids, leading to DH. However, pinpointing structural defects in a supercooled liquid is a challenging task. In this presentation, I will introduce a newly proposed order parameter, the softness of a mean-field caging potential, described in terms of pair structure, and demonstrate that i) the overall dynamics of the system can be described using the average softness parameter and ii) the local dynamics is causally related to the local structure in the supercooled regime, where a separation between short and long time dynamics occurs, enabling a static description of the cage. Using this structural metric, I will then illustrate how the correlation between structure and dynamics can be employed to investigate various phenomena, such as differences in dynamics in systems interacting via attractive and repulsive potentials. Lastly, I will discuss a recent

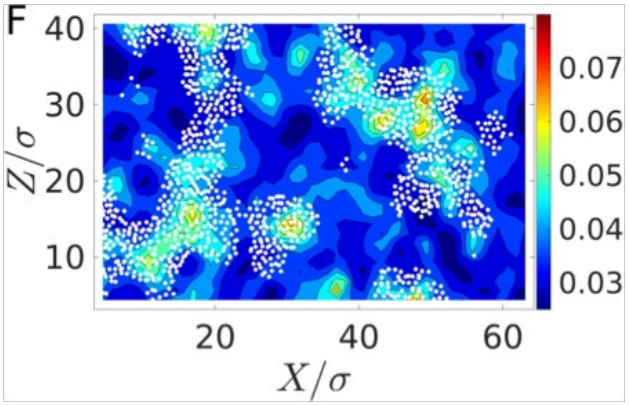

Figure 1. Contour plot of averaged softness of the particle, overlaid with the location of particles (with circles) whose mobility is high in experimental colloidal system under shear [5].

study that showcases the utility of this structural metric in experimental colloidal systems for characterising local structural heterogeneity and its connection to dynamics in both quiescent and sheared systems.

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Mao, Xiaoming (S2.4)

Title: Frustrated assemblies as incompatible graphs

Abstract: Geometric frustration shows up in many self assembly problems in terms of incompatibilities of shapes and interaction potentials, and leads to a rich set of complex hierarchical structures in nature and engineered systems from biomineralization to nanoparticle assemblies. In this talk, we introduce a graph theory formulation for the statistical mechanics of frustrated assembly, where mechanical stress due to geometric frustration maps to cycles and incompatible flow fields on the graphs, enabling not only convenient mathematical descriptions of the complex kinetic processes, but also connections to statistical mechanical models on graphs. We apply these tools to lattice models and find unique nonequilibrium statistical

mechanics features including self-organized divergent length scales and generation of complexity.

Milliron, Delia (C2.4)

Title: Interactions and assemblies of colloidal nanocrystals

Abstract: Controlling the arrangement of inorganic nanocrystals in assemblies allows realization of materials whose properties depend both on the distinctive characteristics of their colloidal nanoscale building blocks and on their organization. We assemble gel networks from colloidal nanocrystals that absorb infrared light due to their composition-tunable plasmonic resonance. Nanocrystal gels are interesting because their porous, percolating structures can in principle lead to structure-tunable material properties with dynamic reconfigurability. However, determining structure and measuring interactions is less straightforward for soft, disordered materials like colloidal gels, motivating the development of experimental systems that minimize complexities, except those deliberately introduced to analyze their effects, and of systems designed to make quantitative measurements of structure and thermodynamics possible. Inorganic nanocrystals offer a versatile platform for fundamental studies of colloidal assembly, being high uniform in size and morphology and having customizable surface functionality, where capping ligands can be exchanged to direct their interactions. For instance, oleate-capped indium oxide nanocrystals were analyzed by small angle X-ray scattering and shown to interact as hard spheres, making them an ideal colloidal system for controlled introduction of attractions—by depletion or chemical linking—to induce assembly. Further, by using colorimetric metal coordination links to assemble nanocrystals into networks, we enable thermodynamic analysis of the linking chemistry to establish the structural basis for thermoreversible gelation in plasmonic doped indium oxide nanocrystal networks. Plasmon coupling upon assembly causes a large shift in the infrared optical absorption, so these gels are thermally switchable optical materials. Their optical spectra also contain hints about the gel structure that we unravel by using large-scale simulations based on many-bodied coupling between their induced dipoles. The development of such near-ideal experimental systems presents opportunities to validate theoretical frameworks and to experimentally realize materials that are computationally designed or optimized for a specific optical response.

Nakagaki, Toshiyuki (B2.6)

Title: Adaptable network of veins to environmental complexity in a huge amoeboid organism of *Physarum plasmodium*

Abstract: A giant amoeboid organism of plasmodial slime mold *Physarum polycephalum* grows to several centimeters and drastically changes its body shape in response to the complexities of the field environment. For example, this creature create functional transport networks that connect food grains scattered here and there. The current-reinforcement rule is known to be one of the mechanisms that bring about the self-organization of such environmentally adaptive networks. Here, this rule is a local rule of growth of flow channel in which flow channels develop when flow is fast, and otherwise decline. Since deformation of amoeboid body is based on the control of sol-gel conversion of polymeric solutions, called protoplasm, the current-reinforcement rule is to be attributed to the interaction between sol-gel conversion and flow. In this presentation, we will show how the highly functional morphogenesis of this interesting amoeba-like organism occurs in a few hours. First, we will present experimental results on the ability of the amoeba to form a transport network connecting scattered food-grains, and discuss mathematical modeling of this ability. Then, the mechanism of current reinforcement will be discussed from a hydrodynamic point of view.

Okumura, Ko (I2.6)

Title: A hydrodynamic analog of critical phenomena: an uncountably infinite number of universality classes

Abstract: When a solid object starts falling into a viscous fluid from air-liquid interface, air is entrained into the liquid and eventually detaches from the solid. Such detachment could occur with or without topological change. Recently, it was found that the former case (i.e., breakup, a form of singular transitions) is observed in a confined geometry but the topology change is suppressed in a more confined geometry, by falling a metal disk in a vertically stood Hele-Shaw cell filled with a viscous liquid with the disk axis perpendicular to the direction of gravity. In this talk, we discuss the results when we tune a confinement parameter, the thickness difference between the cell and the disk, with fixing another confinement parameter, the disk thickness. As a result, we find that the present hydrodynamic case possesses a strikingly close analogy with critical phenomena. Critical phenomena have widely been observed in nature, and the concept of universality class, which has emerged from our understanding of critical phenomena, has guided the recent development of physics. Accordingly, identifying a rich variety of universality class is a major issue in modern physics. Here, we remarkably find the present hydrodynamic analog of critical phenomena reveals the existence of an uncountably infinite number of universality classes, by showing that critical exponents, which define a universality class, depend on continuous numbers characterizing the confinement.

Olvera De La Cruz, Monica (N2.3)

Title: Controlling the structure and function of confined electrolytes

Abstract: Controlling the Structure and Function of Confined Electrolytes M. Olvera de la Cruz Charge containing molecules are ubiquitous in energy and biotechnology applications and offer remarkable capabilities in the design of biomimetic materials. We investigate the physical properties, including transport in different external conditions, of electrolyte solutions confined in channels, as well as electrolytes in nanoparticle assemblies and in polyelectrolyte gels.

Osuji, Chinedum (L1.1)

Title: Polymer self-Assembly and liquid demixing in the presence of liquid crystals

Abstract: Liquid crystals possess structural order that is intermediate between that of fully isotropic liquids and three-dimensionally periodic solids. They are intriguing soft matter systems that display a rich collection of physico-chemical phenomena that are of fundamental interest, but that are also useful for the engineering of useful materials and devices. Here, we explore the influence of liquid crystallinity on macromolecular self-assembly (microphase separation) and on the demixing of simple binary systems (macrophase separation). The presence of mesogens attached to block copolymers (BCPs) or blended with BPCs can result in a rich interplay of self-assembly on multiple length scales, and provides new opportunities to control nanostructure development. This talk explores the self-assembly and directed self-assembly of a variety of mesophase forming systems. These systems display rich phase behavior, including the formation of highly persistent domains, gyroid morphologies and strongly asymmetric phase diagrams, and we encounter systems with structural periodicities as small as ~6 nm. The stimuli responsiveness of LC mesophases represents a useful handle via which to control ordering processes, and we examine this in the context of a photoresponsive and magnetoresponsive systems, including field-induced symmetry breaking. Finally, we explore phase separation due to thermally induced demixing in binary mixtures of mesogens with a hydrocarbon solvent. In the presence of sufficiently elastic mesophases, demixing occurs via the formation of filamentous intermediates that exhibit lower elastic free energy relative to the canonical spherical domains or droplets seen during conventional liquid-liquid phase separation. We detail the subsequent cascade of events as filaments grow and collapse into flat drops that form a ramified smectic network around which active flows are established as the phase separation proceeds.

Palacci, Jérémie (B4.6)

Title: Bacteria as blacksmiths

Abstract: Here we will show that an active bath of swimming E. Coli bacteria direct the aggregation of sticky colloids into forming unconventional gels. In addition to the dynamics of aggregation being accelerated due to enhanced diffusion in the active bath, a key aspect is the emergence of chiral rotation of the aggregations due to the chirality of the flagella rotation of E. Coli. Our experiments are quantitatively captured by a coarse-grained model highlighting the effect of this chiral rotation. Our results show that the activity of the bath can control the phase diagram of materials. Active (bacterial) baths constitute a potent tool to translate the ideas of annealing/quenching of metallurgy into the design of soft materials.

Ramaswamy, Sriram (A5.1)

Title: Bulk condensation by an active interface

Abstract: My talk will present experiments, supported by mechanically detailed simulations, on bulk condensation and sublimation of non-motile beads by a tiny population of orientable motile grains. I will offer an understanding of our findings through a theory with a naturally non-reciprocal Cahn-Hilliard structure.

Safran, Sam (B1.4), coauthors: Gonen Golani and Amit Kumar

Title: Novel mesoscale properties of protein condensates: Non-equilibrium activity and conformational freedom

Abstract: We discuss recent observations [1, 2] of large (10's-100 nm's) protein assemblies in the one-phase regime that precedes LLPS in protein-water-salt solutions in terms of an analytical theory of these protein assemblies based on analogies with other mesoscale structures in amphiphilic (surfactant or lipid) systems where core-shell assemblies are observed. What is unique about intrinsically disordered proteins is that the same protein can – via its different conformations [3] -- act as both the "inner phase" and "amphiphilic surface layer." A statistical mechanical model of the cluster size distribution is compared with experiment to elucidate the nature of the interactions in the core and shell. Another novel aspect of liquid-liquid phase separation of proteins in cells, is that proteins are being produced and degraded over time, via enzymatic activity involving ATP, which makes these systems inherently non-equilibrium. We show theoretically [4] that this results in a steady-state of mesoscale condensates where the size is determined by the ratio of the bare interfacial tension and the kinetic coefficients. In the case of lamellar condensates, the effective tension that includes both the equilibrium and kinetic effects, can be zero and the domains are stabilized by their resistance to bending. Both the conformational and non-equilibrium effects may be related to recent experiments [5, 6] that measure an ultra-low tension and a bending modulus of the order of kBT for protein condensates in cells.

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Šarić, Andela (B3.5)

Title: Shape-shifting soft matter across evolution

Abstract: Biological cells are inherently soft and able to change their shape to fulfil their function such as to move, divide, connect with partners, or exchange material. Today I will present our recent research on computational modelling of non-equilibrium physical processes that drive cell shape changes across the tree of life. I will particularly focus on cell reshaping driven by chemical exchanges with friends or foes within an ecological community. Then I will address cell shape changes during cell division at different points in evolution. Beyond their biological context, our results can help guide the design of artificial structures that are able to mimic life at the nanoscale.

Schulman, Rebecca (B5.4)

Title: Programmed spatiotemporal dynamics and pattern recognition in soft materials with synthetic biochemical signaling networks

Abstract: Reaction-diffusion processes can lead to the emergence of patterns such as Turing patterns or traveling waves in soft materials. In biological tissues, the coupled cell signaling reactions and soluble factor diffusion processes underlying cell-cell communication play critical roles in wound healing, morphogenesis, and recognition of global states such as infection. These observations suggest how reaction-diffusion processes inside soft materials could also direct complex concerted actions and sense overall environmental state. Inspired by cell-cell communication and collective cell behavior, we ask how biochemical reactions coupled to diffusion processes might be programmed to produce arbitrary stable or dynamic micron- to centimeter-scale spatial patterns in response to specific spatial inputs and how materials might respond to spatially distributed inputs to compute functions such as a consensus or pattern recognition. To do so, we rely on a modular material architecture in which material "nodes" each produce and respond to specific biochemical signals. We develop a library of more than ten biomolecular signals that can communicate information without crosstalk and a simple yet robust signal processing architecture that relies on signal amplification and thresholding. A key insight is that these signals must be propagated over a specific radius of influence; this principle enables both reliable signal propagation and separate physical neighborhoods in which computations occur without interference. These methods could provide new means for programming autonomous soft robots, smart coatings, or biomaterials to perform complex actions such as locomotion or healing and allow materials to adapt to their global state such as their physical orientation or type of environment by classifying distributed patterns of mechanical, chemical, or light stimulation.

Sharma, Prerna (C1.2)

Title: Programmed spatiotemporal dynamics and pattern recognition in soft materials with synthetic biochemical signaling networks

Abstract: Rods exhibit a variety of partially ordered liquid crystalline phases unlike spherical colloids. The monolayer smectic phase of rods which we call as colloidal membranes, deserves special attention as it is an ideal realization of a two-dimensional thin elastic sheet or a membrane that has fluid like dynamics at the level of constituents. I will present our recent efforts in sculpting these model membranes by inducing phase transitions which in turn are controlled by microscopic physical properties of the constituent rods such as aspect ratio, flexibility and chirality. These equilibrium phase transitions can also be induced dynamically by changing the temperature of colloidal membranes, thereby enabling the observation of kinetic pathways of transformation. Overall, our studies present novel mechanisms that are relevant to remodeling biological membranes.

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Smalyukh, Ivan (L2.3)

Title: Vortex reconnections in knotted chiral meta matter

Abstract: Knots of vortex lines within physical fields were postulated to behave like particles already starting from Gauss and Kelvin, and recently topological order and phases represent an exciting inter-disciplinary research frontier [1]. I will describe knotted vortices that emerge in the physical order parameter fields of chiral liquid crystals. A combination of numerical modeling and nonlinear optical imaging uncovers the internal structure and topology of individual vortex knots and the various hierarchical organizations that they form via different reconnections. I will discuss their stability in molecular and colloidal liquid crystals of different symmetries and will show how low-voltage electric fields can switch between different types of behavior. Finally, I will discuss how this emergent paradigm of dynamic knotted meta matter could allow for imparting new designable material properties and physical behavior [2-4].

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Soto, Rodrigo (A4.4)

Title: Kinetic theory for active Brownian particles

Abstract: Active Brownian particles (ABPs) have become a prototype for active matter due to their simplicity and ability to display many of the phenomena present in active matter. Despite the importance of this model, a kinetic theory for ABPs has not been derived, mainly due to the finite duration of particle encounters resulting from motion persistence. Here we show that it is possible to build a Boltzmann-Enskog-like kinetic theory that is quantitatively correct in its predictions.

When two ABPs collide, they slide along each other until they can continue their free motion. For persistence lengths much larger than the particle diameter, the directors do not change in the process, but the collision can be modeled as producing a net displacement on the particles compared to their free motion in the absence of the encounter. This displacement at each collision is, on average, opposite to the direction of motion, generating an effective reduction of the velocity.

With these elements, a Boltzmann-Enskog-like kinetic theory is built. Collisions are effectively instantaneous, implying that the equation is local in time. A linear stability analysis of the homogeneous state predicts a density instability associated to the motility induced phase separation (MIPS). The density threshold, computed entirely from microscopic parameters, is in excellent agreement with agent-based simulations. It is equal to the simpler prediction from the effective velocity reduction described above.

Stone, Howard A (Plenary Session F)

Title: Physicochemical hydrodynamics and soft matter: From thin films to molecular biology to swimming cells

Abstract: The principles of fluid dynamics and physical chemistry are applicable to a wide range of soft matter systems. In this talk, I highlight several such themes that arise in our recent work, including (i) thin film flows that exhibit self-similarity (both expected and unexpected), (ii) the role of biomolecular condensates in formation of the mitotic spindle, and (iii) the interplay of mechanics, motility, and transport phenomena to understand the transcriptional response of planktonic bacterial cells in shear flows.

Suo, Zhigang (Plenary Session N)

Title: Mechanical behavior of a tanglemer–a polymer network in which entanglements greatly outnumber crosslinks

Abstract: Polymers inevitably entangle, and do not disentangle in a crosslinked network. This talk describes methods to synthesize a tanglemer, a polymer network of dense entanglements and sparse crosslinks, so that entanglements greatly outnumber crosslinks. We discover that crosslinks and entanglements act differently when a crack grows in the network. At the crack tip, crosslinks concentrate stress, but entanglements deconcentrate stress. The deconcentration of stress leads to outstanding mechanical behavior. In particular, a tanglemer reinforced with rigid particles amplifies fatigue threshold by an order of magnitude. Tanglemers illustrate how network topology affects mechanical behavior.

Tirrel, Matthew (P2.1)

Title: Molecular arrangement in polyelectrolyte complex coacervates

Abstract: Polyelectrolyte complex coacervation is an associative liquid-liquid phase separation process in systems of oppositely charged polyelectrolytes driven by concomitant entropic processes of water reorganization and counterion release. Typically, droplets of the coacervate phase form suspended in a continuous supernatant phase. As the droplets contain a large volume fraction of water, and all their molecular constituents are individually water-soluble, the interfacial tension is very low and can be made extremely low by adding salt to approach a critical salt concentration. Therefore, complex coacervation has been known and used practically for decades as a method of encapsulation or surface adhesion, relying on these interfacial properties, albeit with readily available but poorly characterized constituents. In the last decade, this process has become the object of intense focus in the fundamental polymer physics community, and simultaneously, of the molecular biology community, in several respects. The polymer physics community has focused on the formation, structure and dynamics of polyelectrolyte complexes. The biology community has recognized that polyelectrolyte complexes give rise to many previously unrecognized compartments and condensates within cells. There is also an enduring curiosity about the possible role of complex coacervation in the formation of protocells with the capacity to evolve compartmentalized RNA synthesis in prebiotic environments.

Our own group has produced rigorous new data on phase diagrams and on the effects of chain charge density on phase separation. Recently published, or as-yet unpublished, work from our group has (1) demonstrated positional correlation between polyanions and polycations in coacervate phases *via* small angle neutron scattering; (2) shown that multi-component mixtures of different charge densities form multi-compartment coacervate droplets, which could be relevant to biological compartmentalization; (3) observed that exposure of coacervate droplets deionized water leads to the formation of electrostatic crosslinks on the interface of coacervate droplets that not only suppress droplet fusion indefinitely but also allow the spatiotemporal compartmentalization of RNA on a time scale of days, leading to speculation that such non-fusing membrane-less coacervate droplets could potentially act as protocells.

Valentine, Megan (B4.1)

Title: New approaches to designing and deploying hydrogels for force sensing and control

Abstract: Photocured hydrogel materials, such as those formed from poly(ethylene glycol) diacrylate (PEGDA), hold great promise as tissue replacements and drug delivery agents due to their biocompatibility, mechanical tunability, low cost, and relative ease of manufacturing, including with microfluidic processing or 3D printing. While these gels are a common choice for biomedical engineering applications, we have a very poor understanding of the relationships between composition, processing, and mechanical properties of PEGDA gels due to their extremely complex microstructures and intrinsic heterogeneity. This limits our ability to design gels with tailored mechanical and structural properties for user-driven applications. To address this need, we combine data obtained using uniaxial compression, high-throughput microrheology and indentation studies with data-driven and physics-informed modeling to understand how synthesis parameters, such as the molecular weight and initial PEGDA concentration, and processing parameters, including light intensity and duration, influence the linear and nonlinear mechanical responses of PEGDA hydrogels. We then apply this understanding to develop hydrogel-based materials and devices that allow us study and control the dynamic restructuring of active cytoskeletal composites formed using actin, microtubules, motor proteins, and crosslinkers. Our high degree of synthetic control enables us to investigate the relationships between hydrogel geometry and stiffness, and the resultant cytoskeletal response in order to reveal and interrogate the mechanobiological circuits that underpin cytoskeletal contraction dynamics. At the same time, these devices offer exciting new opportunities to direct nanoscale contractions and amplify their action into deformations and motions at significantly larger scales.

Vlassopoulos, Dimitris (F2.3)

Title: Rheological challenges with polymeric melts and gels

Abstract: The fundamental understanding of the link between molecular structure and processing performance of polymeric materials relies, in part, on our ability to control their rheological properties. The latter is restricted, at the experimental level, by current measurement limitations in the nonlinear regime, which is relevant to processing. We discuss three challenges, the reliable measurement of material functions in entangled polymers at high shear rates, the use of appropriate protocols to tailor or erase the kinematic memory in polymeric gels and the effects of pressure on supramolecular gels.

Edge fracture instabilities are the main limiting factor in rotational rheometry. We present our attempts to reduce it and extend the measurement range of shear and normal stresses, inspired by recent theoretical developments. The use of the cone-partitioned plate geometry combined with an outer ring collar provides an optimum solution for a wide range of macromolecules and yields robust results that are consistent with predictions from simulations and modeling.

Shear startup sequences, developed long ago to study relaxation mechanisms in entangled polymers, are shown to be a powerful protocol to manipulate kinematic memories in macromolecular gels. We demonstrate this for the case of an amphiphilic pentablock copolymer that forms a hydrogel comprising bridged micelles. This generic protocol can be particularly useful in controlling the flow of thixotropic materials with yield stress.

Dynamic light scattering measurements at high pressures (kbar scale) yield the microrheological linear spectrum of macromolecular networks. We show examples that allow using pressure fields to tailor their viscoelastic response and extract scaling dependence for the dynamics as a function of pressure, and phase diagrams.

Wang, Zhen-Gang (P2.4)

Title: Origin of the entropic driving force in polyelectrolyte complex coacervation

Abstract: Mixing two solutions of oppositely charged polyelectrolytes under appropriate conditions results in a liquid–liquid phase separation into a polymer-rich coacervate phase and a coexisting polymer-poor supernatant phase. This polyelectrolyte complex coacervation (PCC) has received considerable attention in recent years due to its relevance to membraneless organelles in biology, and applications in biomedical and biomimetic systems. The complexation of oppositely charged polymers has been widely believed to be driven by the entropy gain due to counterion release. In this talk, we show that a large portion of the entropy change is due to solvent (water) reorganization, which we can extract by exploiting the temperature dependence of the dielectric constant. For weakly-to-moderately charged systems under common conditions (monovalent ions, room temperature in aqueous solvent), the solvent reorganization entropy, rather than the counterion release entropy, is the primary entropy contribution. We use this framework to examine the two elementary stages in the symmetric PCC—the complexation between a polycation and polyanion, and the subsequent condensation of the polycation–polyanion pairs by computing the potential of mean-force (PMF) using molecular dynamics simulation. From the calculated PMF, we find that the supernatant phase consists predominantly of polyion pairs with vanishingly small concentration of bare polyelectrolytes, and we provide an estimate of the spinodal of the supernatant phase. Finally, we show that prior to contact, two neutral polyion pairs weakly attract each other by mutually induced polarization, providing the initial driving force for the fusion of the pairs.

Yang, Shu (Plenary Session L)

Title: Responsive liquid crystalline elastomeric droplets and particles

Abstract: Nature provided us diverse examples of microparticles that have unique surface textures and can be responsive to the environment. In my talk, I will present several examples of diverse and unique droplets assembled from liquid crystal oligomers (LCOs) using a microfluidic device, where polydispersity of the chain lengths is a feature. We show that spherical LCO drops can undergo dramatic shape transition to a rich variety of non-spherical morphologies with unique internal structures upon cooling from the isotropic state to the nematic state, where molecular heterogeneity *promotes* and stabilize the reversible transitions. When shape-changing, spindle-shaped liquid crystal elastomer (LCE) microparticles synthesized from LCOs are spatially encoded in a conventional elastomer film, we realize complex shape morphing from 2D to 3D. When these particles are placed in a periodic lattice, we can reconfigure the lattice from chiral to achiral, then to chiral again, without breaking the translational symmetry.

Yeomans, Julia (A2.4)

Title: Active nematics: a useful approach to mechanobiology?

Abstract: Active materials mirror biological systems in operating out of thermodynamic equilibrium. Dense active nematics show both spontaneous coherent flows and mesoscale turbulence, the emergence of chaotic flow structures characterized by high vorticity and self-propelled topological defects. I shall discuss how we are investigating ways in which models based on the physics of active nematics might be extended to better describe the collective dynamics of epithelial cells, in confluent layers and in tissues. Specific directions include decoupling stress and shape order parameters and replacing substrate friction by internal dissipation. The long-term goal is to contribute to amalgamating mechanic, chemical and genetic approaches to understand embryogenesis, wound healing and the growth and spread of tumors.

Zamponi, Francesco (G1.2)

Title: Creating equilibrium glassy states via random particle bonding

Abstract: Creating amorphous solid states by randomly bonding an ensemble of dense liquid monomers is a common procedure that is used to create a variety of materials, such as epoxy resins, colloidal gels, and vitrimers. However, the properties of the resulting solid do *a priori* strongly depend on the preparation history. This can lead to substantial aging of the material; for example, properties such as mechanical moduli and transport coefficients rely on the time elapsed since solidification, which can lead to a slow degradation of the material. It is therefore important to understand under which conditions random monomer bonding can lead to stable solid states, that is, long-lived metastable states whose properties do not change over time. I will present a theoretical and computational analysis of this problem and introduce a random bonding procedure that ensures the proper equilibration of the resulting amorphous states. This procedure, which belongs to a broader class of free-then-freeze algorithms, also provides a new route to investigate the fundamental properties of glassy energy landscapes by producing translationally invariant ultrastable glassy states in simple particle models.

Zumer, Slobodan (L1.2)

Title: Creating equilibrium glassy states via random particle bonding

Abstract: In the last decades, understanding of the emergence and consequences of topological constraints has been growing immensely in numerous areas of physics. Here we focus on the anisotropic soft matter, a fluid characterized by orientational molecular ordering that includes liquid crystals and some biological systems. Considerable advances have been made in the description of the interplay between the topological and physical properties of these systems. Thanks to the integration of sophisticated experiments and theoretical approaches with increasingly effective numerical simulations and promising technological applications, topological soft matter—the often-used name for this research field—is an exciting area of research attracting scientists from a broad range of fields. Topological soft matter, due to its softness, rarely exhibits homogenous orientational order. Most of the frustration caused by the conflicting effects of chirality, anisotropic elasticity, confining geometries, surface anchoring, and external fields leads to stable and metastable point defects, disclination lines, and solitons in the orientational order parameter field. The dynamics occurring in the presence of activity, mobile ions, or temperate, pressure, and concentration gradients range from stationary to chaotic flows. In contrast to the well-known use of liquid crystals in displays, where defects are undesired objects, the development of techniques that allow researchers to control the formation and interaction of defects in diverse liquid crystal systems opens new possibilities for applications of topological soft matter in photonics, plasmonics, sensorics, and bio-related systems. The basic concepts with theoretical and simulation approaches needed to deal with experiments in topological soft matter will be briefly given and illustrated by a few examples.

- The interaction of topological and bouncing optical solitons in unwound chiral nematic layers based on the momentum transfer from light to matter and the force due to the nonlocal orientational elasticity of chiral liquid crystals enables the dynamical control and spatial localization of topological solitons. The interplay of both types of solitons is expected to be useful for soft photonics and optomechanics.

- Topologically constrained three-dimensional extensile activity-driven nematodynamics was first studied in spherical confinement, where low-activity stationary dynamic defect structures with increasing activity undergo transitions from stationary to chaotic 3D motions—active nematic turbulence. The synchronization of dynamics in two active nematic shells entangled by a disclination in a surrounding passive nematic was demonstrated to critically depend on the activity.

- The nematic order of muscle tissue in the heart is related to its functionality and its formation during the growth process. Using sliced, specially prepared hearts obtained from youngsters who died in the perinatal period allowed a partial determination of the director field in 2D. With the knowledge of 3D nematic ordering, elasticity, and defect structures, 2D images were converted into the 3D director field and disclinations.

Studies were done in collaboration with groups from Ljubljana, Boulder, Montpellier, Paris, and Grenoble.

Contributed Talks

Active Matter

SELF-PROPULSION AT THE NANOSCALE: Exploiting Molecular Energy Relaxation Mechanisms

Mr. Carles Calero, Arnau Jurado-Romero, Rossend Rey

A1.2: Carles Calero, Self-propulsion at the nanoscale, Room 306 BC, July 30, 2024, 10:30 AM - 12:00 PM

Controlling the transport of micro and nano particles in liquids is a fundamental problem with the potential to revolutionize different emerging technologies [1]. The use of self-generated thermal gradients has been theoretically proposed and demonstrated in experiments to be a promising strategy to induce transport of microparticles in liquids [2]. Here we show that the anisotropic dissipation of excess molecular energy into the surrounding solvent can lead to the propulsion of nanoparticles [3]. We use all-atomic models of excited nanoparticles and of the solvent to investigate with molecular dynamics simulaFtions the emergent particle propulsion as the excess energy is dissipated into the solvent. We report results in liquid water from: (i) nanoparticles functionalized with excited fluorophores [3]; (ii) high energy vibrationally excited molecules [4]. In both cases we find a marked energy flux anisotropy during relaxation which results in a temperature gradient across the nanoparticle and in a net propulsion that leads to significant enhanced diffusion when periodic excitations are applied. In contrast to most models of self-phoresis, we find that propulsion occurs via short ($\lesssim 0.5$ps) impulses. From our all-atomic description, we identify the source of propulsion as a transient force imbalance with the surrounding solvent when hydrogen bonds are broken because of the prescribed molecular excitations. Finally, strategies to direct the motion of functionalized nanoparticles in a given direction using confined environments are also discussed.

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Tunability and Switchability of Nanomotor Modes of Motion Utilizing Biocompatible Actuation Methods

Suzanne Ahmed, Tahniat Afsari, Kyle Nowlin, Cynthia Weissing

A1.3: Suzanne Ahmed, Tunability and switchability of nanomotor modes of motion utilizing biocompatible actuation methods, Room 306 BC, July 30, 2024, 10:30 AM - 12:00 PM

Nanomotors and micromotors have captured the imagination of researchers due to their potential to carry out a variety of functions in a wide spectrum of applications. Among the most prominent of these applications are biomedical ones, such as drug delivery and microsurgery. To actualize this potential, it must be possible to have fine control over the mode of nanomotor motion with facile switchability between different modes. Additionally, it must be possible to utilize biocompatible actuation methods. In this work we demonstrate several unique modes of nanomotor motion with a high level of tunability of the modes. The nanomotors are propelled using biocompatible ultrasonic and magnetic fields which allow for the non-contact, external control of motion.

Nanorod motors are metallic and synthesized by electrochemical deposition within porous anodic alumina templates. The nanorods are grown to be 300 nm in diameter and a few micrometers in length. A magnetic segment is incorporated within the gold nanorod motor to confer magnetic responsiveness. The nanomotors are placed within an ultrasonic chamber surrounded by an external magnetic setup. The acoustic chamber is composed of a piezoelectric transducer fixed to a silicon wafer on one side and a cylindrical cell on the other. A glass coverslip serves as a reflector. The nanorods are dispersed in water and placed in the ultrasonic chamber where a standing wave is established and the nanorods propel in the levitation plane. Tunability of their modes of motion is accomplished by externally varying the ultrasonic and magnetic signals. Modes of motion include translational, rotational and multiple combined translational-rotational modes of motion. Independent control over the mode of motion and the spatial position of the nanomotors is also accomplished.

Physical networks become what they learn

Dr. Menachem Stern, Dr. Marcelo Guzman, Mr. Felipe Martins, Prof. Andrea Liu, Prof. Vijay Balasubramanian

A2.2: Menachem Stern, Physical networks become what they learn, Room 306 BC, July 31, 2024, 10:30 AM - 12:00 PM

Physical networks may adapt to have diverse desired functions or properties, whether by design, evolution or learning. The adaptation process is expected to alter the functionality of the network and its own physics. For networks that naturally minimize a physical scalar, e.g. an energy function, adaptation of function is a double descent problem, minimizing both a physical and a learning cost function. We study how the process of physical adaptation couples the associated two landscapes. In linear systems, such as self-learning resistor networks, we show how adaptation links the physical and learning Hessian matrices, suggesting that the physical responses of the network to perturbations hold much information about the functions it adapted to perform.

Memory-induced spontaneous symmetry breaking

Dr. Shengkai Li, Dr. Trung Phan, Dr. Luca di Carlo, Dr. Gao Wang, Dr. Van Do, Prof. Liyu Liu, Prof. Robert Austin

A2.3: Shengkai Li, Memory-induced spontaneous symmetry breaking, Room 306 BC, July 31, 2024, 10:30 AM - 12:00 PM

From genetic encoding in DNA to memory processing in neural networks, information storage in living systems significantly influences collective behaviors, leading to phenomena from evolution to political polarization. Here we use robotic active matter to investigate how decisions based on individual memories can influence their collective behavior. We show that a collective of active agents with two rotational states can spontaneously break the symmetry with sufficiently large individual memory. Each agent we use is a spinning disk (spinner) on an airbed that either spins counterclockwise or clockwise. Thanks to the feature that a pair of same-direction spinners drop their spins upon interaction while a pair of opposite-direction spinners do not, a gyroscope in the microcontroller we mount on each spinner can infer the other spinners around it to some correctness. When each spinner is programmed to follow the majority's spin by checking a list of past interactions with other spinners they keep in the microcontroller, the collective can fall into an all-same-direction state and lock in that state for a very long time when the list size is sufficiently large. A theory considering the the memory evolution and the resultant states well captures the population dynamics of the two states and shows how memory can induce spontaneous symmetry breaking.

New Mechanisms of Active Particle Propulsion Powered by Temporally Asymmetric AC Fields

Nidhi Diwakar, Dr. Gilad Yossifon, Dr. Touvia Miloh, **Dr. Orlin Velev**

A3.3: Orlin Velev, New mechanisms of active particle propulsion powered by temporally asymmetric AC fields, Room 306 BC, August 1, 2024, 10:30 AM - 12:00 PM

AC electrokinetics offers convenient means of powering the motion of active or “self-propelling” microparticles that draw energy from the external field to perform rationally designed and precisely controlled motion. The simplest way to achieve such propulsion is to use particles with an asymmetric polarization pattern. Our group reported earlier how an AC-field induced charge electrophoretic effect, ICEP, emerges when the symmetry of the system is broken by having Janus metallodielectric particles (PRL 100:058302, 2008) or by particles with asymmetric conductance (Nat. Mater. 6:235, 2007). While these effects have been used in many active particle studies, we recently found that there is a third basic effect of symmetry breakdown and particle propulsion. We will present a new electrohydrodynamic effect termed Asymmetric Field Electrophoresis (AFEP) in which spatially homogeneous, but temporally non-uniform AC signals drive field-collinear motion of any types of particles. A systematic voltage sweep revealed an unusual power law dependence of particle velocity on field strength ($U \propto E^n$, $2 < n < 3$). The temporal reversal of the AC signal results in a reversal in direction of motion without a change in speed. Further, the particle velocity drops steeply with increasing frequency ($U \propto 1/\omega$) and increasing particle size. The propulsion is a result from the

imbalance in counterion motion due to signal asymmetry. The experimental velocity data as a function of field strength, frequency, and signal asymmetry are supported by models of asymmetric ionic concentration-polarization. The direction of particle migration exhibits a size-dependent crossover in the low frequency domain, which can be harnessed for simple and efficient on-chip sorting. The AFEP can be combined with other AC electrohydrodynamic effects, such as induced-charge electrophoresis (ICEP), enabling the formation of multiaxially controlled active particle systems.

Light-driven transformations in entangled active matter

Dr. Nitesh Arora, Mr. Aarsh Desai, Mr. Harry Tuazon, Dr. Saad Bhamla

A3.4: Nitesh Arora, Light-driven transformations in entangled active matter, Room 306 BC, August 1, 2024, 10:30 AM - 12:00 PM

California blackworms (Lumbriculus variegatus) are freshwater aquatic worms that entangle with one another, forming aggregate structures commonly referred to as worm blobs. Biologically, the entangled state of worms helps them in the efficient execution of vital functions such as temperature maintenance, moisture control, oxygen regulation, and collective locomotion. From the active matter perspective, these tangled worm blobs represent a remarkable material that can autonomously self-assemble, shape-shift, and exhibit other emergent collective functions. Here, we investigate the response of these worm blobs to light exposure. It had been shown previously that blackworms are negatively phototactic, i.e., they tend to move away from light. We leverage this behavior of worms to control their collective motion through a remotely applied stimulus. To this end, we study the dynamic
response, shape transformation, and locomotion of entangled living matter as the function of programmed light. Moreover, blackworms show the tendency to entangle with passive material present in their proximity, due to thigmotaxis. The interplay of these blackworms' intrinsic behaviors can be harnessed to develop strategies aimed at light-guided material transportation through the utilization of entangled active matter.

Active fractal networks with stochastic force monopoles and force dipoles unravel sub-diffusion of chromosomal loci

Dr. Rony Granek, Dr. Sadhana Singh

> A4.2: Rony Granek, Active fractal networks with stochastic force monopoles and force dipoles unravel subdiffusion of chromosomal loci, Room 306 BC, August 1, 2024, 3:30 PM - 5:30 PM

Motivated by the well-known fractal packing of chromatin, we study the Rouse-type dynamics of elastic fractal networks with embedded, stochastically driven, active force monopoles and force dipoles that are temporally correlated [1]. We compute, analytically -- using a general theoretical framework -- and via Langevin dynamics simulations, the mean square displacement (MSD) of a network bead. Following a short-time superdiffusive behavior, force monopoles yield anomalous subdiffusion with an exponent identical to that of the thermal system. In contrast, force dipoles do not induce subdiffusion, and the early superdiffusive MSD crosses over to a relatively small, system-size-independent saturation value. In addition, we find that force dipoles may lead to ``crawling" rotational motion of the whole network, reminiscent of that found for triangular micro-swimmers and consistent with general theories of the rotation of deformable bodies. Moreover, force dipoles lead to network collapse beyond a critical force strength, which persists with increasing system size, signifying a true first-order dynamical phase transition. We apply our results to the motion of chromosomal loci in bacteria and yeast cells' chromatin, where anomalous sub-diffusion, with exponent $\nu \simeq 0.4$, were found in both normal and ATP-depleted cells, albeit with different apparent diffusion coefficients. We show that the combination of thermal, monopolar, and dipolar forces in chromatin is typically dominated by the active monopolar and thermal forces, explaining the observed normal cells vs the ATP-depleted cells behavior.
[1] https://doi.org/10.48550/arXiv.2307.12310

Environment-stored memory in active matter: a framework for extra-cellular matrix remodeling

Ram M. Adar, Jean-François Joanny

A4.3: Ram Adar, Environment-stored memory in active matter: a framework for extra-cellular matrix remodeling, Room 306 BC, August 1, 2024, 3:30 PM - 5:30 PM

Many active systems display nematic order, while interacting with their environment. We explain how environment-stored memory allows active nematics to create an effective external field that aligns them. This leads to substantial modifications of the known phase diagram and dynamics, including nematic order at arbitrarily low densities and arrested domain coarsening. We are motivated mainly by cells that remodel fibers in their extra-cellular matrix (ECM), while being directed by the fibers during migration. Our predictions indicate that remodeling promotes cellular and ECM alignment, and possibly limits the range of ordered ECM domains, in accordance with recent experiments. Our findings are generic and imply that the understanding of standard active matter may not apply in a dynamic environment, highlighting the need for further investigation and adaptation of existing theories.

Phase behavior and transport of active colloids under extreme confinement

Dr. Stewart Mallory

A4.5: Stewart Mallory, Phase behavior and transport of active colloids under extreme confinement, Room 306 BC, August 1, 2024, 3:30 PM - 5:30 PM

Using computer simulation and analytical theory, we study an active analog of the well-known Tonks gas, where active Brownian particles are confined to a periodic one-dimensional (1D) channel. By introducing the notion of a kinetic temperature, we derive an accurate analytical expression for the pressure and clarify the paradoxical phase behavior where active Brownian particles confined to 1D exhibit anomalous clustering but no motility-induced phase transition. More generally, this work provides a deeper understanding of pressure in active systems as we uncover a unique link between the kinetic temperature and swim pressure valid for active Brownian particles in higher dimensions. In addition, we provide an analytical theory for computing transport coefficient under such confined conditions and derive expressions for the long and short-time self-diffusivity as a function of packing fraction and activity.

Asymmetry in Active-Passive Phase Separation

Mr. Paarth Gulati, Dr. Fernando Caballero, Mr. Liang Zhao, Dr. Itamar Kolvin, Prof. Zvonimir Dogic, Prof. Cristina Marchetti

A4.6: Paarth Gulati, Asymmetry in active-passive phase separation, Room 306 BC, August 1, 2024, 3:30 PM - 5:30 PM

Combining experiments and continuum theory, we examined the interfacial behavior of a phase separated mixture of an active microtubule-based liquid crystal and a passive fluid. The active stresses generated by kinesin motor proteins in the bulk of the liquid crystalline phase drive active flows that deform the interface, producing new morphologies qualitatively different from those found in equilibrium systems. At low and intermediate activities, the interface between the active and the passive fluids remains intact. However, the active interfacial fluctuations are strongly asymmetric, characterized by broad smooth peaks that push into the passive fluid and sharp deep valleys that push into the active phase. We suggest that this asymmetry arises from activity-driven interfacial anchoring of the liquid crystal. The asymmetry of the resulting flows then tends to pinch in the valleys and widen the peaks. Above a critical activity, passive droplets are invaginated in the active phase against gravity, resulting in a dynamical steady state of a “perforated” active fluid. The continuum model suggests universal behavior at the transition to the perforated active phase, which may therefore be understood in terms of the geometrical properties of the interface fluctuations. This work shows how activity can provide a new handle for controlling the morphology of fluid interfaces and the geometry of phase separation.

The hydrodynamics of active matter in inhomogeneous environments

Dr. Gwynn Elfring

A5.3: Gwynn Elfring, The hydrodynamics of active matter in inhomogeneous environments, Room 306 BC, August 2, 2024, 10:30 AM - 12:00 PM

This talk focuses on active matter systems where the active particles are very small, for example bacteria or chemically active colloidal particles, such that the inertia of the particles and the fluid flows that they generate is negligible. The motion of small active particles in homogeneous Newtonian fluids has received considerable attention, with interest ranging from phoretic propulsion to biological locomotion, whereas studies on active bodies immersed in inhomogeneous fluids are comparatively scarce. In this talk I will show how the dynamics of active particles can be dramatically altered by the introduction of mechanical inhomogeneity in the fluid. Specifically, I will discuss the effects of spatial variations of fluid viscosity (leading to viscotaxis) and density (leading to densitaxis) in the context of biological locomotion.

Biological Matter

Rigidity percolation predicts tissue viscoelasticity scaling with fibrillar collagen based on collagenase kinetics imaged by SHG

Dr. Dennis E Discher

B1.1: Dennis Discher, Rigidity percolation predicts tissue viscoelasticity scaling with fibrillar collagen based on collagenase kinetics imaged by SHG, Room 305 AB, July 30, 2024, 10:30 AM - 12:00 PM

Many processes in mature and developing tissues are impacted by physical properties that conceivably reflect an underlying gelation transition. Here, we show that rigidity percolation of collagen-fiber networks within fresh tissues provides a robust means to predict pan-tissue scaling of mechanical properties. Progressive degradation of fibers in diverse tissues is imaged by label-free second harmonic generation (SHG) and paired with viscoelasticity measurements to reveal a gel-to-sol critical transition brought about by small reductions of fiber density above critical levels. Importantly, a pan-tissue percolation exponent ($z \sim 1.4$) predicts a similar power-law exponent for scaling of elasticity, viscosity, and plasticity with collagen-fiber density across adult and embryonic tissues – including perturbations to tissue contractility and collagen-crosslinking. Water content and cell-density variations across tissues also reveal a rigidity transition. Verification of collagen-I protein scaling with SHG signal forms the basis for a simple contractile-strain stabilized feedback loop, which predicts scaling of collagen-I RNA with tissue stiffness. Universality of collagen-fiber percolation further predicts results for organ-size scaling with body-weight, from mouse to elephants, and provides matrix-based metrics for live tissue health, pathology, and regeneration.

Modeling active contractility in fibrous living matter

Dr. Kinjal Dasbiswas

B1.2: Kinjal Dasbiswas, Modeling active contractility in fibrous living matter, Room 305 AB, July 30, 2024, 10:30 AM - 12:00 PM

Fibrous networks occur ubiquitously in living matter ranging from the cytoskeleton to the extracellular matrix. Due to their disordered structure and the propensity of slender fibers to bend and buckle, these biomaterials exhibit unique mechanical properties such as elastic nonlinearity and heterogeneous force transmission. Here, we describe the active deformation of such networks induced by force dipoles modeling myosin motor or cell contractility. We model the fibers as elastic bonds in a connected network which can stretch, bend, and buckle. We predict that predominant fiber bending effectively screens force propagation, resulting in weaker macroscopic contractility and inter-dipole mechanical interactions. Further, we predict an atypical fiber buckling-induced softening regime under intermediate external shear, before the well-characterized stiffening regime. Both these predictions are supported by experiments on crosslinker-inhibited fibrin in platelet-contracted blood clots. We will also provide qualitative comparison with in vitro actomyosin networks.

Diffusion in a Multiscale Model for the Stratum Corneum

Dr. Peter D. Olmsted, Dr Oleh Tovkach, Dr Gustavo S. Luengo, Dr Fabien Leonforte, Dr Ann Detroyer, Dr Sebastien Gregoire

B4.2: Peter Olmsted, Diffusion in a multiscale model for the Stratum Corneum, Room 305 AB, August 1, 2024, 4:00 PM - 5:30 PM

Skin is an effective barrier against the penetration of external molecules (either harmful or beneficial). During topical application the performance of a particular ingredient requires understanding how its chemical nature, together with the skin's structure, guide its diffusion, and its final fate in the tissue. We present a coarse-grained multi-scale modeling approach for studying transport in the outermost barrier of skin, the stratum corneum (SC). This formalism projects from atomistic calculations on a nm scale to diffusion on a 50 micron scale, and accounts for anisotropic transport in the layered lipid matrix that comprises the SC. We introduce a new method for calculating layering of lipids within the cells (corneocytes) which naturally captures realistic patterns of the lamellar ordering, and is generalizable to arbitrary geometries. We calculate the effective permeability of model SC structures for the a wide range of partition coefficients and diffusivity ratios, and demonstrate penetration pathways that range from hydrophobic (lipid) to hydrophilic (corneocyte) regions, as well as intermediate states with a uniform flux throughout the SC. The approach can be generalized to arbitrary SC morphologies (e.g. depending on the body part, age, hydration state). We show how that the 'hydrophilic' pathway can, surprisingly, be preferred by hydrophobic molecules that are sufficiently more mobile (hydrophilic) in the cornecytes than in the lipid region. We discuss the special relevance of this work for not only transport through the SC, but also wider analogous transport in other complex composite media

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Collective behavior of platelets in fibrin fiber clots

Dr. Alexander Alexeev, Dr. Yueyi Sun, Dr. Wilbur Lam

B2.2: Alexander Alexeev, Collective behavior of platelets in fibrin fiber clots, Room 305 AB, July 30, 2024, 3:30 PM - 5:30 PM

Blood clots play a critical role in restoring hemostasis and regulating thrombosis in the body. Upon vascular injury, a cascade of events culminates in the formation of a soft plug of fibrin fiber mesh with distributed anucleate blood cells called platelets. Activated platelets undergo active contraction within fibrin fiber mesh causing the clot to shrink the overall size, modifying the internal clot structure, and altering clot mechanics. We developed an experimentally informed mesoscale computational model of fibrin-platelet blood clots to gain insights into the contraction of blood clots and to examine the interactions among different clot elements. We show that the simulations correctly predict clot contraction for platelet concentration ranging over four orders of magnitude. The simulations reveal that platelets utilize a new emergent behavior to enhance volumetric material contraction and to magnify contractile forces. We refer to this behavior as asynchrono-mechanical amplification and show that it is triggered by the heterogeneity in the timing of platelet activation. We demonstrate the connection between the forces produced by individual platelets nested within fibrin mesh and the macroscopic forces generated by the clot and show how the clot forces depend on network properties. We also prob the ability of contracting colts to entrap and retain red blood cells and the impact these cells have on the clot internal structure and mechanics. The results of our work provide now insights into the biomechanics of blood clots and reveal valuable guidelines for designing advanced synthetic and hybrid materials with platelet-inspired distributed actuation.

Cell packing in the notochord

Sharon Lubkin, Evan Curcio

B2.4: Sharon Lubkin, Cell packing in the notochord, Room 305 AB, July 30, 2024, 3:30 PM - 5:30 PM

Cells inside the notochords of early zebrafish embryos have been shown to pack in a small number of stereotyped patterns. Mutations or treatments which disrupt the typical patterning are associated with developmental defects, including scoliosis. The dominant wild-type “staircase” pattern is the only regular pattern displaying transverse eccentricity. Morphometry and pattern analysis have established a length ratio λ governing which patterns will be observed. Physical models of cell packing in the notochord have established relationships between this geometric ratio λ, a mechanical tension ratio Γ, the transverse aspect ratio α, pattern, pressure, and taper.

Since a major function of the early notochord is to act as both a column and a beam, we aim to understand the overall resistance to compression and bending in terms of these mesoscale cell/tissue properties. To frame the relationships between these properties, we have developed a model of the notochord as an elastic closed-cell foam, packed in either the “staircase” or “bamboo” pattern. Flexural rigidity is shown to be independent of the ratio of membrane stiffnesses of cells and the notochord sheath, but strongly dependent on internal pressure and packing configuration. Our results suggest a specific developmental advantage to the wild-type staircase packing pattern.

Connectivity and Contraction in Cytoskeletal Networks

Dr. Julio Belmonte, Michael Norman, Annamarie Leske

B2.5: Julio Belmonte, Connectivity and contraction in cytoskeletal networks, Room 305 AB, July 30, 2024, 3:30 PM - 5:30 PM

The cytoskeleton's ability to contract and propagate forces is the fundamental mechanism behind cell morphology, division and migration. This can only happen if the network is sufficiently connected, but a rigorous description of the connectivity requirements has never been provided. In this work we focused on the polarity-sorting contraction mechanism and showed that connectivity is not determined by filament spatial distribution alone, but by the interconnectivity between the dual network of filaments and motors. We developed a method to quantify filament-motor connectivity as a function of motor length and filament length distributions, and the densities of each component. With it, we were able to derive a general theory that qualitatively predicts when a random network is sufficiently connected to allow global or local contraction. We validate our predictions with computer simulations and a novel metric to distinguish between these outcomes. All results are independent of filament rigidity, making our findings applicable to both actin and microtubule networks. Lastly, we discuss how those outcomes are affected by the introduction of crosslinking proteins, which, despite not actively generating forces of their own, can promote global contractility at small doses even for networks made of short and/or rigid filaments.

Multiscale Lattice Modeling and Simulations of Heterogeneous Membranes

Dr. Oded Farago, Dr. Tanmoy Sarkar

B3.1: Oded Farago, Multiscale lattice modeling and simulations of heterogeneous membranes, Room 305 AB, July 31, 2024, 3:30 PM - 5:30 PM

Mixtures of lipids and cholesterol (Chol) have been served as simple model systems for studying the biophysical principles governing the formation of liquid ordered raft domains in complex biological systems. These mixtures exhibit a rich phase diagram as a function of temperature and composition. Much of the focus in these studies has been given to the coexistence regime between liquid ordered and liquid disordered phases which resembles rafts floating in the sea of disordered lipids. In the talk, I will present a new lattice model of binary [1] and ternary [2,3] mixtures containing saturated and unsaturated lipids, and Chol. Simulations of mixtures of thousands of lipids and cholesterol molecules on time scales of hundreds of microseconds show a very good agreement with experimental and atomistic simulation observations across multiple scale, ranging from the local distributions of lipids to the macroscopic phase diagram of such mixtures. Importantly, we find that the liquid ordered domains are highly heterogeneous and consist of Chol-poor hexagonally packed gel-like clusters surrounded by Chol-rich regions at the domain boundaries. The presence of such nano-domains within the liquid ordered regions appears as a characteristic feature of the liquid-ordered state and makes the interpretation of scattering data ambiguous in mixtures not exhibiting macroscopic phase separation.

[1] T. Sarkar and O. Farago, Minimal lattice model of lipid membranes with liquid-ordered domains, Phys. Rev. Res. 3, L042030 (2021).

[2] T. Sarkar and O. Farago, A lattice model of ternary mixtures of lipids and cholesterol with tunable domain sizes, Soft Matter 19, 2417 (2023).

[3] T. Sarkar and O. Farago, Characterizing the heterogeneity of membrane liquid-ordered domains, Eur. Phys. J. E 46, 99 (2023)

Competition-based selection of universal DNA ligands for antibody fragments

Dr. Valeria Milam, Ms. Mary Catherine Adams

B3.2: Valeria Milam, Competition-based selection of universal DNA ligands for antibody fragments, Room 305 AB, July 31, 2024, 3:30 PM - 5:30 PM

In contrast to oligonucleotide probes used to detect other oligonucleotide targets, single-stranded DNA ligands called aptamers are self-folded, single-stranded DNA sequences that act as a probe or ligand for a particular non-nucleotide target. Here, the non-nucleotide target is the constant fragment, Fc, found in all IgG antibodies. Due to their intended target-binding function, aptamers are often considered to be substitutes to antibodies which are more expensive and susceptible to irreversible denaturation. Rather than treating aptamers as rivals to antibodies, here the antibody itself is the target for aptamer screening. The overall goal is to find one or more aptamers that can capture any IgG antibody, independent of its bivalent antigen binding fragments. To find suitable aptamer candidates for a particular fragment shared among all IgG called Fc, the Milam group developed a competition-based screening platform called CompELS or “Competition-Enhanced Ligand Screening” to circumvent complications arising from the conventional, yet laborious evolutionary aptamer screening approach called SELEX or "Systematic Evolution of Ligands by EXponential enrichment." Following the completion of CompELS, the screening library, target-bound “winners” as well as nonbinding “losers” were evaluated using next generation sequencing (NGS) analysis. Data analysis indicates a majority of the initial screening library emerge as losers, but the winners are numerous and surprisingly diverse in their sequence composition. Moreover, NGS analysis reveals that there is little sequence overlap between library members and either the winners or losers. Thus, while NGS resulted in large sequence data sets of 10^5 or more each category of library, winners, and losers, the sequence data itself is likely incomplete. As a modern analytical tools in the aptamer community, recognizing the likelihood that NGS data sets – even large ones – may be incomplete. Ongoing work includes additional one-pot competition experiments to rank Fc aptamers as effective ligands and to characterize binding affinities of select winners. As DNA continues to gain prominence as ligands and probes for both oligonucleotide targets and non-nucleotide targets, this study reveals several aspects to the practicality or ligand screening and sequence analysis.

Sequence programmable nucleic acid condensates

Dr. Ankur Jain

B3.3: Ankur Jain, Sequence programmable nucleic acid condensates, Room 305 AB, July 31, 2024, 3:30 PM - 5:30 PM

Nature uses bottom-up self-assembly to build structures with remarkable complexity and functionality. Understanding how molecular-scale interactions translate to macroscopic properties remains a major challenge and requires systems that effectively bridge these two scales. Here, we generate DNA and RNA liquids with exquisite programmability in their material properties. Nucleic acids are negatively charged, and in the presence of polycations, they may condense to a liquid-like state. Within these liquids, DNA and RNA retain sequence-specific hybridization abilities. We show that intermolecular hybridization in the condensed phase cross-links molecules and slows chain dynamics. This reduced chain mobility is mirrored in the macroscopic properties of the condensates. Molecular diffusivity and material viscosity scale with the intermolecular hybridization energy, enabling precise sequence-based modulation of condensate properties over orders of magnitude. Our work offers a robust platform to create self-assembling programmable fluids and may help advance our understanding of liquid-like compartments in cells.

Adapt to Bend: Ant Cooperative Transport of Soft Rods

Dr. Atanu Chatterjee, Dr. Hillel Aharoni, Dr. Ofer Feinerman

B3.4: Atanu Chatterjee, Adapt to bend: Ant cooperative transport of soft rods, Room 305 AB, July 31, 2024, 3:30 PM - 5:30 PM

Local interactions, external constraints, and an influx of information affect collective behavior in animal groups. In the context of cooperative transport in ants, a trade-off exists between the well-coordinated pull of uninformed pullers and the directional information from the informed leaders. When transporting rigid cargo, ants exhibit strong coupling to the load, each perceiving identical local forces, thus ensuring perfect communication with zero delays. With flexible cargo, the material's compliance interferes with this coupling, introducing a delay in force perception among ants. This lag in communication gives rise to complex emergent group behavior. Through experiments and theory, we investigate the mechanisms by which ants continue to transport large flexible cargo efficiently despite constrained communication.

Phagocytic synthetic cells: non-living predators to fight bacteria

Dr. Cesar Rodriguez Emmenegger

B3.5: Cesar Rodriguez Emmenegger, Phagocytic synthetic cells: non-living predators to fight bacteria, Room 305 AB, July 31, 2024, 3:30 PM - 5:30 PM

I will introduce Phagocytic Synthetic Cells (PSCs) that recognize, capture, engulf and kill antibiotic-resistant bacteria without generating selection pressure for resistance recapitulating the most salient steps of phagocytosis. The PSCs are synthetic vesicles that can selectively bind to bacteria and exploit the binding energy to drive engulfment. From a thermodynamic point any vesicle can engulf a bacterium if the adhesive energy surpasses the bending energy of vesicle's membrane. However, the high curvature intermediates present during engulfment have prevented the use of the state-of-the-art vesicles for this task. We invented a new family of biomimetic vesicles, called i-combisomes that, despite having the same flexibility of superflexible liposomes, exhibited unsurpassed ability to quantitatively engulf nano- and micro-objects including bacteria which they killed upon engulfment. This superpredatory behavior is rooted in the statistic nature of the molecular topology of their building blocks, ionically-linked comb polymers. When assembled in water, their collective behavior follows a mean-field description, smearing the heterogeneity by forcing molecules with non-zero spontaneous curvature into a flat membrane acquiring a strained conformation, with the concomitant local-mean curvature mismatch. When engulfment begins, these molecules migrate to the non-zero curvature regions and adopt their more favorable conformation, therefore reducing the kinetic barriers, a trait that membranes assembled from a single low molecular weight amphiphile cannot achieve. By the same token, few minutes after engulfment of an antibiotic-resistant bacterium, the close apposition of the phagosome and bacterial membranes resulted in their fusion and the death inside the i-combisome. The remarkable element of this concept is that the killing occurs inside the PSCs, separated from the environment and because it targets a highly conserved element of the pathogen, its membrane, the killing action cannot be avoided by evolution. Remarkable, the PSCs could be engineered to be safe for eukaryotic cells and human organoids.

Gastric mucin promotes the spread of a growing bacterial swarm on agar surface

Dr. Jay Tang, Mr. Christopher Pawul

B3.6: Jay Tang, Gastric mucin promotes the spread of growing bacterial swarm on agar surface, Room 305 AB, July 31, 2024, 3:30 PM - 5:30 PM

Inoculated on the surface of soft agar containing nutrients, many species of motile bacteria can grow into a dense population, capable of spreading on the agar surface, defined as a swarm. We study the swarming behavior of Enterobacter Sp. SM3, which was isolated from the intestinal tissue of mice resistant to Inflammatory Bowel Disease (IBD). One focused study is on how incorporating mucin into agar affects the swarming motility of SM3. We found that mucin enhances SM3's swarm rate, defined as the rate at which bacteria cover an agar surface. It also helps retain a circular-mat swarm morphology in conditions where the colony spread becomes dendritic, indicative of deficiency in swarming. Measurement of the growth rate of SM3 in liquid media using an optical density-relative density conversion method shows that SM3's growth rate does not significantly change in the presence of mucin even as the swarm rate increases. The increase in swarm rate can be accounted for by the reduction of surface tension due to mucin, which facilitates the spread of the swarm front akin to wetting. The reduction of surface tension is confirmed by measuring the contact angle when droplets of liquid medium were applied on the surface of agar containing mucin. We also tested mucin's effects on the evaporation of covered agar plates, confirming a significant reduction in mass loss due to evaporation compared to the plates of agar without mucin. This finding suggests a secondary mechanism of mucin in preserving a high swarm rate over time, via better retention of moisture on agar surface. The overall results of our study show that mucin acts as a biosurfactant to promote swarming motility.

Coupling During Collective Cell Migration is Controlled by a Vinculin Mechanochemical Switch

Dr. Brenton Hoffman

B2.1: Brent Hoffman, Coupling during collective cell migration, Room 305 AB, July 30, 2024, 3:30 PM - 5:00 PM

Collective cell migration (CCM) plays important roles in development, physiological, and pathological processes. A key feature of CCM is the dynamic mechanical coupling between cells, which enables both long-range coordination and local rearrangements. This coupling requires the ability of cell-cell adhesions to adapt to forces, but a limited understanding of how mechanical forces and biochemical regulation interact to affect coupling has been a major obstacle. This is partly because of the drastically different length scales at which biochemical regulators and mechanical properties are studied. To bridge this gap, we developed a multi-scale approach that integrates experiments using molecular biosensors and quantitative migration assays with models of adhesion mechanics. We applied this approach to the ubiquitously expressed mechanical linker protein vinculin, which is a critical mediator of adhesion strengthening at cell-cell contacts and plays key roles in CCM-associated processes like embryogenesis and cancer invasion. We used FRET-based biosensors to probe the molecular loads (vinculin tension sensor, VinTS) and autoinhibitory conformation (vinculin conformation sensor, VinCS), key aspects of vinculin function, in migrating Madin-Darby Canine Kidney (MDCK) epithelial cells. We found that mutation of S1033, a known phosphorylation site, toggles vinculin between closed/unloaded and open/loaded states at cell-cell adherens junctions (AJs). By rescuing CRISPR Vcl KO MDCK cells with non-phosphorylatable or phosphomimic mutants, we found that this switch concomitantly controlled the speed and long-range coupling of CCM. In the context of physical models of CCM, these kinematic perturbations suggested changes to friction within the system. To test this, we developed a molecularly specific model of adhesion-based friction at AJs that considers the force-sensitive bond dynamics of key proteins and enables biochemically-regulatable reinforcement. In this model, activation of the vinculin switch increased friction at the AJs in a tunable manner, which matched experimentally observed effects on both vinculin molecular tension and CCM dynamics. Together, this work reveals a regulatory molecular switch for controlling cell coupling. It also develops a formalism for linking mechanosensitive, molecular-scale processes with changes in adhesion mechanics and cell migration dynamics that can be applied to the plethora of other mechanical linker proteins to enable future studies in mechanobiology.

De-novo ATP independent contractile protein network

Xiangting Lei, Dr. Carlos Floyd, Dr. Saad Bhamla

B4.3: Xianting Lei, De-novo ATP independent contractile protein network, Room 305 AB, August 1, 2024, 3:30 PM - 5:30 PM

In addition to conventional cytoskeletal motors like myosin, ciliated protists utilize novel Ca2+ -powered motors that do not require ATP to generate force, leading to the fastest acceleration observed in nature. Despite the promising applications which such a mechanochemical machinery offers for synthetic biology, this system has not yet been studied in vitro. In this study, we performed experiments to gain control over a reconstituted Ca2+ -powered network, we used continuum modeling to elucidate the system’s dynamics, and we applied these system to rapid particle transport and programmable vesicle delivery.

Tcb2, a filament protein from the cortex of Tetrahymena which comprises an EF-hand Ca2+ -binding site, has recently been identified for its ability to contract in response to calcium. We used a light-responsive chelator to spatiotemporally control the release of Ca2+ at a micron scale, which then triggers binding and contraction of the Tcb2 filaments. Under a long continuous release of Ca2+, we observe that a contractile active Tcb2 boundary is formed, which at long times transitions to a quiescent gel phase.

To overcome this transition to quiescence, we next studied the response of the system to pulsating light. We observed periodic contractility with pulsating light. In contrast to continuously released Ca2+, with Ca2+ pulses the gel-phase network exhibits more long-lived contractility, a larger active boundary area, and amplified contracting velocity. We also observe surprising dynamical features such as a reversal of the contraction direction from radially inward to outward as the network continues developing.

To understand these features of chemical network growth and elastic contraction, we developed a novel chemo-mechanical model which tracks the concentrations of all chemical components as well as the 2D strain fields. We couple the mechanics to the chemical dynamics by extending previous theoretical work on related systems in contracting protists. The model semi-quantitatively recapitulates many of the experimentally observed phenomena mentioned above. In particular, it explains the transition from radially inward to outward contraction as resulting from density-dependent elastic forces which are not present in standard elasticity theories, but which are important here due to strong accumulation of bound Tcb2 near the network periphery. These density-dependent contractile forces may also be relevant for understanding more traditional soft active matter systems in biology, such as actomyosin or microtubule-kinesin networks.

In addition to these experimental and theoretical explorations of Ca2+-powered network dynamics, we also consider some preliminary applications of this system in synthetic biology contexts. We find that the network can be used to move embedded rigid polystyrene particles and soft-deformable liposomes, as it can sustain hundreds of contraction cycles and can apply stresses of up to ~100 pN/micron2. With a trained reinforcement learning model, we designed the light pattern and cycle to move simulated micron-sized particles/liposomes hundreds of times their body size in minutes with the Tcb2 protein network. These applications suggest that Ca2+-powered networks based on Tcb2 could, in the near future, be used to experimentally exert mechanical forces at micron and second scales within living cells.

Computational engineering of responsive metaparticles

Dr. Ioana Ilie, Massimiliano Paesani

B4.4: Ioana Illie, Computational engineering of responsive metaparticles, Room 305 AB, August 1, 2024, 3:30 PM - 5:30 PM

Nanoparticles (NPs) find applications in a variety of fields, ranging from drug delivery to cosmetics and material design. As drug carriers, NPs need to overcome complex biological barriers to successfully deliver their cargo inside the diseased cell. Typically, NPs consist of a core platform decorated with ligands to enhance specificity. The composition of the core as well as the conformations of the ligands contribute to the mechanical properties of the nanoparticle, i.e. they modulate the intrinsic flexibility of the NP. Conventional models often omit the effect of particle flexibility and its response to the biological environement and, hence, the mechanisms of cellular uptake remain elusive.

Here, we introduce a novel coarse-grained model that captures the intrinsic flexibility of nanoparticles, aiming to ultimately create the ideal nanoparticle, a metaparticle. This metaparticle can respond to environmental changes and traverse the cellular membrane in a non-invasive manner. We used Brownian dynamics simulations to propagate the dynamics of the system [2].

Our results show that the metaparticles are responsive to applied stress. The response correlates with the size and the intrinsic topology of the metaparticles in a non-linear manner. Additionally, we found that the deformation and relaxation times vary with particle topology.

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Cell-derived matrix hydrogels with tunable mechanics for donor-derived microphysiologic systems

Dr. William Polacheck, Dr. Elizabeth Doherty

B4.5: William Polacheck, Cell-derived matrix hydrogels with tunable mechanics for donor-derived microphysiological systems, Room 305 AB, August 1, 2024, 3:30 PM - 5:30 PM

The extracellular matrix (ECM) in tissue provides both chemical and mechanical cues to cells that can affect cellular behavior such as migration and mechanoresponsive behaviors. Structural proteins such as collagens can have an impact on the mechanical and compositional properties of the ECM. Mutations in the genes that encode these proteins impact the microarchitecture of the resulting matrix and lead to devastating clinical consequences for patients. However, studying these changes in the ECM using traditional techniques has been limited by the use of animal-derived single-component ECM substrates. Decellularized extracellular matrix (dECM) scaffolds and hydrogels have been commonly used tissue engineering to recapitulate the native microenvironment more faithfully, but the use of human dECMs has been limited due to the availability of human tissue. Cell-derived matrix (CDM) can be generated from a variety of human cell types in vitro and provides a platform to study the biophysical and biochemical properties of ECM. Here, we report on recent developments to generate hydrogels with tunable viscoelastic mechanical properties, and we demonstrate their use toward the development of donor-derived microphysiologic systems for individualized disease modeling and drug screening.

We previously developed a donor-derived CDM platform to study the impact of COL3A1 mutations on ECM mechanical, compositional, and structural properties. We found that a glycine mutation in COL3A1 resulted in the production of CDM that had vastly different elastic and time-dependent mechanical properties and resulted in the slower migration of endothelial cells compared to CDM produced by healthy cells. While the composition and structure are mimic that of native human ECM, the two-dimensional nature of this CDM platform fails to recapitulate the three-dimensional environment of cells in human tissue. To address this inconsistency, in this study we utilize CDM grown from human dermal fibroblasts to develop CDM composite hydrogels for use within three-dimensional microphysiological models of the vasculature. Using proteomic techniques, we assess the composition of the CDM through multiple processing steps as it is made into a CDM pre-gel solution that can be used to form a hydrogel. CDM composite hydrogels were formulated with this pre-gel solution to include either genipin, a natural cross-linker, rat tail collagen-I, or bovine fibrin. We then characterize these several hydrogel formulations by assessing the gelation kinetics measured by absorbance, the mechanical properties measured by nanoindentation, and the microstructure analyzed by scanning electron microscopy. We demonstrate the utility of these CDM composite hydrogel formulations to foster endothelial cell attachment and growth as two- and three-dimensional substrates, and observe differences in cellular cytotoxicity, spreading, and morphology. Further, we pattern these CDM composite hydrogels for use within microfluidic devices to fabricate both single vessel and vascular network vasculature-on-chip platforms that incorporate human endothelial cells. Interestingly, we find that CDM composite hydrogels are enriched in proteins associated with vascular morphogenesis, and functional analysis demonstrates pro-angiogenic signatures in endothelial cells cultured in these hydrogels. The results of this study suggest that human-derived CDM composite hydrogels could address technical gaps in the development of human organs-on-chip and serve as substrates to promote vascularization.

Neutrophil Extracellular Traps (NETs) in Muco-Obstructive Pulmonary Disease.

Dr. Farnaz Fazelpour, Dr Mahmud Raihan, Lindsey Hill, Dean Bowman, Jean Felix, William Kissner, Dr Kaitlyn Rouillard, Dr Matthew Markovetz, **Dr. David Hill**

B5.1: David Hill,Neutrophil Extracellular Traps (NETs) in Muco-Obstructive Pulmonary Disease, Room 305 AB, August 2, 2024, 10:30 AM - 12:00 PM

Rationale: Hyperconcentrated mucus that is associated with muco-obstructive pulmonary diseases (MOPD) results from the combination of dehydration of the airway surface layer and mucin hypersecretion. This pathologically thickened mucus obstructs the airways and hinders clearance leading to infections and inflammation, which in turn recruit large numbers of immune cells such as neutrophils. A large portion of neutrophils undergo programmed cell death to expel their DNA and form neutrophil extracellular traps (NETs), a process termed NETosis. We hypothesize that for NETs to adversely affect both mucus rheology and removal from the lung via mucociliary clearance, the DNA released in NETs must spread through mucus such that it overlaps with DNA from adjacent NETs.

Methods: Mucus was harvested from human bronchial epithelium (HBE) cell cultures and prepared to concentrations that mimic healthy (1% organic solids (os)) and pathological (5% organic solids (os)) mucus conditions. To mimic inflammatory conditions, neutrophils were isolated from saliva, added to mucus, and stimulated to undergo NETosis. The spreading rates of NETs in mucus over a 48-hour period were measured by fluorescence microscopy. The macro- and microrheology properties of mucus with and without NETs were measured during the NETs spreading process by cone and plate and particle tracking microrheology (PTMR) respectively. Mucociliary transport rates were measured by particle tracking velocimetry on mucociliary transport devices. Results from adding NETs to mucus were compared to adding commensurate concentrations of purified DNA to mucus.

Results: Hyperconcentrated mucus had a negative impact on the spreading rate of NETs, i.e., NETs spread faster in 1% organic solids (os), healthy like mucus, than in 5% os that is associated with MOPD. Further, at 24 hours, the complex viscosity (η^*) of 1% mucus was increased roughly 2-fold, while at 48 hours, η^* was increased 10-fold. This 10-fold increase is the same we have previously reported for the difference in η^* for mucus harvested from HBE culture compared to CF sputum at the same concentration. We found that mucociliary transport rates were likewise decreased by the addition of NETs and DNA to mucus at concentrations great enough to ensure overlap of DNA.

Conclusions: The spreading of NETs through mucus creates new interactions between the polymeric mucus structure and the DNA in NETs, consequently resulting in higher viscosity as measured by η^*. The rate at which NETs spread through mucus via diffusion is dependent on the concentration of mucus and the molecular weight of DNA. These results may indicate that a threshold concentration of DNA is required to facilitate the need for therapeutic DNA-cleaving agents.

Dr. Meera Ramaswamy, Dr Alejandro Martinez-Calvo, Dr Carolina Trenado Yuste, Prof. Ned Wingreen, Professor Sujit S Datta

B5.3: Meera Ramaswamy, Morphodynamics of bacterial communities proliferating in three dimensions, Room 305 AB, August 2, 2024, 10:30 AM - 12:00 PM

In nature, bacteria often grow as communities in three-dimensional (3D) environments, with multiple

different cell types cooperating or competing for resources. While many studies have investigated how

proliferation drives the spatial organization of multi-strain/species communities in two dimensions, little is known about the morphology of these communities in three dimensions. Here, we use two different strains of E. coli suspended in a transparent jammed packing of microgel particles to investigate the morphodynamics of communities with multiple cell types proliferating in 3D. Unexpectedly, even though the strains are initially well-mixed, we find that they proliferate into segregated microcolonies within the overall community, with the size and shape of each microcolony determined by the initial cell density and colony width. We rationalize these results by considering the interplay between proliferation, competition for space, and competition for nutrients. Taken altogether, our results help to shed new light on the morphodynamics of mixed microbial communities, as well as other forms of proliferating active matter, in 3D.

Bacterial Dynamics at the Swarm Front

Ms. Danielle Germann, Dr. Jay Tang

B5.4: Danielle German, Bacterial dynamics at the swarm front, Room 305 AB, Fri, Aug 2, 2024
10:30 AM-12:00 PM

Swarming behavior is a trait observed in many species of flagellated bacteria. It occurs when a growing population of motile cells expands on an agar surface, resulting in collective motion. We investigate the swarming behavior of Enterobacter sp. SM3, a gut bacterium that has recently been identified and shown to provide a physiological benefit to lab mice suffering intestinal inflammation. When SM3 bacteria swarm, they form dynamic packs, featuring transient but strong cell-cell interactions. We found that these interactions are highly sensitive to cell length, velocity, aerial density, along with local fluid thickness and viscosity. Therefore, measurements of cell density, size, as well as individual cell position and orientation within dynamic packs, are all necessary to model the cell-cell interactions that govern the observed bacterial collective dynamics. The aim of our ongoing experiments is to acquire essential parameters for computer simulations with the goal of capturing the underlying physics of bacterial swarming behavior.

Colloidal Matter

Diffusiophoretic Transport of Colloids in Disordered Media
Dr. Amir Pahlavan

C1.4: Amir Pahlavan, Diffusiophoretic transport of colloids in disordered media, Room 302 BC,
July 30, 2024, 3:30 PM - 5:30 PM

Gaining control over the motion of colloids in complex environments is essential in a wide range of applications, from cell sorting and drug delivery to filtration and water purification. Recent studies have demonstrated the utility of diffusiophoresis, i.e., the motion of colloids due to solute gradients, in manipulating and steering colloids in simple microfluidic geometries. Yet, it remains a question whether diffusiophoresis could play an important role in more complex environments, with spatiotemporal gradients in solute gradients and flows. Here, combining experimental observations and numerical simulations of microfluidic channels patterned with obstacles, we study the competition between phoretic and convective migration of colloids and discuss its implications on the transport, dispersion, and steering of colloids on macroscopic length scales.

Engineering the Electrical Response of Conductive Suspensions

Dr. Jeffrey Richards

C1.5: Jeffrey Richards, Engineering the electrical response of conductive suspensions, Room 302 BC, July 30, 2024, 3:30 PM - 5:30 PM

Understanding how suspensions of electrically conductive nanoparticles respond to flow is of fundamental importance to engineering next generation electrochemical energy storage technologies. In this talk, I will show rheo-electric measurements, the simultaneous acquisition of electrical properties and rheological data, on model suspensions of silver-coated nano- and microspheres suspended in non-conductive oil. These suspensions' electrical properties arise because of the complex interplay between the electrical diffusivity and self-diffusion of the particles. By combining measurements with simulations and theory, we conclude that the electrical diffusivity far exceeds the particle self-diffusivity when the dynamics are dominated by both Brownian and shear-induced motion. I will end by outlining how these insights combined with colloidal synthesis can be used to engineer functional suspensions for applications.

Assembly of particles under orthogonally applied electric and magnetic fields

Dr. Ning Wu, Mr Xingrui Zhu, Mr Yuanxing Zhang

C1.6: Ning Wu, Assembly of particles under orthogonally applied electric and magnetic field, Room 302 BC, July 30, 2024, 3:30 PM - 5:30 PM

Colloids can be used either as model systems for directed assembly or as the necessary building blocks for making functional materials. Previous work primarily focused on assembling colloids under a single external field, where controlling particle-particle interaction is limited. This talk will present our recent results under a combination of electric and magnetic fields. When these two fields are orthogonally applied, we can independently tune the magnitude and direction of the dipolar attraction and repulsion between the particles. As a result, we can obtain colloidal structures not possible under one type of field only. For example, we can obtain homochiral colloidal clusters with tunable handedness on demand when the building blocks are anisotropic colloidal dimers. For isotropic microspheres, we have obtained well-aligned, highly dense, but individually separated linear chains with hierarchical structures at intermediate particle concentrations. We will report our experimental observations, underlying mechanisms, and tunability of the assembled structures. In addition, we have also performed Monte Carlo and Brownian Dynamics simulations in which the electric and magnetic dipolar interactions and electrohydrodynamic interactions are involved to gain a more fundamental understanding of our experimental results. Our method provides a convenient route for producing complex and hierarchical structures that are challenging to make using one field only.

Machine-assisted design of effective potentials and surface ligand patterns for colloidal self-assembly

Dr. Gaurav Arya, Dr. Yilong Zhou, Mr. Po-An Lin

C1.7: Gaurav Arya, Machine-assisted design of effective potentials for colloidal self-assembly, Room 302 BC, July 30, 2024, 3:30 PM - 5:30 PM

Colloidal self-assembly provides a scalable route to creating nanomaterials with new architectures and functions. Molecular models and simulations have played an integral role in our understanding of the solvent-mediated interactions between colloidal particles, the assembly morphologies that emerge from these interactions, and the self-assembly process itself. However, detailed molecular models of the building blocks and the solvent are not ideal for exploring assembly behavior or constructing phase diagrams, as the simulations are computational expensive, and the colloidal design space is often vast. Furthermore, the relationship between assembly morphology and design is often complex, so the "inverse design" of particles targeting a given assembly morphology also requires brute-force exploration of the design space. Here, we will demonstrate how machine learning can speed up both the exploration and the targeted design efforts in colloidal assembly. We will discuss the development of an analytical potential based on permutationally invariant polynomials for describing the effective multibody interactions between spherical polymer-grafted nanoparticles in a polymer melt [1]. The potential reduces the computational cost of assembly simulations by several orders of magnitude, allowing us to explore assembly behavior over large length and time scales and thereby obtain phases such as strings and hexagonal sheets that cannot be assessed using two-body potentials, and discover novel phases such as networks, clusters, and gels. We will also discuss the implementation of a neural adjoint framework for inverse-design of DNA-origami building blocks that can self-assemble into periodic superstructures based on patches of hydrophobic brushes introduced at specific locations on the origamis [2].

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Confined Brownian Motion of Soft Colloids

Mr. Nicolas Fares, Dr. Zaicheng Zhang, Dr. Maxime Lavaud, Dr. Yacine Amarouchene, Dr. Thomas Salez

C2.2: Nicolas Fares Confined Brownian motion of soft colloid, Room 302 BC, August 2, 2024, 10:30 AM - 12:00 PM

Confined motions are ubiquitous in microbiology. Examples at the micro- and nano-scales include blood cells flowing in vessels, antibody recognition, mechano-sensing of glia cells or confined diffusion of synaptic receptors. These situations contain viscous flows coupled to charged and soft confining entities, in presence of thermal fluctuations.

Aiming at unravelling the link between softness and thermal, i.e. Brownian, motion, we combine holo-

graphic microscopy and a statistical inference algorithm [1]. The technique allows for a precise experimental characterization of the 3-dimensional motion of a single free Brownian spherical colloid diffusing in a viscous liquid near a charged rigid glass wall, with a nanometric precision.

Already in the case of a micrometric rigid polystyrene sphere, striking differences compared to bulk

Brownian motion are measured and quantified. Namely, the statistics of displacements deviates from Gaussian distributions, which is quantified through high-order cumulants [2]. Also, femtonewton-resolved surface forces, which include electrostatics repulsion and weight, are extracted from Brownian trajectories.

The case of a deformable micro-sphere is even more puzzling. Specifically, we study the confined

Brownian motion of a low-surface-tension viscous oil droplet. Interestingly, at equilibrium, these soft droplets behave similarly as their rigid counterparts. However, they seem to display visco-capillary features [3] at smaller time scales. Specifically, we observe the emergence of a transient inertia-less lift force acting on the droplets [4]. If confirmed, this force could explain spontaneous migration strategies.

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& Dean, D. S. (2023). Non-Gaussian diffusion near surfaces. Physical Review Letters, 130(7), 077101.

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particle moving towards a thin fluid film. Journal of Fluid Mechanics, 977, A50.

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Coupling Between Thermal Fluctuations and Softness. Submitted.

Light-controlled colloidal crystallization

Dr. Steven Van Kesteren, Mr. Shihao Zang, Prof. Stefano Sacanna

C2.3: Steven van Kesteren,Light-controlled colloidal crystallization, August 2, 2024, 10:30 AM - 12:00 PM

Colloidal crystals, formed from the assembly of tiny particles, offer exciting possibilities for creating new materials with remarkable properties. Traditional views of self-assembly, which focus on combining particles with predefined interaction strengths, do not fully capture the diverse array of structures that can emerge. In reality, colloidal crystallization is a dynamic phenomenon influenced by the specific assembly pathways involved. Our study introduces a new system of oppositely charged colloids whose interactions can be precisely controlled with light. This system gives us unprecedented spatial and temporal control and allows us to observe their assembly in real time using confocal microscopy. Our experiments reveal fascinating behaviors, such as the ability to trigger crystal formation in specific spots, control transitions from gel to crystal, and rapidly anneal crystals. Hereby, we showcase the power of dynamic control in colloidal self-assembly, enabling the precise manipulation needed for tailored material properties.

Fluid Dynamics, Rheology

Memory of shear flow in soft jammed materials.

Dr. Véronique Trappe, Dr. H.A. Vinutha, Dr. Manon Marchand, Dr. Marco Caggioni, Dr. Vishwas V. Vasisht, Prof. Emanuela Del Gado

F1.1: Véronique Trappe, Memory of shear flow in soft jammed material, Room 302 BC, July 31, 2024, 10:30 AM - 12:00 PM

Cessation of flow in simple yield stress fluids results in a complex stress relaxation process that depends on the preceding flow conditions and leads to finite residual stresses. To assess the microscopic origin of this phenomenon, we combine experiments with largescale computer simulations, exploring the behavior of jammed suspensions of soft repulsive particles. A spatiotemporal analysis of microscopic particle motion and local particle configurations reveals two contributions to stress relaxation. One is due to flow induced accumulation of elastic stresses in domains of a given size, which effectively sets the unbalanced stress configurations that trigger correlated dynamics upon flow cessation. This scenario is supported by the observation that the range of spatial correlations of quasi-ballistic displacements obtained upon flow cessation almost exactly mirrors those obtained during flow. The second contribution results from the particle packing that reorganize to minimize the resistance to flow by decreasing the number of locally stiffer configurations. Regaining rigidity upon flow cessation then effectively sets the magnitude of the residual stress. Our findings highlight that flow in yield stress fluids can be seen as a training process during which the material stores information of the flowing state through the development of domains of correlated particle displacements and the reorganization of particle packings optimized to sustain the flow. This encoded memory can then be retrieved in flow cessation experiments.

Shear Banding as a cause of Non-Monotonic Stress Relaxation

Dr. Vanessa Ward, Prof. Suzanne Fielding

F1.2: Vanessa Ward, Shear Banding as a cause of Non-Monotonic Stress Relaxation, Room 302 BC, July 31, 2024, 10:30 AM - 12:00 PM

Soft glassy materials arise widely in nature and technology. These elastoplastic materials respond as soft solids at rest, but flow as liquids under external shear, displaying a shear-induced solid-to-liquid transition. When flow subsequently stops, they recover their solid-like properties. However, due to the liquid-to-solid transition, there is often only a partial relaxation of the internal stresses, which typically follow a monotonic decay towards a residual stress. Residual stresses affect both linear and nonlinear material responses, and are significant for the mechanical properties of a broad range of materials. Soft glassy materials can demonstrate a memory effect, where the residual stresses are a signature of the plastic deformation history of the sample.

Several recent experiments on different systems have shown a remarkable non-monotonic stress relaxation towards a residual stress, following the switch-off of a steady imposed shear flow. In this work, we show that the Soft Glassy Rheology (SGR) model – a mesoscopic approach widely used to interpret experiments on soft matter – can capture this experimentally observed non-monotonic stress relaxation. We offer a mechanistic understanding, showing that non-monotonic stress relaxation can arise under certain conditions when shear banding is present. Accordingly, we argue that this effect may be generic across many different materials.

Electrolubrication in flowing liquid mixtures

Roni Kroll, **Dr. Yoav Tsori**

F2.1: Yoav Tsori, Electrolubrication in flowing liquid mixtures, Room 302 BC, August 1, 2024, 3:30 PM - 5:30 PM

We describe the “electrolubrication” occurring in liquid mixtures confined between charged surfaces. For a mixture of two liquids, the effective viscosity decreases markedly in the presence of a field. The origin of this reduction is field-induced phase separation, leading to the formation of two low-viscosity lubrication layers at the surfaces. The thickness of the lubrication layers depends on the Debye length and the mixture correlation length. These layers facilitate larger strain at a given stress. The effect is strong if the viscosities of the two liquids are sufficiently different, the volume fraction of the less viscous liquid is small, the gap between the surfaces is small, and the applied potential is large. The maximum liquid velocity and flux are increased a factor α. In most liquids, α ∼ 1 – 10, and in mixtures of water and glycerol α ∼ 80 – 100 under relatively small potentials.

References

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Electrolubrication of liquid mixtures between two parallel plates
J. Fluid Mech. (2024).

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Electrolubrication in flowing liquid mixtures
Phys. Fluids 33, 073306 (2023).

Nanodiamond-stabilized Pickering Emulsions: Microstructure and Rheology

Dr Barbara Farias, **Dr. Saad Khan**

F2.2: Saad Khan, Nanodiamond-stabilized Pickering emulsions: Microstructure and rheology, Room 302 BC, August 1, 2024, 3:30 PM - 5:30 PM

Pickering emulsions stabilized by nanodiamonds at various particle concentrations were explored in terms of their stability, morphology, and rheological properties. While the low toxicity, high surface area, inertness and easy functionalization is making nanodiamonds attractive in biomedical applications, its use as a Pickering emulsion stabilizer, which would open new application platforms such as in topical drug delivery, and personal care, remains unexplored. We investigated fundamental aspects related to the effect of ND-OH concentration on the mean droplet size and fraction of water resolved after stabilization. We found that as we increase the particle loading from 0.5 wt.% to 2 wt%, the droplets sizes reduced by two thirds, while the fraction of water resolved depended on both the ND-OH content and network formation in the emulsion. Rheological measurements show that the elasticity of the emulsions follows a power-law behavior with an exponent of 0.75 when plotted as a function of ND-OH concentration, which is lower than the range observed for other Pickering emulsions and colloidal systems (3.0 – 5.6). When scaled with the Laplace pressure, the systems show a power-law behavior with an exponent of 1.1, only slightly higher than what has been observed for concentrated surfactant-stabilized emulsions. However, their yielding profile did not follow a power-law behavior, a phenomenon usually observed in colloidal systems. These results suggest that the nanodiamond-stabilized Pickering emulsions combine aspects of typical colloidal gels and traditional surfactant-stabilized emulsion to form a complex system. In addition, while Pickering emulsions yielding behavior was previously studied, their recovery and its sensitivity to applied shear is a unique feature of this work.

We found that the recovered modulus collapses into a single master curve when the applied stress is scaled by the yield stress for each ND-OH concentration. This master-curve reveals two distinct regimes in terms of recovery with a minimum observed closed to ~ τ/τy ~ 1. With increased applied (breakdown) stresses but below τy, the modulus recovery decreased reaching a minimum (~60% recovery) in the range of the yield stress of the sample (τ/τy ~ 1). With larger applied stresses (τ/τy > 1), the microstructure was broken down to small enough units, where the material is able to reform to the network it initially had. This behavior is similar to what has been observed for colloidal systems composed of nanodiamonds and fumed silica in nonpolar media. For even larger applied stresses, the microstructure rearranged into a more evenly distributed structure with the recovered modulus reaching up to 120% its original value. The scaling of our results with the yield stress and the recovery of the modulus to higher values have not been observed previously and opens the door for future work both in terms of further understanding and exploring the universality of the behavior.

Amplification of vorticity fluctuations and stochastic resonance in inertia-less viscoelastic channel flow

Dr. Victor Steinberg

F2.4: Victor Steinberg, Amplification of vorticity fluctuations and stochastic resonance in inertia-less viscoelastic channel flow, Room 302 BC, August 1, 2024, 3:30 PM - 5:30 PM

Linear elastic instability from laminar to single fastest growing normal mode and weakly nonlinear analysis above the instability onset, Wic, in viscoelastic flows with curved streamlines have been successfully applied both experimentally and theoretically in different flow geometries with good quantitative agreement. Here Wi is the Weissenberg number, the control parameter at Re<<1. However, inertia-less viscoelastic channel flow has been proven linearly stable, similar to Newtonian pipe flow, although elastic instability has recently been observed for finite-sized external perturbations. It is also shown that this elastic instability is a non-normal mode, elastic instability, in contrast to the former flows. Both a mechanism of elastic instability onset and further energy pumping to velocity fluctuations at Wi>Wic are driven by "hoop stress", the latter being elastic stress generated by polymers stretched along curved streamlines, causing radial force to trigger instability. However, it becomes ineffective in channel flow, where elastic instability leads directly to chaotic flow due to finite-size perturbations. At Wi>Wic, three chaotic flow regimes are observed and characterized: transition, elastic turbulence (ET), and drag reduction (DR) accompanied by elastic waves. Furthermore, in all flow regimes, counter-propagating streaks of streamwise velocity fluctuations are found to self-organize into a cyclic self-sustaining process synchronized by the elastic waves. These surprising observations provide evidence that the elastic waves play the key role in the energy transfer from the main flow to the wall-normal fluctuating vortices. We propose and experimentally validate the mechanism of amplification of the wall-normal fluctuating vortices by the elastic, which also provides an explanation for the appearance of DR. Furthermore, universal scaling exponent values of the dependence on Wi-Wic in the transition regime independent of the external perturbation strength, urms/U, and the power-law dependence of Wic on urms/U are obtained. Finally, we report on recently discovered experimentally unexpected stochastic resonances (SRs) just above Wic in a restricted subrange

of the existence of very low intensity elastic waves. Originally, SR is a cooperative resonance effect in a stochastic nonlinear dynamical system subjected to external weak periodic forcing, and has been extensively studied over the past forty years. It is the first observation of SR in chaotic flow, which is much more complicated than stochastic dynamical flow. Here we report the characterization of SRs, their relation to elastic waves, the mechanism of their emergence, and their role in the transition to chaotic flow in a viscoelastic channel flow.

Complex Fluids in Confined Flows

Dr. Sara Hashmi

F2.5: Sara Hashmi, Complex fluids in confined flows, Room 302 BC, August 1, 2024, 3:30 PM - 5:30 PM

Intermittency and clogging of complex fluids flowing through small spaces can occur nearly anywhere: in the porous media of the earth, in industrial flows through hoppers, in water filters, 3D printing nozzles, and in some of the worst instances, in our blood vessels. These examples include flows of colloidal particles, granular material, crosslinking polymers, and multicomponent systems. Despite the differences in the type of complex fluid involved, some aspects of clogging are universal, like its stochastic nature and the importance of the constituent material properties. Understanding the nature of clogging is key to controlling or preventing it, and facilitates improved design of filters, hoppers, and diagnostic tools. Our research explores intermittency, clogging, and flow in both microfluidics and in macroscopic hopper flows. We study granular materials, colloids and emulsions, and crosslinking polymers. In colloidal and granular flows, we vary the softness of the constituent particles and the fraction of soft particles in a mixture. In this way we elucidate how softness controls phenomena like clogging and avalanches. Polymers crosslinking in situ in flow through microchannels also exhibit intermittent dynamics reminiscent of avalanches. In these flows, gelation, deposition, and ablation can occur repeatedly and persistently. Intriguingly, despite the low-Re nature of the flow, we find signatures of chaotic behavior as conditions approach regions of complete failure. This model system might represent situations encountered in polymer flows in 3D printing applications, or, in a greatly simplified way, two of the final steps in the coagulation cascade. \

Glasses, Granular, Jamming

Force signatures of creep in a photoelastic granular medium

Dr. Cacey Bester

G1.3: Cacey Bester, Force signatures of creep in a photoelastic granular medium, Room 301 AB, July 30, 2024, 10:30 AM - 12:00 PM

Creep is the subsurface, slow movement of constituents in a granular packing due to applied stress and the disordered nature of its grain-scale interactions, as in the example of slowly evolving sloped hillsides. We explore creep through experiments of quasi two-dimensional piles of disks that are made from a birefringent material, which allows us to use image acquisition to observe both grain movements and grain-scale force networks. Controlled disturbances to the pile are used to instigate creep events. We investigate the evolution of the force network and particle rearrangements to illuminate signatures of these events. We find that shifts in force chains provide a precursor to larger, avalanche-scale disruptions that can predict where an avalanche will occur. In addition, changes in force chain structure manifested at greater depth than any noticeable particle shifts, suggesting that there is a distinct "flowing" layer that transitions to creep behavior deeper in the pile.

Role of Gravity on Granular Drag: From impacting on to digging into sand

Dr. Kai Huang, Dr. Tivadar Pongo

G1.4: Kai Huang, Role of gravity on granular drag: From impacting on to digging into sand, Room 301 AB, July 30, 2024, 10:30 AM - 12:00 PM

`Nothing is built on stone; all is built on sand, but we must build as if the sand were stone.' Jorge Luis Borges, vividly describes the influence of sand grains on the civilization process happening throughout the past century, and continuing till now. However, do we really understand the mechanism behind granular rigidity and its dependence on the `microscopic' properties of individual sand grains and interactions in-between? In this talk, I will use projectile impact [1] and auger drilling [2] as two examples to illustrate how granular media respond to external intruders with an emphasis on applications in space exploration. In addition, I will also provide a brief overview of how to effectively trace objects embedded in a granular medium with an overview of challenges and opportunities associated [3].

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Impact of Chain Connectivity and Covalent Bonding on the Local Glass Transition Temperature of Polymers

Dr. Connie Roth, James Merrill

G2.1: Connie Roth, Impact of chain connectivity and covalent bonding on the local glass transition temperature of polymers, Room 301 AB, August 1, 2024, 3:30 PM - 5:30 PM

How exactly chain connectivity and covalent bonding in polymers alter the glass transition is still an unsolved question. Polymers exhibit much of the same glass phenomenon as small molecules and other glass forming systems such that theoretical efforts can frequently treat the polymer as

an effective system of disconnected spheres. The well-known saturation of the glass transition temperature Tg with increasing chain length is best understood in terms of how chain flexibility sets the size of the effective average conformational unit for cooperative motion and activation energy for alpha-relaxation events. Free chain ends are more flexible, compared with monomer segments within the chain, such that numerous free chain ends reduce the average size of the effective conformational unit. In contrast, numerous advanced applications involve polymers with tethered chain ends: ionomers, vitrimers, and chains grafted to nanoparticles. These tethered chain ends will have hindered mobility that would be expected to increase the size of the effective conformational unit, thereby slowing dynamics and increasing Tg. We are experimentally interrogating the impact that chain tethering and covalent bonding has on the local glass transition by using a simplified sample geometry with planar interface, where pyrene fluorescence is used to measure the local Tg of polystyrene (PS) matrix chains intermixed with PS chains grafted to silica substrates. The grafting density is kept low such that the chains still retain their ideal gaussian conformations. We find that the covalent bonding of a small number of chain ends to the silica substrate significantly increases the local Tg of the matrix chains by ≈45 K above the bulk value for PS
suggesting a slowing of the segmental dynamics by at least ~10 orders of magnitude [ACS Macro Letters 12, 1-7 (2023)]. The silica substrate is a neutral interface for PS that does not independently alter Tg without chain grafting, meaning this effect is entirely topological in origin resulting from the covalent bond to the substrate interface. In addition, by assembling specific multilayer sample geometries, we map the profile in local Tg(z) as a function of position away from the substrate interface as it decays down to the bulk value at distances sufficiently far from the interface. Interestingly, this strong perturbation to the local Tg extends far beyond, 6 to 10 times, the extent of the grafted chains. Possible causes for this long-ranged phenomenon will be discussed.

Anomalous behavior of ultrastable glasses and the implications for the glass “transition”

Dr. Gregory Mckenna, Dr. Dejie Kong, Dr. Amer El Banna, Dr. Yan Meng

G2.2: Gregory McKenna, Anomalous behavior of ultrastable glasses and the implications for the glass “transition”, Room 301 AB, August 1, 2024, 3:30 PM - 5:30 PM

For over a century the difficulty of achieving equilibrium in normal glasses has created a conundrum for the physical science community. Two major behaviors have been used to construct the modern views of the glassy state. First, the viscosity of a glass-forming liquid can vary by upwards of 14 orders of magnitude in a narrow temperature range as described by the Vogel-Fulcher(VF) equation in which the equilibrium viscosity extrapolates to infinity at a finite temperature T^0, i.e we see “super-Arrhenius” behavior. Second, extrapolation to low temperatures of equilibrium entropy data seems to give violations of Nernst’s 3rd law at a temperature now referred to as the Kauzmann temperature Tk. These temperatures are often close to one another, though not always. The combination has led to various explanations, many of which are based upon the concept of an “ideal” glass transition that keeps the third law from being violated and provides a link between the thermodynamics and the temperature dependence of the viscosity giving an apparent divergence at $T^0 \approx Tk$. The difficulty in testing such models is that obtaining equilibrium behavior at temperatures much below the conventional glass transition temperature is not possible because of the rapidly decreasing molecular mobility.

To finesse the long relaxation times, we seek other means to study “ultra-stable” glasses, i.e., those with fictive temperatures Tf very far below the glass transition temperature Tg for which the relaxation time is 100 s. We have created through vapor deposition (VPD) of amorphous perfluoropolymers) and discovered ancient ambers that have fictive temperatures Tf far below the Tg. In the VPD polymer we determined a $Tf<T^0$ by both rapid chip calorimetry and atomic force microscope (AFM) dilatometry. In the case of ancient ambers, we found a 50 million-year-old sample that has a value of $Tf<T^0$ and for which we were able to carry out dilatometry and dynamic mechanical measurements to estimate the dynamics at close to the equilibrium volume of the amber as much as 190 K below the Tg. The results provide strong evidence that the glass transition event is a liquid state phenomenon that is not related to crystallization, thus confirming the Kauzmann view that “…it is operationally meaningless to extrapolate the entropy, energy, and specific volume curves below that temperature…” Though Kauzmann did not foresee a solution to the paradox, per se, we now have evidence from deep glassy state materials that cannot crystallize and form glasses, thus challenging the view that holds the Kauzmann temperature to be fundamental to glass formation. Rather, glass-formation is a liquid state property that is not related to the Kauzmann paradox and possible crystallizable states in a material. We also show evidence that the deep glassy state dynamic response in the nominal equilibrium condition where Ttest=Tf is neither Arrhenius nor super-Arrhenius, rather it is exponential in temperature, i.e., $\tau=\tau_1 \exp(XT)$ over at least 22 orders of magnitude of relaxation time τ.

Acknowledgements

The authors gratefully acknowledge the National Science Foundation under Grants DMR-2022732 and DMR-1610495.

Emergence of preferential flow paths in transport of emulsions in porous media

Dr. Michael Izaguirre, **Dr. Shima Parsa**

G2.5: Shima Parsa, Emergence of preferential flow paths in transport of emulsions in porous media, Room 301 AB, August 1, 2024, 3:30 PM - 5:30 PM

We investigate the dynamics of emulsions within a two-dimensional porous medium using an integrated experimental approach that combines pore-level dynamics of single emulsions and bulk transport properties of the medium. The dynamics of emulsions are highly intermittent despite a small average velocity over the trajectory of an individual emulsion. At low concentrations, emulsions predominantly flow through pores with higher local velocities including pores smaller than the size of emulsion droplets, leading to trapping of emulsions and a decrease in medium porosity. Preferential pathways for the emulsions emerge within the medium once the porosity of the medium decreases significantly.

Interfaces, Surfaces, Membranes

Investigating Viscoelastic Behavior of Lipid Monolayers in Spontaneous Oscillation of Surface Tension Induced by the Marangoni Effect.

Dr. Yohko Yano

I1.2: Yohko Yano, Investigating viscoelastic behavior of lipid monolayers in spontaneous oscillation of surface tension induced by the Marangoni effect, Room 306 BC, July 30, 2024, 3:30 PM - 5:30 PM

Biological membranes are formed by the self-assembly of lipids in aqueous solutions. Consequently, they exhibit fluidity with lipid molecules and proteins diffusing laterally. This fluidity, coupled with structural rigidity, may seem contradictory. Therefore, visualizing the membrane's structure in a flowing state is crucial for understanding its behavior.

The Marangoni effect is a phenomenon that introduces a non-equilibrium state to condensed matter. Marangoni convection, a type of liquid flow, arises from spatial surface tension gradients caused by temperature and composition differences. When a small amount of surfactant is added to water, surfactant droplets can move on the water's surface, a phenomenon known as "Marangoni convection." This occurs as the surface tension decreases locally where the surfactant is added, causing a flow on the water's surface.
On the other hand, when surfactants are introduced into water, the phenomenon of "spontaneous oscillation of surface tension (hereafter referred to as SOS)", wherein the surface tension periodically decreases and increases, can be observed. This phenomenon was extensively researched around the year 2000. It was found that surfactants in water repeatedly generate Marangoni convection on the water surface by spreading onto it and then dissolving back into the water, inducing oscillation of surface tension. A numerical study revealed that the characteristics of the oscillation are strongly dependent on the system’s geometry and surfactant species. Furthermore, it was also found that SOS is more likely to occur when a surfactant, which is insoluble in water, is applied to the water surface in advance. However, the reason why this is more likely to occur remained a mystery.

Previously, we have examined the structure and dynamics of an insoluble surfactant monolayer under SOS at the molecular level using X-ray reflectometry[1]. We have repeatedly observed that surfactant molecules at the air-water interface become regularly oriented normal to the surface synchronously with changes in surface tension. The orientational change is driven by the periodically generated Marangoni flow, which pushes the insoluble surfactant outward. In this system, we discovered that two types of collective motion interact to produce rhythmic behavior.

Building on this research, we derive further insights from SOS profiles resembling damping oscillations. We aim to discuss the viscoelastic behavior of insoluble surfactant monolayers and analyze in detail the elastic motion of a lipid monolayer under Marangoni convection, towards understanding the behavior of biological membranes exhibiting both structural rigidity and high lateral fluidity.

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Porous Thin Films Facilitate Rapid Evaporation of Water Droplets

Dr. William Ducker, Mohsen Hosseini

I1.3: William Ducker, Porous thin films facilitate rapid evaporation of water droplets, Room 306 BC, July 30, 2024, 3:30 PM - 5:30 PM

Small liquid droplets form spherical caps on impermeable surfaces and therefore experience a low rate of evaporation. Low evaporation is important in applications where the droplet is being used to deliver a solute and the solvent needs to be removed, or where the droplets are used for cooling. Here we describe how application of a thin porous wetting coating can be used to speed evaporation. The key is for the coating to be thin, which forces the liquid to spread rapidly near the vapor–liquid interface. We examined coatings that are about 30–100 µm thick, fabricated from hydrophilic silica or glass, with pore sizes in the range 3–8 µm. These coatings improve the rate of evaporation of water by a factor of about 8 compared to an impermeable solid, and a factor of 37 compared to a bulk porous material of the same chemistry at the same temperature. In this work, we describe how the evaporation varies as a function of temperature, humidity, size and polydispersity of the pores, and contact angle. Results are compared to Hu and Larson's equation for impermeable solid and to a modified version for permeable surfaces. We also find that transport within the pores is important for evaporation and describe the coffee ring effect in these systems.

Thin films under an electric field

Dr. Di Jin, Prof. Jacob Klein, Dr. Yu Zhang, Dr. Nir Kampf, Prof. Liraz Chai, Prof. Yongyun Hwang, Prof. Ran Tivony

I1.5 Di Jin, Thin films under an electric field, Room 306 BC, July 30, 2024, 3:30 PM - 5:30 PM

Biological thin films such as lipid membranes and boundary water thin films are nano systems that are ubiquitous in biological systems. They play key roles in various physiological processes, such as hydration lubrication at asperity contacts between cartilage surfaces, the hemifusion processes with drug-delivery vesicles, or the interaction between colloidal particles that are often heterogeneously charged (if surfactant coated). Many of these processes are localized, either at micro-scale asperities as in the scenario of cartilage lubrication or initiated through a nano-scale contact point as in the case of hemifusion. In such a scale, within the complex biological environments, localized instantaneous perturbation often arises. Transverse electric fields are such a case, which arise from localized ion gradient. As revealed by our recent studies, transverse electric fields impose nontrivial effects on the macroscopic properties on lipid membranes as well as liquid thin films.

Experimentally, we have observed and characterized the dependence of macroscopic properties of thin films on transverse electric fields of order 0.1 V/nm using a state-of-art technique—surface force balance. It allowed us to quantify the "viscoelectric effect" –the change of viscosity in presence of an electric field of nano-confined ultra-pure water thin films, which has been a challenge experimentally in the past 80 years. We also measured the change in friction coefficients between lipid bilayers when turning on the electric field and discovered a significant increase up to two orders of magnitude in the friction coefficients. The threshold pressures to the hemifusion of lipid membranes, a metric for the robustness of the bilayer-stack against load, also reduces in presence of an electric field. These observations suggest that electric fields provide as a platform for in-situ manipulation of the mechanical properties of lipid membranes.

Theoretically, we interpret these results using equilibrium and non-equilibrium all-atom and coarse-grained molecular dynamics simulations, which allow us to quantitatively relate the measured macroscopic properties to the molecular structural changes of the thin films. We also extend from the established theoretical framework to predict thin film properties. Specifically, we seek to systematically investigate the correlation of lipid membranes' compositions to their mechanical properties, and by using cutting-edge techniques such as machine learning, we expect to predict and design lipid membranes with macroscopic properties tuned for biomedical applications.

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Deposition of Complex Colloidal Assemblies from Drop Evaporation

Dr. Jacopo Vialetto, Théophile Gaichies, Dr. Sergii Rudiuk, Dr. Mathieu Morel, Prof. Dr. Damien Baigl

I1.6 Jacopo Vialetto, Deposition of complex colloidal assemblies from drop evaporation, Room 306 BC, July 30, 2024, 3:30 PM - 5:30 PM

Microfabrication strategies designed to produce ordered arrangements of colloidal particles on solid supports are of great interest in materials science and technology due to their wide range of applications, from colloidal lithography, to plasmonic and biomimetic surfaces or tags for anti-counterfeiting and goods identification.1 Existing methods allow excellent control over particle organization yet share various degrees of complexity in terms of equipment or chemicals required, hampering their straightforward implementation.2

In this talk, I will present a drastically simplified methodology to achieve ordered particle deposition, consisting in adding micromolar amounts of cationic surfactant to a colloidal suspension drop and let it evaporate in an upside-down configuration.3 In previous works we exploited additives4,5 (such as positively charged surfactants) to promote the spontaneous adsorption of colloids from their dispersion in water to the fluid interface, and control their assembly into crystalline or amorphous structures.

In evaporating hanging drops deposited on solid substrates, we show that promoting adsorption of particles to the air/water interface enables their 2D confinement and induces their assembly into ordered crystals. These assemblies are then transferred on the substrate upon solvent evaporation, producing highly ordered structures displaying vivid, orientation-dependent structural colors. We demonstrate the versatility of the method with various kinds of particles (silica, polystyrene) with diameters in the range 300 nm – 5 µm on different target substrates (polystyrene, polydimethylsiloxane, glass). The size and morphology of the deposit, from single-crystals to multi-crystalline patches, can be controlled by the curvature of the drop and the total number of particles, while more complex colloidal structures, like colloidal crystal “alloys” with Moiré patterns or “irises” can be achieved by successive depositions, co-crystallization or double flipping, demonstrating its potential practicality for a variety of processes.3

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Investigating Viscoelastic Behavior of Lipid Monolayers in Spontaneous Oscillation of Surface

Pearling, buckling, and wrinkling instabilities of multicomponent vesicle threads

Dr. Vivek Narsimhan, Anirudh Venkatesh, Aman Bhargava

I2.1: Vivek Narsimhan, Pearling, buckling, and wrinkling instabilities of multicomponent vesicle threads, Room 306 BC, July 31, 2024, 3:30 PM - 5:30 PM

Vesicles are sacs of fluid enclosed by a lipid bilayer membrane. In nature, vesicles play a key role in molecular trafficking and compartmentalization in cells, while in industry vesicles are commonly used in drug delivery and consumer products. Vesicles behave fundamentally differently than liquid droplets in flow due to the elastic membrane separating the inner and outer compartments. Moreover, multi-component lipid membranes give rise to phase separation, which plays a key role in biological processes such as vesicle budding and fusion in cells. Despite recent progress, we lack a complete understanding of how flow alters thermodynamics and kinetics of membrane phase separation, and how such phase behavior in turn alters the deformation and instabilities (e.g., breakup) of vesicles in flow. Understanding these behaviors will improve our ability to process such materials for the industrial applications mentioned above, and will provide crucial understanding on how cell membranes behave in non-equilibrium situations.

In this talk, we will discuss our recent work characterizing an instability found on a cylindrical vesicle thread, similar to the beads-on-thread structure found in the Rayleigh-Plateau instability for liquid jets. We perform a linear stability analysis on a cylindrical thread containing multiple phospholipids that can phase separate. The lipids have different bending rigidities, and line tension between phase-separated domains. We solve the Stokes equations along with the Cahn-Hilliard equations to develop the linearized dynamic equations governing the vesicle shape and surface concentration fields. We show that multicomponent vesicles can undergo beads-on-string structures (e.g., pearling) similar to a Rayleigh Plateau instability for liquid treads. However, these vesicles can also exhibit buckling and wrinkling instabilities under tension, which is a significantly different result from studies on single component vesicles as well as liquid jets. This behavior arises due to the competition between the free energies of phase separation, line tension, and bending for this multi-phospholipid system. We supplement our results with an energy analysis that shows the sources for these instabilities, and show that the trends qualitatively match recent experiments.

Polarized resonant soft X-ray scattering measurements in polymer-grafted nanoparticles

Dr. Dean Delongchamp

I2.2: Dean DeLongchamp, Polarized resonant soft X-ray scattering measurements in polymer-grafted nanoparticles, Room 306 BC, July 31, 2024, 3:30 PM - 5:30 PM

Orientation and conformation in nanoscale amorphous regions often dominate the properties of soft materials. Robust correlations between structure in these amorphous regions and important properties are not well developed due to a lack of measurements with high spatial resolution and a sensitivity to molecular orientation. For example, radial polymer chain orientation with significant spatial variation is typically predicted in computational models of polymer-grafted nanoparticles (PGNs), but it has not been validated due to insufficient measurements. I will describe our approach to solving this issue using polarized resonant soft X-ray scattering (P-RSoXS), which combines principles of soft X-ray spectroscopy, small-angle scattering, and data fusion with real-space imaging to produce a molecular scale structure measurement for soft materials.

I will focus on the P-RSoXS of polymer-grafted nanoparticles (PGNs). The most unique structural motif of PGNs is the high-density region in the corona where polymer chains are "stretched" under significant confinement. We apply our approach to measure the orientation of polystyrene (PS) chains grafted to gold nanoparticles. In conjunction with a pattern simulation approach, we measure the thickness of the anisotropic region of the corona and the extent of chain orientation within it. Radial chain orientation is observed that decays in magnitude away from the particle, and differences in this nanoscale orientation landscape are observed between particles of different graft density. The shape of this nanoscale orientation landscape can be reconciled with recent computational predictions, and quantitative agreement is possible with data fusion that incorporates experimental data from other measurements, coarse-grain simulation results, and atomistic conformation information. These results demonstrate the power of P-RSoXS to quantify and discover orientational aspects of structure in PGN systems and illustrate a framework that can be applied broadly to semicrystalline or amorphous polymers with a range of chemistries and chemical heterogeneity.

AFM force clamping and extension spectroscopy studies of velvet worm slime proteins at different pH and buffer conditions

Dr. Yendry Corrales Ureña, Reinaldo Pereira, Dr José Vega-Baudrit

I2.3: Yendry Corrales Urena, AFM force clamping and extension spectroscopy studies of velvet worm slime proteins at different pH and buffer conditions, Room 306 BC, July 31, 2024, 3:30 PM - 5:30 PM

Velvet worms secrete a white, adhesive slime onto their prey, effectively immobilizing it. This slime undergoes rapid hardening upon mechanical agitation, further ensnaring struggling prey. Similar to viscous egg yolk, it transforms into a robust solid resembling nylon within seconds.

Before mechanical stimulation, the expelled slime forms nanoglobules, which, upon mechanical agitation, transition into crystalline fibers. Upon redissolution, they can revert to nanoglobules.

Understanding the chemo-mechanoresponsive properties of velvet worm slime proteins provides insights for developing recyclable, eco-friendly biopolymers.

Previous studies have shown that velvet worm slime contains crystalline microparticles (carbonates and phosphates), silicates, dissolved sodium chloride, proteins, lipids, and carbohydrates. Shear stress induces rapid dissolution of discharged microparticles, raising pH and ionic strength, initiating gelation, and influencing phase separation of the slime. It's hypothesized that salt dissolution affects protein unfolding and protein-protein interactions. To investigate the impact of salts and pH, stable adsorbed films of velvet worm slime proteins were prepared on a silicon oxide substrate, confirmed by contact angle and XPS. Unfolding behavior of interfacial proteins was examined under varying pH, buffer conditions, and with a DTT reducing agent, utilizing atomic force clamp and force extension spectroscopy techniques. The velvet worm slime is formed by heterogeneous polyproteins, linked by disulfide bridges, comprising protein units with varying stiffness, correlated with β-crystallites and disordered region structures. Following external mechanical stimulation, most crystalline domains unfold, leading to fiber formation.

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Avalanches and extreme value statistics of a moving contact line

Dr. Penger Tong, Dr Caishan Yan, Prof. Dongshi Guan, Dr Yin Wang, Prof. Pik-Yin Lai, Prof. Hsuan-Yi Chen

I2.3.1: Penger Tong, Avalanches and extreme value statistics of a moving contact line, July 31, 2024, 4:15 PM - 4:30 PM

Avalanche dynamics is widely observed in various out-of-equilibrium disordered systems, ranging from the seismic activities of tectonic plates to the plastic deformation of crystalline materials and the proceeding of a domain wall in the ferromagnets. As a yield response to a smoothly varying external force, the avalanche dynamics manifests itself as a unique collective behavior of multiple defects in a disordered system, where the depinning from a single defect triggers a large-scale avalanche involving many nearby defects. Among the systems that exhibit avalanche behaviors, the moving contact line (CL) between a liquid interface and a solid substrate, which is often pinned by the physical roughness and/or chemical inhomogeneity on the solid surface, is an ideal system for the study of the avalanche dynamics. This is because the moving CL is a one-dimensional system with a better geometry for a stringent test of the theory on avalanche dynamics. In this talk, we present our recent experimental efforts in developing a mesoscale "long needle" AFM (atomic force microscope) to study the stick-slip dynamics of a moving three-phase contact line [1]. From a large volume of individual avalanche events collected over a wide range of sampling rates and long durations, we established, for the first time, three statistical laws of the avalanche dynamics at the critical state, in the forms of the probability density functions (PDFs) of the slip length \Delta z_slip, the maximal force F_c needed to trigger the avalanches and the local force gradient k' of the pinning force field. This work bridges the gap between the microscopic behavior of individual depinning events and the macroscopic laws of contact angle hysteresis and thus represents a breakthrough in our understanding of the avalanche dynamics of a moving CL.

*This work was supported in part by the Research Grants Council of Hong Kong SAR and by the Ministry of Science and Technology of Taiwan.

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Direct measurement of the hydro-capillary lift force acting on sphere moving along liquid interfaces

Dr. Abdelhamid Maali, Mr. Hao Zhang

I2.4: Abdelhamid Maali, Direct measurement of the hydro-capillary lift force acting on sphere moving along liquid interfaces, Room 306 BC, July 31, 2024, 3:30 PM - 5:30 PM

I will present a first direct measurement of the lift force acting on a particle moving in a viscous fluid along the liquid interface that separates two liquids. The force is due to the hydro-capillary coupling between the viscous flow induced by the movement of the particle and the capillary deformation of the liquid interface. In these experiments, we used the device we developed previously to study soft solids [1]. We measured the hydro-capillary lift force as a function of the distance between the sphere and the interface between the liquids [2]. The force increases as the distance between the sphere and the interface decreases and saturation is observed at a very small spacing distance[2]. We studied various liquid interfaces, sliding speeds and two different sphere radii. The experimental results are in excellent agreement with the theoretical model and numerical calculations developed within the framework of the theory of soft lubrication [2].

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Effect of Surface Chemistry on Conformation and Aggregation of Amyloidogenic Peptides

Dr. David Cheung

I2.5: David Cheung, Effect of surface chemistry on conformation and aggregation of amyloid peptides, Room 306 BC, July 31, 2024, 3:30 PM - 5:30 PM

The formation of dense, linear arrays (fibrils) by biomolecules is the hallmark of many degenerative diseases, such as Alzheimer's and type-2 diabetes. Protein fibrils have also attracted interest as building blocks for new materials. It has long been recognised that surfaces can affect the fibrillation process, with the effect of surfaces dependent on both surface chemistry and protein structure. As the behaviour of proteins on surfaces depends on the complex interplay of many different effects (e.g. protein sequence, surface physiochemical properties, protein mobility) and understanding this requires detailed microscopic information. While this is challenging to investigate experimentally, molecular dynamics simulations provide direct insight into the microscopic realm and so are ideally suited to investigate this.

In this presentation we will discuss recent simulation results investigating the behaviour of archetypal fibril forming proteins, amyloid-beta [1,2] and human islet amyloid polypeptide [3], on surfaces. In both cases hydrophobic surfaces reduce the number of conformations adopted by these proteins and favour the formation of conformations that are unlike those found in bulk solution. On hydrophobic surfaces they also aggregate into structures that unlike those found in bulk solution. Understanding the relationship between surface properties and protein conformation and aggregation can help us decipher the mechanism of protein fibrillation on both naturally-occurring (e.g. cell membrane) and synthetic surfaces.

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Liquid Crystals

Moiré effect enables versatile design of topological defects in nematic liquid crystals

Dr. Xinyu Wang, Prof. Jinghua Jiang, Dr. Juan Chen, Ms. Zhawure Asilehan, Mr. Wentao Tang, Prof. Chenhui Peng, Prof. Rui Zhang

L1.3: Xinyu Wang, Moiré effect enables versatile design of topological defects in nematic liquid crystals, Room 305 AB, July 31, 2024, 10:30 AM - 12:00 PM

Recent advances in surface-patterning techniques of liquid crystals have enabled the precise creation of topological defects, which promise a variety of emergent applications. However, the manipulation and application of these defects remain limited. Here, we harness the moiré effect to engineer topological defects in patterned nematic liquid crystal cells. Specifically, we combine simulation and experiment to examine a nematic cell confined between two substrates of periodic surface anchoring patterns; by rotating one surface against the other, we observe a rich variety of highly tunable, novel topological defects. These defects are shown to guide the three-dimensional self-assembly of colloids, which can conversely impact defects by preventing the self-annihilation of loop-defects through jamming. Finally, we demonstrate that certain nematic moiré cells can engender arbitrary shapes represented by defect regions. As such, the proposed simple twist method enables the design and tuning of mesoscopic structures in liquid crystals, facilitating applications including defect-directed self-assembly, material transport, micro-reactors, photonic devices, and anti-counterfeiting materials.

Functional soft materials from the directed self-assembly of liquid crystals

Dr. Kushal Bagchi, Dr. Tadej Emersic, Dr. Juan de Pablo, Dr. Paul Nealey

L1.4: Kushal Bagchi, Functional soft materials from the directed self-assembly of liquid crystals, Room 305 AB, July 31, 2024, 10:30 AM - 12:00 PM

Liquid crystals (LCs) combine the structural anisotropy of crystalline solids with the fluidity of liquids. While controlling the structure of simple liquid crystalline phases, such as nematics is well-understood, alignment of complex liquid crystals such as blue-phases and discotics is more challenging. We present here two methods to align complex liquid crystalline phases, namely chemo- and grapho-epitaxy. These techniques involve making chemical and topographical patterns using nanolithography. Chemo and grapho-epitaxy are well established techniques in the field of block copolymers. We present here extensions of these techniques for assembly of liquid crystalline phases. We demonstrate how directed self-assembly of blue-phase and discotic liquid crystals can be used to prepare polymeric photonic single crystals (1,2) and biaxially textured crystals of organic semiconductors (3), respectively.

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Interparticle friction in sheared, dense suspensions of rod-like particles: Simulations

Mr. Christopher Quinones, Mr. Peter Olmsted

L2.1: Christopher Quinones, Interparticle friction in sheared, dense suspensions of rod-like particles: Simulations, Room 305 AB, August 1, 2024, 10:30 AM - 12:00 PM

The complex interplay between nematic order, frictional contacts, and flow in dense suspensions of rigid rods has yet to be fully elucidated. Here, we present simulations of suspensions of non-Brownian hard sphere chains under shear, with Coulomb contact friction and lubrication between particles. A new model adapting the Cundall-Strack friction model for spheres to rod-like sphere chains is derived. We measure rod-to-rod contacts at varying nematic order, volume fraction, and aspect ratio; and investigate a modified form of Philipse's random contact equation. We also make connection to the Wyart & Cates model for spheres by modelling the viscosity as a function of a jamming fraction and nematic order.

Chiral doping of a colloidal liquid crystal phase in cellulose nanocrystal suspensions

Dr. Thomas Parton, Mr Kevin Ballu, Dr Richard Parker, Dr Bruno Frka-Petesic, Professor Silvia Vignolini

L2.2: Thomas Parton, Chiral doping of a colloidal liquid crystal phase in cellulose nanocrystal suspensions, Room 305 AB, August 1, 2024, 10:30 AM - 12:00 PM

Cellulose nanocrystals (CNCs) are bio-sourced rod-like nanoparticles that form a lyotropic cholesteric mesophase in colloidal suspension. This helicoidal arrangement of CNCs can be preserved upon drying to create structurally colored films, which have attracted growing interest as a sustainable source of coloration. However, despite intensive research on CNCs over the past few decades, the origin of their mesophase chirality is unclear. While the underlying chiral crystalline structure of naturally-derived cellulose is widely believed to play a crucial role, most CNCs are not strongly twisted, and samples exhibit considerable polydispersity in both particle size and shape.

In an initial study, we performed advanced statistical analysis of CNC morphology, based on transmission electron microscopy (TEM) and atomic force microscopy (AFM) images, while gradually tuning their size and shape using high-intensity ultrasound. This analysis allowed quantitative relationships between colloidal liquid crystalline behavior in suspension and the morphological distribution of individual CNC particles to be established. In particular, we showed that the cholesteric mesophase is highly sensitive to the presence of “bundles” (clusters of laterally-bound cellulose crystallites) in the suspension, as indicated by the divergence in cholesteric pitch as the bundles are broken apart by ultrasonication. These CNC bundles thus act as colloidal chiral dopants, analogous to those used in molecular liquid crystal systems, providing the missing link in the hierarchical transfer of chirality from the molecular to the colloidal scale.

We then compared common ways to induce aggregation in CNC suspensions (e.g., centrifugation or excess ionic strength). This investigation revealed that the formation pathway significantly affects the morphology of the bundles and thus their effectiveness as chiral dopants. These findings demonstrate that the "making" and "breaking" of crystallite bundles offers a facile way to tailor the self-assembly behavior of CNC suspensions.

Parton, T. G. et al (2022). Nat. Commun, 13, 2657. DOI: 10.1038/s41467-022-30226-6
Ballu, K. et al (2024) arxiv:2404.04171

Networks & Gels

Highly polydisperse colloidal gels

Dr. Eric Weeks, Ben Lonial

N1.1: Eric Weeks, Highly polydisperse colloidal gels, Room 301 AB, July 30, 2024, 3:30 PM - 5:30 PM

We experimentally study colloidal gels composed of highly polydisperse particles. Much prior work has focused on gels composed of mono- or bi-disperse particles as the backbone, perhaps with a third species acting as a depletant. Our samples are made from highly polydisperse particles (the ratio of sizes between largest and smallest particle being approximately 10:1) suspended in a density matched organic solvent, which spontaneously gel due to the van der Waals force. We study the effect polydispersity has on the dynamics and structures that form. Larger particles are more sensitive to the depletion force, and the depletion force acting on a small particle in proximity to a large particle is larger still (an effect similar to the enhanced depletion for particles near a wall). Thus, large particles act like nodes around which clusters of smaller particles will congregate. Our work demonstrates the role that polydispersity plays in the structure of colloidal gels.

A universal strategy for decoupling stiffness and extensibility of polymer networks

Dr. Liheng Cai

N1.2: Liheng Cai, A universal strategy for decoupling stiffness and extensibility of polymer networks, Room 301 AB, July 30, 2024, 3:30 PM - 5:30 PM

Polymer networks represent one of the most ubiquitous materials in modern society. They are essential components in automobiles and home appliances and are increasingly important in healthcare, wearable electronics, and soft robots. Since the invention of polymer networks in the 19th century (e.g., crosslinked natural rubber by Goodyear), it has been a dogma that stiffer networks are less stretchable, a trade-off inherent to the molecular nature of polymer network strands. Here, we report a universal strategy for decoupling the stiffness and extensibility of single-network elastomers. Instead of using linear polymers as network strands, we use foldable bottlebrush polymers, which feature a collapsed backbone grafted with many linear side chains. Upon elongation, the collapsed backbone unfolds to release stored length, enabling remarkable extensibility. By contrast, the network elastic modulus is inversely proportional to the network strand mass and is determined by the side chains. We validate this concept by creating a series of unentangled single-network elastomers with nearly constant Young's modulus (30 kPa) while increasing tensile breaking strain by 40-fold, from 20% to 800%. We show that this strategy applies to networks of different polymer species and topologies. Our discovery opens an avenue for developing polymer networks with extraordinary mechanical properties.

Characterizing dynamic heterogeneities and properties of degrading polymer networks

Dr. Olga Kuksenok, Mrs. Zafrin Ferdous Mira, Ms. Rupali Sharma, Dr. Vaibhav Palkar

N1.4: Olga Kuksenok, Characterizing dynamic heterogeneities and properties of degrading polymer networks, Room 301 AB, July 30, 2024, 3:30 PM - 5:30 PM

Understanding degradation of polymer networks is critical for a range of applications. In particular, photo-controlled bond scission permits localized and dynamic control of gel properties. We focus on hydrogels formed by end-linking of four-arm polyethylene glycol precursors with photolabile groups and characterize structural and dynamical heterogeneities in these gels during photodegradation. We use our recently developed dissipative particle dynamics framework that captures bond scission and diffusion of degraded fragments at the mesoscale. Breaking elastically active network strands during degradation leads to a decrease in elastic modulus and structural and dynamic heterogeneities. We quantify the elastic modulus of degrading gels as a function of the proximity to the reverse gel point. Our approach allows us to model behavior of the degrading network without making a-priori assumptions typically made in continuum theories regarding network deformations.

To quantify spatiotemporal fluctuations in local dynamic behavior, we calculate the self-part of van-Hove correlation function for the network junctions and reactive end groups. We demonstrate strong deviations from the Gaussian behavior during the degradation and quantify variations in the non-Gaussian parameter with the proximity to the reverse gel point. We show that the peak in the non-Gaussian parameter is observed significantly earlier than the reserve gel point. Our approach allows one to quantify mechanical properties of degrading hydrogel material and correlate structural and dynamic heterogeneities in these systems. Our results could provide guidelines for future design of reactive materials with dynamically controlled mechanical properties.

This work was supported by the National Science Foundation under NSF award no. 2110309

Rapid, non-linear diffusio-phoretic swelling of chemically responsive hydrogels

Dr. C. Nadir Kaplan, Dr. Peter Korevaar, Chinmay Katke

N1.5: C. Nadir Kaplan, Rapid, non-linear diffusio-phoretic swelling of chemically responsive hydrogels, Room 301 AB, July 30, 2024, 3:30 PM - 5:30 PM

Poly-acrylic acid hydrogels can store chemical signals, such as copper or calcium divalent ions, and release them upon adding acid. While the hydrogel interface is fully permeable to the released ions and acid, interactions between the free ions and the gel polymer network lead to a diffusio-phoretic gel actuation at a rate faster than the characteristic poroelastic deformation rate. We have recently shown this effect theoretically and experimentally by focusing on linear deformations [1]. However, in light of potential applications such as hydrogel-based soft robotics and drug delivery, comprehending large diffusio-phoretic deformations in hydrogels is imperative for increased strain rates and power output. I will present a continuum nonlinear poroelastic theory to model large diffusio-phoretic gel swelling, induced by high acid concentrations or by steady acid flow at arbitrary rates. The theory incorporates the interplay between nonlinear poroelasticity, variable hydrogel permeability, and the diffusio-phoretic swelling along with the transport dynamics of chemical agents within the gel.

[1] C. Katke, P. A. Korevaar, C. N. Kaplan, Phys. Rev. Lett. in press (2024).
https://doi.org/10.48550/arXiv.2309.05165

Dynamical and structural behaviour of PNIPAM based microgels

Dr Roberta Angelini, Dr Valentina Nigro, Dr Silvia Franco, Dr Elena Buratti, **Dr Barbara Ruzicka**

N2.1: Barbara Ruzicka, Dynamical and structural behaviour of PNIPAM based microgels, Room 301 AB, August 2, 2024, 10:30 AM - 12:00 PM

The novel class of responsive microgels has recently become very popular since their smart responsivity to external stimuli makes them very attractive for industrial applications and excellent model systems for exploring the exotic behaviours emerging in soft colloids since their softness allows to explore high density states well beyond random close packing.

In the last years we have deeply investigated a dual responsive Interpenetrated Polymer Newtork (IPN) microgel composed of poly(N-isopropylacrylamide) (PNIPAM), a temperature sensitive polymer, and poly(acrylic acid) (PAAc), a pH sensitive polymer [1]. The system, with multi-stimuli responsiveness and rationally designed properties, can be finely controlled through different experimental parameters. PNIPAM-PAAc IPN microgels is investigated as a function of sample concentration, temperature and PAAC content that permit to tune ad hoc the formation of arrested states.

Combining the dynamical (through Dynamical Light Scattering and X-ray Photon Correlation Spectroscopy) [2] and structural (through Small Angle X-ray Scattering and Small Angle Neutron Scattering) behaviour, together with rheology [3], we distinguish three different states: liquid, glass and jammed.. The possible molecular mechanisms driving the formation of these states are discussed and a preliminary T- Cw phase diagram is drawn [4].

[1] V. Nigro, R. Angelini, M. Bertoldo, E. Buratti, S. Franco and B. Ruzicka, Plymers 13, 1353 (2021).
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[4] S Franco, E Buratti, V Nigro, M Bertoldo, B Ruzicka, R Angelini, Polymers 14 (1), 115 (2022).

Cellulose microfibrils: Properties and application in complex fluids and soft materials

Dr. Krassimir Velikov

N2.2: Krassimir Velikov, Cellulose microfibrils: Properties and application in complex fluids and soft materials, Room 301 AB, August 2, 2024, 10:30 AM - 12:00 PM

Native cellulose microfibrils are unique highly shape anisotropic semi-flexible particles found in plants, also produced by some bacteria and algae. The cellulose microfibrils are attractive and can form space filling networks at low volume fractions, which can be used to control textural of various consumer products. Their ability to be mixed with emulsifiers, proteins, polysaccharides, or other dispersed systems (e.g. particles, droplets) give rise to various soft mater systems. In this talk, several examples of structured fluids, hybrid gels, and particle-assisted foams and emulsions will be presented.

Ultratough Ionogels

Dr. Michael Dickey

N2.4: Michael Dickey, Ultra tough ionogels, Room 301 AB, August 2, 2024, 10:30 AM - 12:00 PM

Ionogels are compelling materials for energy storage devices, ionotronics, and actuators due to their excellent ionic conductivity, thermal and electrochemical stability and nonvolatility. However, most existing ionogels suffer from low strength and toughness. Here, we report a simple one-step method to achieve ultra-tough and stretchable ionogels by randomly copolymerizing two common monomers in ionic liquid. Copolymerization leads to a single covalent network with controllable polymer- and solvent-rich phases that form in situ due to the phase behavior of the polymer in ionic liquid. The polymer-rich phase forms hydrogen bonds that dissipate energy and thereby toughen the ionogel during extension, while the solvent-rich phase remains elastic to enable large strain. The copolymer ionogels composed of acrylamide and acrylic acid exhibit extraordinary mechanical properties (see photograph below), including fracture strength (12.6 MPa), fracture energy (~24 kJ m-2), and Young's modulus (46.5 MPa), setting new records among reported ionogels. The tough ionogels are highly stretchable (~600% strain) and possess good self-recovery, as well as excellent self-healing and shape-memory properties. This concept extends to other monomers and ionic liquids, which offers a promising and general way to tune microstructure in situ during one-step polymerization that solves the longstanding mechanical challenges in ionogels.

Correlated orientational disorder in crystalline assemblies of hard convex polyhedra

Dr. Avisek Das, Mr. Sumitava Kundu, Mr. Kaustav Chakraborty

N2.5: Avisek Das, Correlated orientational disorder in crystalline assemblies of hard convex polyhedral, Room 301 AB, August 2, 2024, 10:30 AM - 12:00 PM

Entropy driven self-assemblies of hard convex polyhedra into simple and complex crystals have been valuable model systems for understanding colloidal crystals and superlattices formed by anisotropic nanoparticles. The nonspherical shapes of the building blocks lead to the possibility of crystalline phases with purely orientational disorder. Here, despite maintaining a regular arrangement in terms of positions of the centers of geometry, particles adopt different orientations, with no discernible relationships with the underlying crystal structure. We report computational evidence of a new type of orientational phase in the cubic crystals formed by certain hard convex polyhedra. Despite the lack of order, particle orientations are not random and exhibit strong correlations. The novel forms of orientational correlations observed in multiple systems seem to follow a common pattern characterized by certain conserved features. The rotational motions of particles are found to be restricted in a small set of unique orientations with three properties: 1) the number of such orientations is a property of the shape and nothing else; 2) irrespective of external pressure, particles are always equally distributed, within statistical error, among the unique absolute orientations; 3) pairwise differences between unique orientations are fixed, and are solely the property of the shape. The result of the correlations is a “discretely mobile” phase at low packing fractions and an orientationally arrested state at high pressures, where each particle is frozen in one of the unique orientations. The newly found phase is qualitatively different from the well characterized plastic crystal phase, which, in the hard particle systems, is completely random in terms of single particle orientations. We have decided to characterize the phase as a “correlated orientationally disordered” phase because of the presence of both attributes, and novel forms of correlations defined by the conserved quantities. The origin of orientational correlations appears to stem from an underlying symmetry consideration involving the point group symmetry of the anisotropic particle and the rotational symmetry of the cubic unit cell. It was empirically observed that for each particle in the system, the orientation is such that the highest order rotational symmetry axis of the particle point group is always parallel to any one of the rotational axes of the crystallographic point group of the corresponding unit cell. This finding seems to provide a straightforward justification for the presence of distinct orientations and the number of such special orientations. The main factor determining the presence of this phase is the mismatch of two kinds of symmetries mentioned before. Shapes with point groups with orders much smaller than that of the full octahedral point group of cubic crystals tend to form this phase. A systematic variation of particle shapes further indicates that symmetry and not any other geometrical properties of the shape, is the sole determinant of the existence of this phase. In the broader context of fundamental understanding of self-assembly processes, our findings underscore the versatility of entropy as an organizing principle and particle shape as a design principle.

Polymers

Multi-material additive manufacturing of polymeric composites with seamless soft-hard interface integration from molecular bonding

Dr. Daniel Rau, Baiqiang Huang, Alexander Church, Dr. Baoxing Xu, Dr. Liheng Cai

P1.2: Daniel Rau, Multi-material additive manufacturing of polymeric composites with seamless soft-hard interface integration from molecular bonding, Room 302 BC, July 30, 2024, 10:30 AM - 12:00 PM

Multi-material additive manufacturing (AM) enables the fabrication of functionally graded three-dimensional (3D) structures by integrating multiple materials with dramatically different properties. However, it remains a grand challenge to develop a robust multi-material AM process that enables joining parts with distinct mechanical properties. Here, we report multi-material stereolithography (SLA) printing of polymeric composites with seamless soft-hard interface integration from molecular bonding. Exploiting our recently discovered foldable bottlebrush polymer networks, we develop photocurable resins with Young's modulus ranging by more than three orders of magnitude from ~40 kPa to ~150 MPa. Importantly, all resins are cured by the same chemistry, such that polymers of dramatically different stiffness can be bonded at the molecular level. We customize an SLA platform to print these resins into multi-material tensile bars, which exhibit remarkable stretchability (with tensile breaking strain >700%) determined primarily by the softer material. Further, we demonstrate printing multi-material polymeric composites with spatially resolved mechanical properties and seamless soft-hard interface integration. The developed polymeric resins and multi-material SLA process open an avenue for manufacturing highly functional 3D multi-material polymeric structures and devices for a wide range of applications.

3D Printing of Polymeric and Composite Porous Scaffolds for Biomedical Applications

Dr. Alina Kirillova

P1.3: Alina Kirillova, 3D Printing of polymeric and composite porous scaffolds for biomedical applications, Room 302 BC, July 30, 2024, 10:30 AM - 12:00 PM

In the realm of regenerative medicine, synthetic biomaterials play a crucial role. These materials are the foundation for creating scaffolds and implants, made from polymers, ceramics, and metals – often combined as composites. For instance, biodegradable polymers are used to construct scaffolds and medical devices that gradually degrade after implantation, aiding defect reconstruction and tissue healing. Additionally, bioceramic-based biomaterials gradually resorb after application, making them appealing for bone repair and eliminating the need for follow-up procedures once bone healing occurs. Meanwhile, metallic materials, known for their robust mechanical properties, find applications in orthopedic contexts requiring high load-bearing capacity. To maximize the benefits of these materials, it's crucial to consider both their mechanical and biological properties, along with associated trade-offs. An effective approach involves creating composite scaffolds by combining different clinically relevant materials. Furthermore, 3D printing offers promise for fabricating scaffolds with intricate, customizable architectures, potentially tailored to individual patients. Careful design of porous 3D-printed scaffolds is essential to optimize their mechanical performance while maintaining sufficient porosity for enhanced biological behavior. These polymeric and composite scaffolds could ultimately improve clinical outcomes in regenerative medicine applications.

Phage probes couple to DNA relaxation dynamics across scales and regimes

Mr. Farshad Safi Samghabadi, Ms. Juexin Marfai, Dr. Mehdi Aporvari, Mr. Philip Neill, Ms. Maede Chabi, Dr. Rae Robertson-Anderson, **Dr. Jacinta Conrad**

P2.2: Jacinta Conrad, Phage probes couple to DNA relaxation dynamics across scales and regimes, Room 302 BC, July 31, 2024, 3:30 PM - 5:30 PM

Microrheology has become an indispensable tool for measuring the dynamics of macromolecular systems. Yet, its ability to characterize polymer dynamics across spatiotemporal scales, which vary among polymers and concentration regimes, is limited by the selection of probe morphologies and sizes. Here, we introduce semiflexible M13 phage as a powerful microrheological probe able to circumvent these constraints to robustly capture the dynamics of polymeric solutions across decades of concentrations, sizes, and ionic conditions. We show that phage mobility directly couples to the relaxation dynamics of DNA solutions of two sizes, 5.9 kbp and 115 kbp, spanning from semidilute to entangled regimes at ionic strengths varying by four orders of magnitude. Phage mobility metrics across a broad range of timescales collapse onto universal master curves that are unexpectedly insensitive to ionic strength and exhibit sharp crossovers from semidilute to entangled regime scaling, not captured by current theoretical models. Our results open the door to the use of phage probes to elucidate the complex dynamics of systems exhibiting a spectrum of thermal and active relaxation processes.

Triggering inorganic crystal deposition from polymer-induced liquid precursors

Mohammed Kayes Patoary, **Thomas Schroeder**

P2.3: Thomas Schroeder, Triggering inorganic crystal deposition from polymer-induced liquid precursors, Room 302 BC, July 31, 2024, 3:30 PM - 5:30 PM

Polyelectrolytes are commonly used to control the deposition of minerals from aqueous solutions; an industrially important application of this class of compounds is as antiscalants that control inorganic buildup on the interiors of pipes. Around 25 years ago, Gower and coauthors discovered that the presence of trace polyelectrolytes can induce the formation of so-called “polymer-induced liquid precursor” phases in solutions of insoluble salts such as calcium carbonate. Such phases are metastable viscoelastic droplets composed of aggregated amorphous mineral granules; in these droplets, the polyelectrolyte additive serves as a kinetic barrier delaying the nucleation of crystals. Since their discovery, the droplets have been found to be capable of coalescing and wicking into (nano)porous scaffolds via capillarity, where they eventually nucleate to form complex crystalline structures in the shape of the pores; they can also wet surfaces to form films. A compelling hypothesis implicates polymer-induced liquid precursors in the formation of bone, which is composed of hydroxyapatite (calcium phosphate) crystals deposited internally within nanoporous collagen fibrils; multiply phosphorylated “non-collagenous proteins” are thought to play the role of the stabilizing polyelectrolyte.

In this work, we present a method of controllably destabilizing such precursors to trigger the deposition of crystalline calcium carbonate on demand. We further discuss the thermodynamic driving forces that act upon such precursors in solution in an attempt to rationalize their behavior.

Stretching bistable linear polymers and loops

Dr. Panayotis Benetatos

P2.5: Panayotis Benetatos, Stretching bistable linear polymers and loops, Room 302 BC, July 31, 2024, 3:30 PM - 5:30 PM

The local bending stiffness of semiflexible polymers may fluctuate due to internal conformational changes (e.g, the helix-coil transition in polypeptides or the thermal denaturation of double-stranded DNA) or due to the reversible attachment/detachment of ligands from the environment (e.g., DNA-binding proteins or hybridization of oligomers). We theoretically analyze the tensile elasticity of a strongly-stretched wormlike chain consisting of N bistable blocks. The bending stiffness of each block is an annealed degree of freedom with two values. We calculate the force-extension relation of this chain in both the fixed-force (Gibbs) and the fixed-extension (Helmholtz) ensemble. We show that, for finite N, there is significant ensemble inequivalence. Under certain conditions, in the Helmholtz ensemble, the tensile compliance becomes negative. (PB, J. Chem. Phys. 157, 2022.) We also consider a rod-like wormlike chain with fluctuating bending stiffness grafted at an angle to a rigid substrate subject to a force at the other end. We show the emergence, under certain conditions, of compliance higher than that corresponding to the two values of the bending stiffness (Gibbs ensemble), as well as negative compliance (Helmholtz ensemble). (M. Razbin and PB, Polymers 15(10), 2023.) In addition, we are going to present an analysis of flexible polymer loops under tension, undergoing reversible transitions between two states: looped and unlooped, or looped and zipped. In the case of a reversible necklace (concatenated reversible loops and zipped chains in the thermodynamic limit) under tension, using the generating function method, we show that the flexibility of the zipped part has a significant effect on the force-temperature phase diagram.

Microwave dielectric relaxation spectroscopy: A technique to inform ion transport in hydrated polymer membranes

Mr. Sean Bannon, Dr. Kevin Chang, **Dr. Geoffrey Geise**

P2.6: Geoffrey Geise, Microwave dielectric relaxation spectroscopy: A technique to inform ion transport in hydrated polymer membranes, Room 302 BC, July 31, 2024, 3:30 PM - 5:30 PM

Providing sustainable supplies of purified water and energy is a critical global challenge for the future, and polymer membranes will play a key role in addressing these clear and pressing global needs for water and energy. Polymer membrane-based processes dominate the desalination market because they are more energy efficient than thermal desalination processes, and polymer membranes are crucial components in several rapidly developing power generation and energy storage applications that rely on membranes to control, selectively, rates of ion transport. Much remains unknown about the influence of polymer structure on basic intrinsic transport properties, and these relationships are important for designing next generation polymer membrane materials.

Key to controlling ion transport in membranes for water purification and energy applications is engineering interactions between ions and the solvated polymer matrix. Microwave dielectric relaxation spectroscopy is a tool that enables study of hydrated polymer membranes because water molecule dipoles can be probed in the microwave frequency region. This technique can provide unique insight into hydrated polymer dielectric permittivity (or dielectric constant) properties, which are critical in emerging thermodynamic modeling of ion transport in hydrated polymers. This presentation discusses the use of microwave dielectric relaxation spectroscopy to uncover structure property relationships in hydrated polymers and, more broadly, presents an overview of research aimed at further understanding fundamental structure/property relationships that govern small molecule transport in polymeric materials considered for desalination and electric potential field-driven membrane applications that can help address global needs for clean water and energy.

Elastomer Mechanics of Cross-linked Ring-Linear Polymer Blends

Dr. Ting Ge, Siteng Zhang, Dr. Daniel Vigil, Dr. Thomas O'Connor, Dr. Gary Grest

P3.2: Ting Ge, Elastomer mechanics of cross-linked ring-linear polymer blends, Room 302 BC, August 1, 2024, 10:30 AM - 12:00 PM

Recent studies have demonstrated the distinctive physical properties of non-concatenated ring polymers, such as the superior softness and stretchability of cross-linked ring polymers. Nevertheless, synthesizing high-molecular-weight ring polymers with high purity has remained demanding in polymer chemistry. Away from the ideal pure limit, a blend of ring polymers with linear polymers occurs more readily in experiments and brings blend composition as a new parameter for the molecular designing of ring-polymer-based materials. Large-scale molecular simulations are performed to investigate the elastomer mechanics of cross-linked ring-linear polymer blends. The tensile stress σ as a function of the stretch ratio λ in a uniaxial tensile test is calculated for varying volume fractions ϕ_R of ring polymers. As ϕ_R increases, both the network shear modulus G and the maximum stretch ratio λ_p before the network failure do not change much until a sufficiently large ϕ_R^c, beyond which G decreases while λ_p increases towards their respective values for the super-soft and super-stretchable pure ring elastomer (ϕ_R=100%). Meanwhile, the network strength characterized by the peak stress σ_p depends on ϕ_R non-monotonically, exhibiting a maximum around ϕ_R^c before decreasing towards the value of the pure ring elastomer. Further analysis of the network topology reveals that the threading of rings by linear chains plays a crucial role in the structure-property relationship for the dependencies of G, λ_p, and σ_p on ϕ_R.

Dynamics of polymers with controlled distribution and density of associative groups

Myoeum Kim, Shalin Patil, Siteng Zhang, Ting Ge, Shiwang Cheng, Li-Heng Cai

P3.3: Myoeum Kim, Dynamics of polymers with controlled distribution and density of associative groups, Room 302 BC, August 1, 2024, 10:30 AM - 12:00 PM

An associative polymer may carry many moieties that can form reversible bonds. For >30 years, the dynamics of unentangled associative polymers have been described by the sticky Rouse model: reversible associations change the shape of linear viscoelastic spectra by adding a rubbery plateau in the intermediate frequency range, at which associations have not yet relaxed and thus effectively act as crosslinks. Our recent study showed that this classical understanding is incomplete for homogeneous associative polymers carrying high fractions of stickers (>0.7/Kuhn segment): the reversible interactions significantly slow down the polymer dynamics but nearly do not change the shape of linear viscoelastic spectra. Yet, it remains to be determined the conditions at which the classical sticky Rouse behavior resumes. Here, we design and synthesize unentangled associative polymers with various densities and distributions of stickers. For associative polymers with randomly distributed stickers, the polymers are a homogenous melt and exhibit the same Rouse dynamics regardless of the sticker densities down to 0.3/Kuhn segment. Remarkably, for a telechelic polymer with only one sticker at each of the two ends, the stickers aggregate into nanoclusters but nearly do not slow down polymer dynamics. Increasing the number of stickers at the two polymer ends forms stronger nanoclusters, resulting in sticky Rouse behavior characterized by a rubbery plateau with a width correlated to nanocluster strength. Our results show that both microphase separation and relatively strong nanoclusters of stickers are required for associative polymers to exhibit sticky Rouse behavior, resolving a long-standing controversy in polymer dynamics.

Self-Assembly

Rational Design of Nanoparticle Surface Patterning for Directed Self-Assembly

Dr. Thi Vo

S1.3: Thi Vo, Rational design of nanoparticle surface patterning for directed self-assembly, Room 301 AB, July 31, 2024, 10:30 AM - 12:00 PM

Designing nanoscale synthons with predictive control over shape, size, and interparticle interactions is a holy grail for materials design. To date, there exists a large space of experimental parameters that can be employed to direct nanoscale assemblies. Tuning such experimental handles produces different modes of interactions such as hard particle packing, soft deformable ligand shells, or patchy/selective attraction. However, a major limitation intrinsic to such building blocks lies in the fixed nature of their pre-programmed interactions. This means that the assembled morphologies are also often static, thereby limiting the a priori design of reconfigurable structures. Here, we present strategies for designing building blocks that address the above limitation. We first discuss theoretical insights into how to imbue secondary interactions into synthesized building blocks that can be toggled on/off via experimentally relevant external stimuli such as temperature, external field, and/or solvent change. We then showcase how synthon reconfigurability shifts the preferred, thermodynamically stable assembly structures, validated by both simulation and experiments. Our works provide unique insights into nanoscale synthesis, allowing for a priori design of complex building blocks that can target novel and reconfigurable assemblies.

Towards controlled self-assembly of curved surfaces

Mr. Andraž Gnidovec, Dr. Simon Copar

S1.4: Andraž Gnidovec, Towards controlled self-assembly of curved surfaces, Room 301 AB, July 31, 2024, 10:30 AM - 12:00 PM

Inverse design problems are ubiquitous in material science as well as in complex biological and biologically inspired systems. In soft materials, design of interactions for self-assembly allows for precise tuning of material structure, properties, and even kinetics. With recent advances in patchy particle synthesis, the scope of attainable structures has greatly expanded. On the other hand, self-assembly of mesoscopic particles, such as synthetic hard particles, proteins or larger biological building blocks, is often affected by the curvature of the substrate. The particles themselves can influence this curvature or even assemble into curved structures on their own. Understanding how to manipulate the curved geometry of assemblies can elucidate new ways of tuning properties of functional soft materials.

We discuss how one can target self-assembly into surfaces with specified Gaussian curvature in systems of model patchy particles. We start by presenting an automatic differentiation-based approach to inverse design that allows us to determine parameter gradients by differentiating through self-assembly kinetics as well as consider arbitrarily complex loss functions. We present some of the challenges that arise when we differentiate through long molecular dynamics trajectories and the ways to mitigate them. Additionally, we discuss the model requirements and hyperparameter choices for successful optimization. We show that the learning predominantly happens at the later stages of the self-assembly process and that the information gathered from a small number of assembly trajectories suffices for generalizable optimized potentials. Finally, we show some results for the self-assembly of vesicles with a given target curvature.

Programming Self-Assembly of Colloidal Gyroids for Advanced Materials

Dr. Dwaipayan Chakrabarti, Dr. Wesley Flavell, Dr. Andreas Neophytou, Mr. Adam Walker, Dr. Angela Demetriadou, Prof. Tim Albrecht

S2.2: Dwaipayan Chakrabarti, Programming self-assembly of colloidal gyroids for advanced materials, Room 301 AB, July 31, 2024, 3:30 PM - 5:30 PM

Gyroid structures have stimulated widespread interest across mathematical, physical, materials, and biological sciences for having intriguing structural features, rich chiroptical properties and exotic topological physics [1-4]. While the double-gyroid morphology as a bicontinuous structure is not uncommon in self-assembled soft materials [5-7], direct self-assembly of single-network gyroids has proven elusive. Notwithstanding their appeal as chiral photonic crystals and metamaterials [8], the single-gyroid structures have largely been ignored as targets for programmed colloidal self-assembly, presumably due to their structural complexity. Instead, colloidal diamond, in its cubic form, has drawn much attention as an attractive target for a photonic crystal at optical frequencies for nearly three decades [9,10]. This presentation introduces an enantiomorphic pair of single-gyroid crystal structures comprising colloidal spheres, and two distinct routes are demonstrated in silico for programmed self-assembly of each single colloidal gyroid enantiomorph from rationally designed patchy spheres [11]. The designer colloidal patchy spheres, which closely hew to their synthetic feasibility, are chiral, having either two staggered rectangular patches at opposite poles or four circular patches arranged in a well-defined geometry. The single colloidal gyroid, as well as its inverse structure, is shown to support a wide complete photonic bandgap and exhibit rich chiroptical properties, making them attractive chiral photonic crystals [11]. Moreover, the presentation illustrates how advanced materials based on colloidal gyroid structures can be developed, while addressing the challenges concerning the synthesis of sophisticated patchy colloids [12].

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Multicomponent liquid-core nanocapsules synthesized with flash nanoprecipitation

Dr. Edward Van Keuren, Sophia Taylor, Yuri Chung, Orelle Bulgin, Sam Becker, Allie Stevens, Dr. Eleni Hughes, Dr. Mauro Mugnai

S2.3: Edward Van Keuren, Multicomponent liquid-core nanocapsules synthesized with flash nanoprecipitation, Room 301 AB, July 31, 2024, 3:30 PM - 5:30 PM

Nanoparticles containing a liquid core surrounded by a solid shell, or nanocapsules, are interesting materials for a number of applications. We have shown that these materials can be synthesized using a simple method known as flash nanoprecipitation, in which a solution of both the shell and core components is rapidly mixed with a miscible non-solvent. We have made nanocapsules comprised of a variety of polymers as shells and both aqueous and non-aqueous liquid cores. We will present our recent work on these materials, including molecular dynamics simulations that give insights into the particle formation, and development of applications including as MRI contrast agents and in nanodrug formulations.

Self-Assembly of Recombinant Elastin-like Polypeptide

Yulia Shmidov, Ashutosh Chilkoti

S2.5: Yulia Shmidov, Self-Assembly of Recombinant Elastin-like Polypeptide, Room 301 AB, July 31, 2024, 3:30 PM - 5:30 PM

Elastin like polypeptides (ELPs) are synthetic intrinsically disordered proteins that exhibit lower critical solution temperature (LCST) phase behavior. In this research we studied how appending self assembling domains onto ELPs influence their LCST and their structure.

To do so, we have synthesized ELPs that are fused—at the gene level—to peptide sequences, that has alternating aromatic and charged residues also known to promote beta sheet formation. Cryogenic transmission electron microscopy (cryo-TEM) revealed nanostructures with distinct morphologies. The morphological difference between these structures had significant effect on the LCST. Work in progress focuses on finding the key parameters for controlling the morphology of the self assembly and potential drug delivery applications. This work could lead to the ‘next generation’ thermoresponsive biomaterials with unique self-assembly structures.

Design of Peptide-DNA Architectures to Build Functional Artificial Cells

Dr. Maggie Daly, Dr. Kengo Nishi, Stephen Klawa, Kameryn Hinton, Yuan Gao, Dr. Ronit Freeman

S2.6: Maggie Daly, Design of Peptide-DNA Architectures to Build Functional Artificial Cells, Room 301 AB, July 31, 2024, 3:30 PM - 5:30 PM

The natural cytoskeleton is a supramolecular polymer network composed of various biomolecules that dynamically and hierarchically organize to perform various tasks within a cell. To engineer artificial cells with life-like properties, generating a cytoskeleton able to organize at distinct locations and modulate its structure and mechanical properties is needed. In this work, we use a simple set of biomacromolecular building blocks, peptides and DNA, to encode weak interactions into dynamic structures that span nano- to micrometer length scales. We leverage an emerging class of materials that combines peptide self-assembly with the programmability of DNA base-pairing. Inspired by the vast array of actin associated proteins and their ability to reversibly crosslink and bundle filaments, we design a library of DNA-peptide crosslinkers varying in duplex length, valency, and geometry. The peptide filaments crosslinked through DNA hybridization give rise to tactoid-shaped bundles with tunable aspect ratios, filament alignment, crosslinker density and mechanics guided by the DNA design. The tunable DNA junctions as well as various solvent and heat treatment pathways allow the formation of a diverse set of hierarchical filamentous networks that are able to transition between structural and mechanical states via the transient Watson-Crick base-pairing, mimicking the dynamic polymorphism of natural actin structures. The modular biodesign of the synthetic cytoskeleton enables control over its spatial localization when confined in cell-sized water-in-oil droplets, directing structures to the cortex or the lumen of the synthetic cells. This tunable spatial arrangement of the peptide-DNA cytoskeleton regulates payload diffusion and cargo load-and-release properties within the synthetic cells. Heat-induced reconfiguration of peptide-DNA architectures triggers droplet deformations that resemble functional cell structures such as filopodia, regulated by tunable DNA melting temperatures. Peptide-DNA nanotechnology as a bottom-up reductionist approach for building synthetic cells is a powerful strategy towards producing new biomaterials with life-like functions.

Dissipative self-assembly within an oscillating energy landscape.

Dr. Kateri DuBay, Dr. Jessica Niblo, Austin Cheng, Jacob Swartley, Dr. Zhongmin Zhang

S3.3: Kateri DuBay, Dissipative self-assembly within an oscillating energy landscape, Room 301 AB, August 1, 2024, 10:30 AM - 12:00 PM

Oscillations in inter-particle potentials can alter self-assembly processes in interesting ways: in some cases they facilitate the relaxation of kinetic traps, and in others they give rise to entirely novel non-equilibrium steady-state structures. Previous theoretical work in the field has shown that, at the limit of fast oscillations of the inter-particle potential, the dynamics of this dissipative self-assembly process should proceed as if the system were under a constant interaction potential equivalent to the time-dependent one, averaged over a single oscillation period. In this work, we use a 2D model of the assembly of a viral-capsid-like structure to demonstrate this correspondence at the fast limit. We then vary the oscillations and investigate how oscillation period and amplitude influence capsid yield by facilitating error correction if oscillations are slow enough to enable local relaxation. We also draw out the implications of earlier theoretical findings at the fast oscillation limit by working through the functional forms of different interaction potentials to show which oscillations may be able to form self-organizing materials that would be inaccessible with static interactions.

Self-Assembly of Recombinant Elastin-like Polypeptide
Yulia Shmidov, Ashutosh Chilkoti

S2.5: Yulia Shmidov, Self-Assembly of Recombinant Elastin-like Polypeptide, Room 301 AB, July 31, 2024, 3:30 PM - 5:30 PM

Elastin like polypeptides (ELPs) are synthetic intrinsically disordered proteins that exhibit lower critical solution temperature (LCST) phase behavior. In this research we studied how appending self assembling domains onto ELPs influence their LCST and their structure.

To do so, we have synthesized ELPs that are fused—at the gene level—to peptide sequences, that has alternating aromatic and charged residues also known to promote beta sheet formation. Cryogenic transmission electron microscopy (cryo-TEM) revealed nanostructures with distinct morphologies. The morphological difference between these structures had significant effect on the LCST. Work in progress focuses on finding the key parameters for controlling the morphology of the self assembly and potential drug delivery applications. This work could lead to the 'next generation' thermoresponsive biomaterials with unique self-assembly structures.

Timed material self-assembly controlled by circadian clock proteins

Dr. Rae Robertson-Anderson

S3.4: Rae Roberson-Anderson, Timed material self-assembly controlled by circadian clock proteins, Room 301 AB, August 1, 2024, 10:30 AM - 12:00 PM

Active biological molecules present a powerful, yet largely untapped, opportunity to impart autonomous regulation to materials. Because these systems can function robustly to regulate when and where chemical reactions occur, they have the ability to bring complex, life-like behavior to synthetic materials. Here, we achieve this design feat by using functionalized circadian clock proteins, KaiB and KaiC, to engineer time-dependent crosslinking of colloids. The resulting material self-assembles with programmable kinetics, producing macroscopic changes in material properties, via molecular assembly of KaiB-KaiC complexes. We show that colloid crosslinking depends strictly on the phosphorylation state of KaiC, with kinetics that are synced with KaiB-KaiC complexing. Our microscopic image analyses and computational models indicate that the stability of colloidal super-structures depends sensitively on the number of Kai complexes per colloid connection. Consistent with our model predictions, a high concentration stabilizes the material against dissolution after a robust self-assembly phase, while a low concentration allows circadian oscillation of material structure. This work introduces the concept of harnessing biological timers to control synthetic materials; and, more generally, opens the door to using protein-based reaction networks to endow synthetic systems with life-like functional properties.

Poster Sessions

Active Matter

2x2 Rotation bit system composed of active matter: pattern and synchronization of self-propelled rotation

Sogo Akiyama, **Dr. Kazuaki Furukawa**

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Sogo Akiyama, Kazuaki Furukawa
School of Science and Engineering, Meisei University, 191-8506, Hino, Tokyo Japan

We have reported that some ion gels exhibit autonomous motion on the water surface (1). We cut the ion gel into a rectangle and make a hole in the center. When this hole is passed through a rotation shaft perpendicular to the water surface, the ion gel undergoes rotation motion on the water surface. The direction of rotation can be guided to either the left or right direction, depending on the initial motion direction. The rotation direction is not determined by the possible asymmetric shape of the ion gel. This bistable rotation represents one bit of information, and we call this a rotation bit.

In the latest conference (2), we reported the conditions under which adjacent rotation bits rotate in opposite directions by adjusting the size of the ion gel and the distance between the rotation shafts. We showed that when the three rotation shafts are arranged in a straight line, the rotation bits alternately rotate in the opposite direction, and when the three rotation shafts are arranged in an equilateral triangle, a phenomenon similar to spin frustration occurs.

In the present study, we arranged the rotation shafts in a 2x2 tetragonal system and investigated the state of four rotation bits. At the start of motion, the state in which the rotation bits in the nearest neighbor rotated in opposite directions was predominant. The angular speed of the rotation bit gradually slows down over time. After a certain period of time, four rotation bits take stationary state and align horizontally or vertically. During this stationary state, the four rotation bits occasionally make a rotational motion all at once, and then return to an aligned state. The timing of taking stationary and rotation states of the four rotation bits were synchronized. We investigated the distribution of durations of stationary and rotation states, and found that these values showed a distribution similar to a normal distribution. We will discuss the origin of the synchronous motions.

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Active-assisted Assembly of Colloidal Crystal

Min Kyung Lee, David Pine

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Colloidal crystals are three dimensional arrays of colloidal particles and are valued for their applications in display technologies and photonics. To realize their full potential, it is important to form large single crystals that are free from grain boundaries and other defects. Attaining large crystalline grains is often impeded by kinetic barriers, which anneal slowly under thermal agitation. Recently, it has been proposed that annealing can be significantly accelerated by doping colloidal crystals with “active colloids” that locally agitate at or near grain boundaries and eliminate defects. Such approaches are known as active-assisted assembly and have been studied using simulations. While simulations show promising results for fast annealing, there have been few experimental studies.

We aim to experimentally study active-assisted self-assembly. We use light-activated colloidal particles that are synthesized with a hematite cube embedded in a TPM (3-methacryloxypropyl trimethoxysilane) particle and partially exposed. The hematite is activated by blue light (λ=450nm) and decomposes hydrogen peroxide dissolved in aqueous solution. This induces self-diffusiophoretic propulsion of the particles. These active particles are studied under various conditions to control swimming speed, including hydrogen peroxide concentration, pH, and light intensity.

We designed and prepared cells to confine both passive and active particles using soft PDMS lithography. A hexagonal pattern mold is deposited on a glass substrate using SU-8 photoresist and UV exposure. The height of the cell wall is controlled by varying the viscosity of the photoresist. Polystyrene (PS) particles are confined in hexagonal PDMS cells to monitor the defect healing process with different swimmer speeds and concentrations. The process is recorded using an optical microscope. Each frame is analyzed by software to detect individual particles and identify the grains and their size. The experimental set-up explores how swimmers heal the defects of PS in the cell. After finding optimal conditions for annealing 2D crystals, we will explore fully 3D crystals.

We also perform experiments using particles activated by an external electric field. We use Janus particles consisting of two coalesced TPM particles with one side coated by gold nanoparticles. The speed of the swimmers is controlled by the electric power and is significantly greater than that of the light-activated particles. Another advantage of this approach is that no chemical reaction is required, which poses fewer constraints on the type of colloidal suspension used. We use the depletion interaction to retain the crystal structure after annealing. This research benefits from continuous feedback between experiments and simulation and target various new 3D colloidal structures.

Activity-enhanced colloidal self-assembly: insights from simulations

Mr. Ravi Gautam, Dr. John F. Braddy, Dr. David J. Pine, Dr. Daphne Klotsa

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Active particles, propelled by mechanisms such as light activation or magnetic fields, offer a promising avenue for modulating self-assembly processes in colloidal systems. Introducing a small fraction of active particles in colloids can accelerate the crystallization kinetics and can anneal defects within polycrystalline structures via the facilitation of rearrangement at grain boundaries. These advancements hold significant potential for engineering materials with tailored properties and functionalities. In this study, we employ Active Brownian Particle dynamics simulations to delve into the underlying mechanics of activity-enhanced self-assembly and to develop strategies for manipulating colloidal crystal architectures. Our work aims to elucidate the fundamental principles governing the interaction between active particles and colloidal assemblies, with the ultimate goal of designing innovative materials for various applications, including photonics, plasmonics, sensing, and catalysis.

Designing Cell-Inspired Microswimmers

Kameryn Hinton

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Nature features various mechanisms in which living systems interact with the environment. Cells are characterized by several hallmarks such as compartmentalization, responsiveness to stimuli, growth and proliferation, adaptiveness, and energy transfer. Inspired by these hallmarks, specifically compartmentality, cargo-loading and surface reactivity, we report on the design of soft, multicompartment micromotors with tunable surface modalities. In this work, we utilize a hydrogel-based microswimmer (120-180 µm) with internalized motor powered by catalytic reaction to drive bubble-propulsion of the swimmers. The motion patterns can be further tuned by changing the amount of payload, concentration of fuel or compartment size in which the payload is situated. We achieve cell-like functionalization of the surface post-fabrication via bioorthogonal chemistries that are spatially separated from the site of the motor. To showcase the functionality of the active design, we incubate complementary payloads with the active microswimmers to showcase enhanced binding of the target probes. We hope this work can help towards developing on-the-fly diagnostic tools, specifically in identifying antibodies in biological fluids to detect diseases.

Effect of background flow on motility-induced phase separation

Ms. Soni Prajapati

The phase separation due to the motile nature of finite-size self-propelling particles is a well-known phenomenon, commonly known as motility-induced phase separation (MIPS). In nature, many motile organisms show a phase separation and MIPS have been used to explain the aforementioned observation. More often than not these organisms grow and thrive in a fluid environment. It is known that when the background flow becomes chaotic it acts as a mixture. Now, the question is how the phase separation due to these motile organisms will be affected by the background flow in which they grow and thrive. To address this question we consider a large number (N) of finite-size isotropic self-propelling particles (SPP), which are being advected by the four-roll mill flow. We have taken this four-roll mill flow because it mixes the scalar field very well even though this flow is laminar. The SPPs follow the active Brownian particle (ABP) dynamics and show MIPS for packing fraction ($\Phi >\sim 0.4$). In this study, we are maintaining a packing fraction value of 0.7. The fluid characteristic velocity and self-propulsion speed of SPP are the two relevant velocity scales. The two relevant time scales are the inverse of fluid characteristic vorticity and rotational diffusivity of SPPs. We define two dimensionless quantities based on the ratio of these four scales: 1) scaled time is the ratio of SPP to fluid time scale; 2) scaled velocity is the ratio of SPP to fluid velocity. Based on these dimensionless numbers, we observe three distinct distribution regimes for SPPs. When scaled velocity is small (<<1) the flow dominates the dynamics of SPPs and shows a homogeneously mixed phase. When scaled velocity is large (>>1) the motility of the SPPs dominates the dynamics and shows the MIPS regime. When scaled velocity is moderate ~1, we observe that based on the time scale, it can either show a moderately mixed homogeneous phase (scaled time is small) or it can show a novel phase, that emerges due to interplay between flow topology and motile, finite-size nature of SPPs at large scales times. We call this novel phase flow-induced phase separation (FIPS). To get a better understanding of the system on the dimensionless number we show a phase diagram in scaled-time scaled-velocity phase space. We have also characterized the drift velocity and diffusivity from the mean-squared displacement, giant number fluctuation, radial distribution function, and cluster-size distribution to develop a detailed understanding of this system.

Emergence of Collective Behavior: An Evolutionary Approach to Vicsek-like Particles with Neural Networks

Mr. Guilherme Giardini, Dr. Carlo daCunha

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Multi-agent systems are widely observed in nature, from colonies of insects to schools of fish and flocks of birds. A common characteristic of these systems is that the individual agents exhibit coordinated motion, giving rise to large-scale structures that can adapt to their environment. This emergent behavior has inspired the development of artificial multi-agent systems, where many interacting agents collaborate to achieve a common goal.

Researchers often create systems of rules and priorities to replicate the multi-agent coordination observed in nature, allowing agents to navigate their environment [1]. A seminal example is C. Reynold's Boids [2]. These simulated entities, inspired by bird flocks, interact with their neighbors according to a set of rules, pioneering the use of artificial agents to model collective motion. T. Vicsek later built upon this concept, introducing a special case of the Boids model specifically for simulating active matter [3,4].

However, these rule-based models suffer from two key limitations: first, their fixed nature hinders adaptation to unforeseen environmental changes or complex tasks. Second, we lack knowledge of the minimal conditions necessary to produce coordination or the reasons why such rules originate in biological systems. These limitations pose challenges for designing artificial systems that mimic the adaptability and self-organization observed in soft matter, where emergent collective behavior arises from simple interactions.

Here we propose a novel model that leverages Boid-inspired agents equipped with trainable neural networks that receive information about their neighbors as input and produce orientation as output, guiding their movement. For neural network training, we draw inspiration from nature and test three fundamental biological principles: grouping, reproduction, and predator avoidance.

Using Vicsek's order parameter, a measure of collective motion, we observed that the vectorial average of learned velocities stabilizes over time for all evolutionary pressure models. Interestingly, Vicsek's model of social conformity, known for rule-based coordination, is not driven by either grouping or reproductive pressures. Future work might explore incorporating more intricate models like Lotka-Volterra to understand the emergence of social conformity in our agent-based system.

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Fiber networks assembled and driven by an active fluid

Mr. Sattvic Ray, Dr. John Berezney, Dr. Itamar Kolvin, Dr. Seth Fraden, Dr. Zvonimir Dogic

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

While the self-assembly of filamentous networks has been extensively studied, methods of harnessing active matter to assemble and drive such networks remain largely unexplored. Cytoskeletal proteins reconstituted in vitro provide a rich set of building blocks for constructing tunable passive and active materials. We study how the chaotic active flows and stresses of a microtubule-kinesin fluid control the structure, mechanics, and dynamics of passive actin-fascin networks. The active fluid reorganizes and drives the passive network across several length and time scales. At the scale of filaments and bundles (tens of microns), active flows coarsen the actin-fascin fiber bundles and drive them into a large, globally-connected network. This network contracts vertically in the quasi-2D sample chambers, forming a sheet at the sample midplane suspended by active flows. The active flows drive in-plane and out-of-plane strain fluctuations of the elastic sheet. Strikingly, these local fluctuations sometimes coarsen into persistent shear oscillations on the order of the system size (several millimeters). These experiments demonstrate novel pathways by which an active fluid can both assemble a passive network and drive its nonequilibrium dynamics.

Non-Markovian Modeling of Nonequilibrium Fluctuations and Dissipation in Active Viscoelastic Biomatter

Mr. Amir Abbasi, Prof. Dr. Roland Netz, Prof. Dr. Ali Naji

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Using a Hamiltonian that accounts for the elastic coupling between a tracer particle and the surrounding active viscoelastic biomatter, we develop a generalized non-Markovian Langevin model to describe the nonequilibrium mechanical response of the tracer. Our analytical formulas for the frequency-dependent tracer response function and positional autocorrelation function align quantitatively with experimental data from red blood cells and actomyosin networks, both with and without adenosine triphosphate, across the entire frequency spectrum. Notably, they accurately capture the low-frequency violation of the fluctuation-dissipation theorem. The extracted viscoelastic power laws, elastic constants, and effective friction coefficients from the experimental data provide clear physical interpretations.

Phase separation kinetics in Two Temperature Induced Phase Separation(2-TIPS)

Ms. Nayana Venkatareddy, Prof Prabal Maiti

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

2-TIPS (Two Temperature Induced Phase Separation) refers to the phase separation phenomenon observed in mixtures of active and passive particles modeled using scalar activity. In scalar models, the activity of the particles is proportional to the temperature of the particles. The active particles are connected to a thermostat at high temperature while the passive particles are connected to the thermostat at low temperature, and the relative temperature difference between "hot" and "cold" particles is taken as the measure of the activity χ of the non-equilibrium system. Using molecular dynamics, we show that the equal binary mixture of hot and cold particles phase separates when the activity χ is greater than a density-dependent critical activity. The phase separation forces the cold particles to form dense crystalline clusters where particles are predominantly arranged in FCC or HCP packing.

Next, we investigate phase separation kinetics in 2-TIPS, where we study the temporal evolution of the binary mixture as it reaches its non-equilibrium steady state. We observe two different mechanisms of phase separation in the binary mixture. At high densities, the phase separation begins immediately after quenching the system into the phase-separated region and proceeds by forming bi-continuous domains rich in hot or cold particles, which grow in size with time. This mechanism closely resembles spinodal decomposition observed in passive systems. Conversely, at low densities, the phase separation takes place by the formation of small clusters of cold particles that grow independently with time. This mechanism is similar to nucleation and growth found in passive systems. To quantify the size of phase separating domains we calculate equal time spatial correlation function of the order parameter from which we calculate the characteristic length of the domains. The spatial correlation functions at different times collapse onto a master curve when the distance is divided by the domain length, showing the self-similar nature of domain growth. The growth of domain length with time occurs in a power-law fashion, with the growth exponent being equal to 1/3. This exponent is universally observed in many phase-separating passive systems. Our results on phase separation kinetics in 2-TIPS show that the universality in phase separation kinetics extends to our non-equilibrium binary mixture beyond the scope of passive systems.

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Self-propulsion of active particles through surface charge asymmetry

Dr. Ahis Shrestha, Professor Monica Olvera de la Cruz

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Charged colloidal particles propel themselves through asymmetric fluxes of chemically generated ions on their surface. We show that asymmetry in the surface charge distribution provides an additional mode of self-propulsion at the nanoscale for chemically active particles that produce ionic species. Particles of sizes smaller than or comparable to the Debye length achieve directed self-propulsion through surface charge asymmetry even when ionic flux is uniform over its surface. Janus nanoparticles endowed with both surface charge and ionic flux asymmetries result in enhanced propulsion speeds of the order of μm/s or higher. Our work suggests an alternative avenue for specifying surface properties that optimize self-propulsion in ionic media.

Shape-shifting gel-based micro-ribbons patterned by e-beam lithography

Yuke Han, Dr. Xinpei Wu, Professor Matthew Libera

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Hydrogel films and ribbons that change their conformation in response to external stimuli offer a promising path to create 3D shape-shifting materials. We have been exploring electron-beam (e-beam) lithography to pattern gel-based shape-shifting ribbons and lines. In contrast to UV photolithography, an e-beam approach can pattern pure homopolymers without photoinitiators or crosslinking agents and do so at high spatial resolution without a mask. We focus on homopolymer thin films of poly(acrylic acid) (PAA) and bilayer films of PAA and polystyrene (PS). Both polymers preferentially crosslink under electron irradiation, though with different dose dependences. Near-surface radiation chemistry is driven in thick films (~0.5 - 2 μm) using low-energy (2 keV) electrons, and the patterned structure is tethered to the underlying substrate at one end using higher energy (10 keV) electrons. Developing (washing) in a good solvent removes unexposed polymer and enables the pattern to adopt an equilibrium shape. We pattern ribbons with typical widths of ~1 - 5 μm and lengths of ~5 - 100 μm. Through-thickness gradients in crosslink density are created by the depth-dependent adsorption of electron energy. In PAA the radiation chemistry also damages acid groups to create a structure comprised of a heavily crosslinked hydrophobic top region and a hydrophilic gel bottom region with a continuous through-thickness variation in between these two extremes. The gel region produces out-of-plane bending stresses. We observe the classic roll-to-helix transition as the ribbon aspect ratio increases, and we see examples of single-loop rolls, multi-loop rolls, and minimal-pitch helices. Increasing pH from below to above the PAA pKa increases the swelling force to an extent that the ribbons deform plastically, which generates helices with a nonminimal pitch. Our most recent work replaces the top region of the PAA film with homopolymer PS. In addition to the ribbon geometry and the incident radiative dose, the PS layer provides another degree of freedom with which to control shape-shifting properties. We vary the ratio of PS and PAA layer thicknesses in films that range from pure PAA to pure PS. In addition to studying the shape-shifting behavior in aqueous buffers with controlled ionic strength and pH, we explore the shape-shifting behavior in organic solvents (e.g., dimethyl formimide) which preferentially swells the PS.

Spatio-temporal dynamics of nutrient exchanges in microbial active matter

Dr. Praneet Prakash

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Microorganisms inhabit highly fluctuating environments and survive in a low-nutrient resource bath. It is now well recognized that symbiotic relationships between microbes play a vital role in their survival. The existence of such interaction raises general questions about the spatio-temporal dynamics of nutrient exchanges. Here we experimentally and theoretically examine a model system of this problem – bacteria, an obligate microbe capable of chemotactic response towards oxygen, in a co-culture with green algae, which produce oxygen when illuminated. Even in their simplest arrangement in a localized illuminated domain, we find a complex dynamics involving nutrient exchanges, enhanced algal diffusivity due to the bacteria, and a stochastic version of "flux expulsion".

The Fluctuating Nature of Mesenchymal Cell Movement: Beyond Velocity Definitions

Mr. Guilherme Giardini, Dr. Gilberto Thomas, Dr. Carlo daCunha, Dr. Rita deAlmeida

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Single-cell migration is a phenomenon observed in wound healing, tissue growth, embryo development, and tumoral invasion, among many other domains. It is usually modeled by a Langevin-like problem consisting of ballistic motion for short periods and random walks for long periods. Conversely, experiments and simulations have revealed a previously neglected random motion at very short intervals, which would rule out the possibility of defining the cell's instantaneous velocity with a robust measurement procedure.

A previous attempt to address this issue considers an anisotropic migration model, which takes into account a polarization orientation along which the velocity is well-defined, and a direction orthogonal to the polarization vector that describes a random walk. Although the numerically and analytically calculated mean square displacement and auto-correlation agree with experimental data for that model, calculating a velocity distribution results in a curve that peaks at zero, which contradicts experimental observations of a constant drift in the polarization direction and a curve peaked at some positive value. Moreover, recent Potts model simulations indicate that instantaneous velocity cannot be measured for any direction.

In this study we propose a dynamical equation for cell polarization that introduces a polarization-dependent displacement, circumventing the problem of ill-defined instantaneous velocity.

Polarization, which can be measured from single pictures does not present the same problems as velocities, it is a well-defined quantity, besides preserving memory for short intervals. We consider cell polarization dynamics to follow a modified Langevin equation that yields cell displacement distribution that peaks at positive values, in agreement with experiments and Potts model simulations.

Furthermore solving the model presents displacement autocorrelation functions with two different time scales, improving the agreement between theoretical and experimental results. Using the normalized Root Mean Square Error nRMSE to estimate the error between experimental data and the resulting fitted model, shows results ranging from 0.18\% to 0.08\%, which at worst is equivalent to previous models and at best is a 2 to 3 times a decrease in error.

Our results contribute to the robustness of experimental measurements with cell migration in general, besides providing a sound basis for theoretical models with their analytical solutions.

Yielding in active granular matter is different than in sheared granular matter

Mr. Adil Ghaznavi, Dr. Lisa Manning

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Our goal is to develop a predictive theory for flow in dense active matter, which models systems including bacterial swarms and biomimetic emulsions. Researchers have identified a direct link between the dynamics of sheared amorphous solids and dense active matter in the limit of small and intermediate strains, where the response is still macroscopically elastic, but it remains unclear whether there is a link at larger strains where materials yield and start to flow. In sheared solids, rapidly quenched systems with low stability exhibit a continuous, “ductile” yielding transition, while slowly quenched systems with high stability fail in a brittle manner via system-spanning shear bands – localized regions where the deformation tensor is large and similar across the band. We analyze the yielding transition in dense active systems with varying stability. We find that there is no brittle failure in dense active matter, even in deeply quenched, highly stable systems. To understand why, we alter the correlation length of the field of active forces, and find that failure becomes more brittle – with larger stress drops at the yielding transition -- as the correlation length increases. We develop a method to identify the equivalent of shear bands in active matter systems, and demonstrate that the size of shear bands increases with increasing stress drop and correlation length of the input field. This suggests that, in addition to material stability, the symmetry and length-scale of the active driving field controls ductility in dense granular materials.

Biological Matter

Active wetting and dewetting dynamics of zebrafish embryonic explants

Owen Blanchard, Usha Kadiyala, Nick Marschlich, Michael Glombitza, Steve Ho, Dr. Vikas Trivedi, Dr. Suraj Shankar, Dr. Qiong Yang

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Wetting and dewetting phenomena are fundamental to numerous morphogenetic processes in development, ranging from mammalian intestinal villi formation to zebrafish epiboly. While previous studies have investigated these dynamics using simple monoculture systems, our work leverages a more complex model: three-dimensional zebrafish embryo explants known as pescoids. This approach allows us to consider the multitude of factors influencing wetting and dewetting in biological tissues within a developmentally relevant context.

We focus on the outer layers of pescoids where high-resolution microscopy is most feasible. Cell segmentation, tracking, and particle image velocimetry (PIV) were used to map strain rates and surface area changes over time. We noticed that the pescoid wetting-dewetting sequence occurs autonomously over ~12 hours at 28°C, similar to the epiboly process in wild-type zebrafish embryos. The dewetting transition is triggered at ~6 hours, which we noticed was strongly coupled with mesoderm onset in the pescoid's center, the area of highest cell density. PIV analysis revealed increased strain rates in the center at dewetting onset followed by contraction of the leading edges, suggesting a potential differentiation-linked trigger for the wetting-to-dewetting transition. This transition, analogous to non-equilibrium complex fluid behavior, compacts the tissue into a spherical geometry. We observed a critical maximum radius of 205 ± 3.7 µm at peak wetting. Strikingly, wetting-dewetting persisted after inhibition of cytoskeletal dynamics with blebbistatin.

Based on preliminary results, we propose that wetting-dewetting dynamics are not driven solely by cytoskeletal mechanics but also by active cell differentiation and dynamic changes in cell density.

Chiral-based Hydrogel Scaffolds Bias Immune Mismatched Skin Transplantation Toward Engraftment Through Humoral Attenuation

Ms. April Espinoza, Ms. Alejandra Suarez-Arnedo, Dr. Holly Lewis, Dr. Tatiana Segura

Organ transplantation requires life-long systemic immunosuppressants with several side effects; injectable biomaterials may offer an alternative approach with tunable properties to enable in situ immunoengineering. Before these therapies can be translated into clinical use, it is important to study their role in tolerance induction. Several researchers have used locally-delivered hydrogels to encapsulate immunologic drugs for pancreatic islet cell and limb transplantation. Our work extends those models, the uniquely-interlinking network of microporous annealed particle scaffolds (MAPS) engages innate and adaptive immunity, while restoring skin strength and native architecture. By leveraging the immunoregenerative properties of soft matter, we will deploy clinically relevant drugs within the transplant microenvironment to study the effects of allogeneic recipient-biomaterial interactions. We hypothesize hydrogel-augmented skin transplants will serve as an antigen-tolerization platform, reduce reliance on intravenous or oral medications, and control the alloimmune response.

Initial transplants were performed in congenic mice (CD45.1+ to CD45.2+), with blinded clinicopathological scoring revealing that MAPS-augmented tissues exhibited non-inferior to slightly-improved engraftment. In a time-dependent fashion, MAPS modulated donor- and host-derived antigen-presenting cells, including T-cell costimulatory markers (CD80, CD86), with recruitment of regulatory T cells to skin-draining lymph nodes and memory compartments. Together, these data demonstrate that MAPS may have a transformative impact as a platform for donor-directed immunotherapy prior to transplantation.

We sought to develop a more clinically-relevant model with mismatched Balb/c donors and C57BL/6 recipients. Grafts rejected over four weeks, as would be expected for allogeneic transplants. Using flow cytometry to study donor-specific antibodies (DSA) after transplantation, we found that MAPS treatment attenuated alloreactive DSA. Although DSA do still develop, MAPS attenuates the rate at which antibodies developed alongside the overall magnitude and variability of the observed alloreactivity. Together, these data show that even without co-delivery of biologic agents, the structural and biochemical properties of MAPS is modulating the immune response in a time- and context-dependent manner. Further studies are underway to conduct site-specific delivery of antibody-based drugs (CTLA4-Ig), a known immunomodulatory agent in transplantation, released via self-assembled scaffolds in hopes of polarizing recipient leukocytes toward tolerogenic phenotypes. MAPS is a powerful platform in assessing allograft-interface interactions and demonstrates promise as a next-generation approach in transplant immunology.

Dissecting the Complexities of Phase Separation in Living and Synthetic Systems

Hongbo Zhao, Amy Strom, Clifford Brangwynne, Sujit Datta, Andrej Košmrlj

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

This poster explores the complexity of phase separation in two distinct biological systems: membraneless intracellular compartments in the cell nucleus and the collective behavior of bacteria. These systems are characterized by their complex interplay of mechanical interactions and nonequilibrium activities. Our work reveals how competition between elasticity and capillarity influences the structural and mechanical properties of chromatin networks, and how motility-induced phase separation coupled with movements along chemical gradients result in novel emergent phenomena in active systems. Looking forward, the theory and methodologies I developed for phase separation in fiber networks and active matter hold immense potential for unlocking new biophysics of living matter in complex and nonequilibrium environments.

Dynamic Display of ECM Ligands Controls Machinery of the Cytoskeleton from the Outside-In

Mr. Kyle Riker, Ms. Shreeya Bhonge, Dr. Mitch Butler, Dr. Maggie Daly, Dr. Qunzhao Wang, Mr. Stephen Klawa, Dr. James Bear, Dr. Ronit Freeman

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Cells have the ability to sense, integrate, and respond to temporospatial changes in their native environment including a variety of extracellular matrix (ECM) bound signals. The ability to respond to changes in these cues is essential for complex behaviors such as embryonic development, wound healing, and cancer metastasis. Many studies have looked at the response of cells to static gradients and shown that they have a remarkable ability to align themselves with and migrate along these predefined paths. However, the ways in which cells respond to dynamic changes in cue presentation as well as how cells make decisions based on cues presented at different locations along and distances from the cell is not well understood. Here we make use of a dynamic cell culture platform based on coiled-coil peptide display and peptide strand displacement to reversibly present ECM bound ligands to cells. We show that changes in the extracellular environment cause sequential changes in an ensemble of intracellular proteins, ultimately leading to large scale reorganization of cytoskeletal components and directed cell movement. When presented with changing gradients of the fibronectin mimetic RGDS, the most immediate response is seen in actin morphology through changes in the Arp2/3 complex, resulting in alternating spreading modes between lamellipodia and filopodia. We further expand this work by engineering a light-responsive coiled-coil pair that allows for spatially controlled presentation of ECM signals. When presented with local and conflicting cues, cells protrude their membranes in response to stabilized ECM ligands and can even polarize in a user-defined manner. These results help to better understand how the steps in the cell’s response to extracellular changes can be controlled and directed towards as specific result. This platform can be used further to integrate multiple cues using orthogonal peptide handles. Additionally, as more and more studies move to explore cell movement in 3D culture settings, peptide strand displacement can easily be extended to a hydrogel environment to explore cell behavior that more closely represents the in vivo setting.

Frustrated Phagocytosis of Beads by Macrophages on Traction Force Q-gels

Jim Fan, Megan Kern, Jeremy Cribb, Mike Falvo, Professor Klaus Hahn, Professor Richard Superfine

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Phagocytosis is a key immune system process where specialized immune cells engulf foreign particles, harmful bacteria, and cell debris. This is also a physical phenomena, where the immune cell makes decisions based on the mechanical properties of the target, and generates forces to dislodge the target cell from its cellular environment to complete engulfment. This biomechanical process proceeds through established steps of probing the environment with thin protrusions, attaching and recognizing surface ligands of the target, forming a cuplike structure around the target and finally enclosing the cup into a phagosome. The process is coordinated by tightly regulated organization and disassembly of the underlying actin cytoskeleton. The actin cytoskeleton itself during phagocytosis has been well studied, but it is still not well understood how the forces are exerted from the earliest stages, to dislodgement to final engulfment. Understanding this force mechanism would give key insights on how macrophages respond to targets like bacteria and cancer cells which have been shown to become stiffly embedded into the surrounding extracellular matrix in vascular epithelium. Our previous experiments probing forces with a combination light-sheet AFM microscope helped gain insight to the inward forces during certain stages of phagocytosis and indicated that a peeling process is at play during dislodgement. Using insights from that we aim to take a new approach by using 2.5D traction force microscopy to capture three- dimensional force vectors around the target and phagocyte (RAW264.7 macrophage) during the process of phagocytosis which would mimic the scenario in the human body of a macrophage engulfing a target on a tissue surface. We aim to achieve this by functionalizing a target bead that will bind to the surface of a traction force gel and then adding cells that will approach and engulf the target while we image with a combination of TIRF, confocal and light sheet microscopy. The insights gained will provide new connections between biology and soft matter physics, and new biological physics that may offer clues to improve therapies.

MELD Accelerated MD: A tool to study DNA-Protein Interactions

Taylor Kranbuhl

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Understanding the structural determinants of protein-DNA interactions can provide insight for advancements in gene regulation, DNA repair mechanisms, as well as the development of therapeutics targeting DNA-binding proteins. Histone-DNA interactions are of particular interest as they are essential for the folding of chromatin which regulates gene expression via controlled access to DNA. The study seeks to apply the methods used in “Structural predictions of protein-DNA binding: MELD-DNA” by Esmaeeli et. al 2023, to generate an understanding of the protocol for binding and structural predictions of protein-DNA complexes. The method introduced utilizes MELD (Modeling employing limited data) to increase the sampling ability of molecular dynamics simulations; this allows the use of larger systems that traditional methods would find too computationally expensive. By applying the same computational framework and parameters, we have reanalyzed the DNA-Protein complexes to assess the reproducibility in order to apply to the Histone-DNA complex in the future.

Probing effects of vimentin on cell cytoskeleton dynamics through Differential Dynamic Microscopy (DDM)

Ms. Renita Saldanha, Yiling Lan, Dr. Rae Robertson-Anderson, Dr. Ryan McGorty, Dr. Alison Patteson

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The cell cytoskeleton is a complex network of actin, microtubules, and intermediate filaments, which play a fundamental role in cellular processes, such as cell polarization, intracellular transport, and cell migration. While microtubules are central to cell-polarization and have been studied in great detail, vimentin intermediate filaments also seem to play a role, as disrupting vimentin impairs polarized cell motion and the directional mobility of vesicles. In our investigation, we employed Differential Dynamic Microscopy (DDM) to explore the dynamic behavior of the microtubules and vesicles in wild-type and vimentin-null mouse embryonic fibroblasts. DDM is a non-invasive method which offers the ability to elucidate cytoskeletal properties like dynamics of networks and transport dynamics by monitoring the movements of subcellular structures through high-speed imaging. Here, we measured the dynamics and spatial organization of microtubule network in presence and absence of vimentin and actin. Our research reveals that cells lacking vimentin show 1.5 times higher decay times compared to cells with vimentin, which suggest that presence of vimentin decreases the dynamics of microtubule filaments in the cell. Our results indicate a role of vimentin in mediating microtubule dynamics, which has important implications for how cells organize and coordinate polarized motion.

Simulation Studies to Predict Protein-Peptide Binding Affinities via MELD accelerated Molecular Dynamics

Maria Ciko

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

In this study, we explore complex formation via protein-ligand binding affinities, a valuable resource in disrupting the interactions that enable cancer growth with respect to drug discovery and structure-based design. Proteins have many degrees of freedom of internal and relative motion that can be captured by Molecular Dynamics (MD), though at a high computational cost. MELD, or Modeling Employing Limited Data, is a probabilistic approach using Bayesian integration of external information to not only locate the most frequent, low-energy conformations and accelerate the process, but facilitate flexibility in protein-peptide interactions. In a study conducted by Morrone, MELD demonstrated correct outcomes in a competitive inhibition environment across the nine systems. Our hypothesis is that we can effectively compute the relative binding affinities in a way that minimizes ligands' steric hindrance and mitigates the effect of slowed diffusion on simulation convergence time. After having confirmed the stability of nine docked systems comprising a MDM-protein and a peptide with a distinctive mutation using RMSD values, we aim to develop efficient MELD protocols to match Morrone's results with limited computational effort.

Substrate stiffness regulates collective colony expansion of the social bacterium Myxococcus xanthus

Ms. Nuzhat Faiza, Roy Welch, Alison Patteson

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Many cellular functions depend on the physical properties of the cell's environment. Many bacteria have different types of surface appendages to enable adhesion and motion on a variety of surfaces. Myxococcus xanthus is a social soil bacterium with two distinctly regulated modes of surface motility, termed the social motility mode driven by type iv pili and the adventurous motility mode based on focal adhesion complexes. How bacteria sense different surfaces and subsequently coordinate their collective motion remains largely unclear. Using polyacrylamide hydrogels of tunable stiffness, we found that wild-type M. xanthus spreads faster on stiffer substrates. Here, we show using motility mutants that disrupt adventurous motility suppresses this substrate-stiffness response, suggesting focal-adhesion-based adventurous motility is substrate-stiffness dependent. We also show that modifying surface adhesion by the addition of adhesive ligands, chitosan, increases the amount of M. xanthus flairs, a characteristic feature of adventurous motility. Taken together, we hypothesize a central role of M. xanthus adventurous motility as a driving mechanism for surface and surface stiffness sensing.

Sustainable Nanoformulations of Anthracyclines

Mr. Nandish Mudegowdru Nagappa

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Cancer has become one of the leading causes of morbidity worldwide and it is estimated that there will be over 13 million deaths because of cancer by 2030. Anthracyclines are the main therapeutics used in various types of cancer treatments, they inhibit the activity of topoisomerase II, an enzyme responsible for DNA transcription and replication, generating unstable, highly active free radicals that damage the DNA and cause cell death, although it has a broad spectrum of antineoplastic activity, adverse events especially cardiotoxicity has limited the usage of conventional anthracyclines like doxorubicin in clinical practice. Numerous data was reported on reducing toxicity of the anthracyclines by developing novel analogs, or using low dose, prolonged, continuous infusion schedules and with the use of liposomal and other encapsulation technologies. Novel drug delivery systems aim to reduce the adverse side effects and enhance the specificity of the chemotherapeutic drugs.

To overcome the above challenges, we want to develop a nanoemulsion drug delivery system for anthracyclines, for this we are using two different surfactants which helps in engulfing the anthracyclines and have desirable properties- THPP and Calixarenes. Tris(3-hydroxypropyl)phosphine (THPP) is demonstrated to be a versatile, water-soluble, and air-stable reducing/protective agent which shows exceptional stability at biological ph. Calixarene has the properties that allow controlled and localized administration of anti-cancer drugs like anthracyclines, due to its extraordinary selectivity, they reduce the toxicity and improve their biodistribution and tolerability. Using tris(hydroxypropyl)phosphine (THPP) and amphiphilic calixarenes reported in our previous study along with co-surfactants, to encapsulate anthracyclines: (i) doxorubicin hydrochloride, (ii) doxorubicin-14-valerate and (iii) valrubicin as well as alizarine dyes as their simulants in the host-guest complexes is reported. The nanoemulsions were fabricated to evaluate envisaged therapeutic effect and determine their cell toxicity profile. The surface tension of the surfactants was measured using Du Nouy method. For encapsulation, a high energy method (ultrasonication) was applied with variable time and energy input. The size and zeta-potential of the aggregates formed was measured using DSC. The nanoformulations revealed minor changes of size and charge for a week(s), giving us an information about stability of the (nano)emulsions prepared for forthcoming cell studies.

The Effects of Nano-plastics on Developmental Stages in Zebrafish & Nano-plastics as MRI Contrast Agents

Mr. Orelle Bulgin

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Our lab specializes in researching the synthesis and application of multicomponent colloidal nanoparticles, which are nanoscale particles ranging from 10 to 1000 nanometers in size and can be composed of various combinations of metals, semiconductors, polymers, or other materials. These nanocapsules offer unique functionalities but also present challenges in terms of growth and colocalization of multiple components. The lab focuses on their use in drug delivery and as contrast agents, employing two main methods of synthesis: mini-emulsion polymerization and flash nanoprecipitation.

One of our research projects involves investigating the impact of nanoplastics nanocapsules on marine life, particularly the development of Zebrafish embryos (Danio rerio). Zebrafish serve as an excellent model organism for studying vertebrate development and diseases like cancer and neurological disorders due to their physiological similarities to humans. There are ongoing experiments involving exposing zebrafish to nanoplastics through their diet and surroundings to investigate their potential impacts/effects.

Eventually the fate of these particles are determined through a process called ICP-MS, determining the mass concentration of particles in the fishes. These Manganese Iron particles amongst others are also being used as potential contrast agents where phantoms are being employed to test the limits of their sensitivity in all hopes of replacing current gadolinium contrast agents which is detrimental to patients with kidney diseases due to the risk of nephrogenic system fibrosis.

The effects of substrates on biofilm growth

Mr. Sounok Ghosh, Dr. Jennifer Schwarz, Dr. Alison Patteson, Dr Antun Skanata

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Bacteria reproduce and generate extracellular polymeric substance (EPS) to form biofilms, multicellular communities of bacteria often found on surfaces. Biofilms are complex systems where individuals perform specific tasks based on their intracellular signaling networks and the environmental cues that they receive. Several experiments have also observed biofilms expand at rates that depend on substrate stiffness, but the exact mechanisms behind this collective behavior are not well understood. We present an agent-based model to address these observations and suggest a possible mechanism for biofilm expansion on substrates characterized by their stiffness, where the individual's tasks are coupled to nutrient availability and substrate properties. We apply our model to current and ongoing experimental studies of biofilm dynamics and growth on dynamical substrates

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Colloidal Matter

Aerosol-assisted particle deposition for solvent-free fabrication of MOF-polymer composites

Darshana Malusare, Dr. Hooman Tafreshi, Dr. Saad Khan

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The increasing focus on sustainable methodologies is spurring the development of multifunctional materials through solvent-free fabrication processes. Metal-Organic Frameworks (MOFs) represent a class of porous multifunctional materials, distinguished by high surface area, tunable pore size, and intricate three-dimensional network structure. MOFs find diverse applications across various fields including gas storage and separation, catalysis, sensing, drug delivery, environmental remediation, and energy storage. However, MOFs typically exist in an agglomerated powder form, necessitating integration into a suitable substrate to enhance their applicability. Polymer-based fibrous mats, renowned for their highly flexible, lightweight, and breathable structures, present themselves as ideal candidates for this purpose. Traditional techniques often rely on organic solvents in the fabrication of MOF-polymer composites. Addressing this challenge, we present a solvent-free technique for deposition of MOFs onto fibrous mats. This method utilizes an in-house aerosolizer specially engineered to disperse MOF particles uniformly by breaking up agglomerates. Our initial study focuses on using analogous adsorbents to study key parameters which influence the deposition process. We systematically investigate aerosolization conditions, substrate morphology, particle size (ranging from 0.5 to 10 µm), and concentration to discern their impact on the uniformity, coverage, and adhesion strength of the particles. We achieve composite materials with up to 30 wt% of analogous adsorbent particles through this process. Our recent investigation focuses on zeolitic imidazolate framework (ZIF-8) MOF (surface area 1800 m2/g) integrated on a unique sheath-core structure of fibers. The aerosolized MOF particles are directed onto the fibrous mat, where they adhere through weak intermolecular interactions. Characterization of the composites includes quantitative analysis via thermogravimetric analysis and BET surface area testing. Additionally, microscopic techniques like SEM are employed to qualitatively examine the deposition of MOF on the mats. Overall, we will discuss the intricacies of our fabrication method, detailing its optimization, comprehensive characterization, and wide-ranging applications of the resulting composites.

Bidirectional currents in confined driven colloids

Dr. Antonio Ortiz Ambriz, Mattia Ostinato, Dr. Pietro Tierno

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The problem of moving colloidal particles in suspension has attracted much attention due to the possibility of using them for sensing, medical diagnosis, and drug delivery. On the other hand, it is well known that matter behaves differently in confined spaces. One example of this is the lubricating properties of a water layer, which acquires a different structure when only a few layers of atoms can fit in the gap between two surfaces.

I will discuss the rich behavior that appears from experimentally bringing a strongly confined colloidal system out of equilibrium by adding a dynamic magnetic field. With this strategy, we can assemble the system in particle pairs, which can be made to rotate synchronously or asynchronously, or we can obtain buckled phases with soft potentials. By adjusting the packing fraction, an intermediate state can be induced in which particle pairs are broken and reassembled with other particles in a continuous exchange of neighbors. In this case, when the field is

spatially isotropic there is no net particle current and the colloids display strongly enhanced diffusive dynamics.
If we add a small in-plane component, this exchange process can be harnessed to produce a “ceilidh”-like bidirectional current with particle transport in a state that is reminiscent of skipping orbits in electronic and molecular systems. These currents can be strongly affected by the presence of defects

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Collision-mediated Transfer Kinetics of Cargo Items Among Mobile Nanocarriers

Faruk Hossain, Dr. Guilherme Bossa, **Dr. Sylvio May**

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Micelles, liposomes, microgels, dendrimers, macrocyclic host molecules, and nanoparticles represent nanocarriers used to transfer cargo items--such as drug molecules--among each other and to a carrier target. We calculate the kinetics of collision-mediated transfer of cargo items within ensembles of chemically distinct mobile nanocarriers that each hosts non-interacting cargo items on discrete and identical sites. Rate equations for collision-mediated transfer of cargo items are expressed in the Gaussian limit as a set of Fokker-Planck equations and solved analytically for arbitrary initial distributions.

Colloids with a Twist: Controlling Filament Helicity and Length to Tune Macroscopic Rheology

Nicholas Cuccia, Daniel Ravicz, Itamar Kolvin, Zvonimir Dogic

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The macroscopic rheological behavior of a dense suspension is intrinsically linked to the microscopic interactions of its constituent particles. Using bacterial flagella, a rigid biological filament, we construct a novel colloidal system that allows control over these interactions from the colloid's shape. Flagella are polymorphic, capable of transforming between several discrete shapes in response to external chemical conditions, temperature, and stress. Straight flagella filaments, for instance, twist into helices with uniform pitch and diameter after mild heating in a particular biocompatible solvent. This morphological transformation is directly imaged using fluorescent microscopy. In a dense suspension, the abrupt change in shape results in intricate collective motion as each coiling particle rapidly entangles with its neighbors. Macroscopically, these entanglements manifest as a dramatic increase in the system's bulk viscosity, which we characterize using a rheometer. Many shape changes are reversed upon restoration of the initial sample conditions, offering a unique way to switch the system's rheological properties between markedly different states. Our findings pave the way for a new category of complex fluids whose viscous properties can be toggled by manipulating their constituent particles' shape.

Data Driven Inference of Colloidal Interactions

Mr. Florian Benedetti, MSc. Tayebeh Saghaei, Dr. Peter van Oostrum, Dr. Emanuela Bianchi

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Florian Benedetti 1, Tayebeh Saghaei 2, and Peter D. J. van Oostrum2, Emanuela Bianchi 1,3

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Forces between colloidal particles cannot generally be measured directly while they contribute to particle movements and ultimately drive self-assembly. We develop methods to infer the forcefield in colloidal systems from experimentally accessible trajectories. According to the Overdamped Langevin Equation (OLE) [1-2], colloidal motion is the sum of two terms: a deterministic motion caused by the total force between the colloids that depends on their (respective) coordinates and a stochastic motion due to the solvent thermal agitation, known as diffusion. Consequently, direct measurement of colloidal motion gives only access to a noisy estimator of the total force and nothing can be said about the different components in the forcefield (i.e external field, pairwise interaction, …). Furthermore, hydrodynamic couplings make the diffusion state dependent and the motion of one colloid becomes correlated with the motion of all the surrounding colloids [3]. Following the core idea developed in [4], we introduce a basis with physical inductive biases to capture the different phenomena behind hydrodynamic couplings. Then, using the inferred hydrodynamic couplings, we decorrelate colloidal motions and apply a similarly designed basis to disentangle the different forcefield components. Within this approach, we validate our method on both passive and active 3D systems simulated using Brownian dynamics with hydrodynamics [5]. We show that we are able to get very good quantitative agreements between the exact and inferred hydrodynamic couplings as well as the self-activity and pairwise interactions.

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Dynamical long-time coupling in binary suspensions of highly charged colloidal particles

Mr. Daniel Weidig, Prof. Dr. Joachim Wagner

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Particles' size dispersity is a crucial issue in real colloial suspensions with impact on these systems' properties. Regularly, particle sizes influence particle interactions and thus both, time-averaged, static properties and dynamic behavior. We investigate the propagation of different mobilities to the time-dependent diffusive motion of interacting particles. The Yukawa-type interaction in highly charged colloidal particles is essentially governed by their effective number of charges. Investigating binary mixtures of equally charged, but differently sized particles with different

short-time diffusion coefficients allows to isolate the effect of different mobilities preserving identical interactions between particles either belonging to the same or different species.
In highly dilute suspensions with next neighbour distances typically one order of magnitude larger the largest particles' diameter, equally charged particles, independently of their actual size, interact via a Yukawa potential with practically identical potential parameters. Hence, in time-average, identical partial pair correlation functions $g_{11} = g_{22} = g_{12}$ result since, due to the long-range electrostatic repulsion, particle distances comparable to the individual particles' diameter do not occur.
According to Brownian dynamics simulations, coupled via electrostatic repulsion, faster fluctuations of more mobile particles influence the long-time dynamics of less mobile particles and vice versa: long-time self-diffusion coefficients normalized to Stokes-Einstein diffusion coefficients of larger particles are enhanced in presence of a more mobile species, those of a faster species are slowed down in presence of a larger, less mobile species. The analysis of size- and number-density-dependence of these effects reveals a nearly linear, universal dependence on the size- and number-density-ratios.
Also collective dynamics, analyzed by partial van Hove functions in reciprocal space and time-domain is influenced by the presence of a differently sized species: Time constants and functional form of the correlation decay, both between identical and different species, are altered in presence of a species with different short-time mobility as quantified by parameters of stretched exponentials used as a first heuristic description of the time-dependence observed in computer experiments.

Effective interactions between colloids: an approach based on the contraction of the bare forces.

Dr. Ramón Castañeda-Priego

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Effective interactions are fundamental for determining the phase behavior of a vast number of materials and colloidal dispersions and have been used for the manipulation of in- and out-of-equilibrium thermodynamic states. In the case of depletion forces, a particular case of effective interactions, their entropic nature is well understood; however, most theoretical approaches, and molecular simulations, work quantitatively at moderate size ratios in diluted systems since large size asymmetries and high particle concentrations are difficult to deal with. The existing approaches for integrating out the degrees of freedom of the depletant species may fail under these extreme physical conditions. Then, the main goal of this contribution is to introduce a general physical formulation capable of evaluating the depletion forces even in those cases where the concentration of all species is relevant. We show that the contraction of the bare forces uniquely determines depletion interactions. Our formulation is tested by studying depletion forces in a vast number of interesting physical situations, even close to non-equilibrium thermodynamic conditions.

Hydrophobic Forces in Foam and Emulsion Films

Dr. Roe-hoan Yoon, **Dr. Aaron Noble**, Dr, Kaiwu Huang

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Hydrophobic Forces in Foam and Emulsion Films

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We used the Scheludko-Exerowa cell to measure the surface forces in the thin liquid films (TLFs) of surfactant-free water confined between two air bubbles and two hydrophobic solvent (toluene) drops by recording the changes in curvature using a high-speed video camera. The recorded interference patterns were analyzed using the Laplace, Reynolds, and DLVO theories to determine the surface forces in the TLFs. It was found necessary to consider the presence of hydrophobic forces in both the foam and oil films in addition to the EDL and vdW forces to obtain disjoining pressure isotherms Π(h) and explain the experimental data obtained at different temperatures and NaCl concentrations. The isotherms measured at lower temperatures shifted to a lower pressure range, suggesting that the attractive hydrophobic forces increase with decreasing temperature.

Analysis of the isotherms obtained at different temperatures (10-20oC) showed that hydrophobic interactions in foam and hydrophobic solvent films are driven by enthalpy rather than entropy, i.e., $|\Delta H| > |T\Delta S|$, which is the opposite to the hydrophobic interactions at molecular scales. However, the free energy changes (ΔG) are small due to significant enthalpy-entropy compensations. It was also found that the hydrophobic forces measured in foam films are weaker than those measured in the hydrophobic solvent films but are longer ranged. Hydrophobic forces in both the foam and solvent films become weaker and shorter ranged at higher NaCl concentrations.

Mie scattering theory applied to light scattering of large nonhomogeneous colloidal spheres

Mr. Christian Balderas, Prof. Dr. Rolando Castillo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Smart microgels, like PNIPAM (Poly(N-IsoPropyl AcrylaMide)) microgel particles, have unique properties that make them attractive for various applications, such as biomedical, water cleaning, and optical switches. Regardless of the application in question, one of the fundamental steps in studying microgel particles is to determine their form factor function to obtain information about their internal structure, where typical experiments, like Small-Angle Neutron Scattering (SANS), Small-Angle X-ray scattering (SAXS), and Static Light Scattering (SLS) are used.

The Rayleigh-Gans-Debye approximation (RGD) models often determine the form factor function in light scattering experiments for small particles compared with the light scattering wavelength. However, they can not be used when the particle diameter is comparable to or larger than the light wavelength used for light scattering experiments or when the difference between particle and solvent refractive index is large. One example is PNIPAM particles, whose size is temperature-tuned and could abruptly change their light scattering from Rayleigh to Mie scattering regime.

In this work, we apply the Mie scattering theory for a multilayer sphere to describe the static light scattering of different core-shell particles, comparing with static light scattering experiments for core-shell particles made of polystyrene hardcore and PNIPAM shell (PS/PNIPAM particles), developed by us, and comparing with experimental data for PNIPAM light scattering from other authors, with excellent results.

Motion of chemically powered Janus colloids in an anisotropic fluid.

Ms. Devika Gireesan Sudha, Ms. Hend Baza, David Rivas, Dr. Sambeeta Das, Prof. Oleg Lavrentovich, Prof. Linda S Hirst

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Platinum-coated Janus colloids exhibit self-propelled motion in aqueous solution via the catalytic decomposition of hydrogen peroxide. Here, we report their motion in a uniformly aligned nematic phase of lyotropic chromonic liquid crystal, disodium cromoglycate (DSCG). When active Janus colloids are placed in DSCG, we find that the anisotropy of the liquid crystal imposes a strong sense of direction to their motion. The Janus colloids move parallel to the nematic director. Motion analysis over a range of timescales reveals a cross-over from ballistic to super-diffusive behavior on timescales below the relaxation time for liquid crystal elastic distortions. Surprisingly we observe that smaller particles roll during ballistic motion, whereas larger particles do not. This result highlights the complexity of phoretically-driven particle motion, especially in an anisotropic fluid environment.

Mpemba effect in terms of mean first passage times

Mr. Matthew Walker, Dr. Marija Vucelja

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Out of equilibrium systems host a variety of complex behavior, but one example that stands out is the Mpemba effect—named after the phenomena when a hotter system might cool faster than an identical, but colder one. Supposedly known to Aristotle, this effect has recently been given a lot of attention. In this talk I will highlight the recent progress in understanding The Mpemba effect, where I focus on an experimentally realizable colloid system that hosts but the strong and weak Mpemba effect. I will show the initial conditions necessary to observe the effect and express the criteria in terms of a first passage time problem.

Nonaffinity in colloidal gels

Mr. Max Jiang

Gels are viscoelastic solids widely used to stabilize fluids. Their space-spanning, highly disordered microstructures make it extremely difficult to understand their bulk rheological properties. Here, we study colloidal gels formed from colloid-polymer mixture to understanding their viscoelastic properties. Using a home-made shear setup with confocal microscope, gel deformation is tracked in single particle level. We find that subjected to cyclic shear, colloidal gels exhibit unexpected nonaffinity localization. Furthermore, this nonaffinity localization can be directed by shear deformation history. We directly visualize how nonaffine deformation of strands happens inhomogeneously in the network. We contribute this surprising nonaffinity localization to the interplay between plastic deformation due to straining and hydrodynamics due to the shear.

Precision measurement of homogeneous crystal nucleation of hard-sphere colloids

Zizhao (Will) Wang, Alexander Young, Dr. Debora Walker, Prof. David Weitz, Prof. Frans Spaepen

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

There is a large discrepancy between theory and experiment in the rate of homogeneous crystal nucleation in hard-sphere systems: copious nucleation has been discovered where MD simulations predict imperceptible values. Since these experiments have been challenging, we have addressed this again by performing high-precision measurements of the rate of nucleation under carefully controlled conditions. Homogeneous nucleation was investigated by confocal microscopy of a density-and-refractive-index-matched colloidal system at a range of volume fractions. By roughening the sample chamber walls, heterogeneous nucleation was suppressed, and all crystals formed at random positions in the builk liquid. Homogeneous nucleation was confirmed from the randomness of the crystal orientations. At each volume fraction, we tracked the evolution of each crystal and determined the crystal growth probabilities as a function of cluster size, as well as the critical nuclei size and the nucleation rate. Good agreement with simulation and classical nucleation theory was observed at volume fractions higher than 52%. At lower volume fractions, we measured higher nucleation rates than seen in the simulations, but lower than in earlier experimental work. We found many crystal nuclei are not compact spheres, as assumed in classical nucleation theory: crystals containing fewer than 30 particles tend to be more non-spherical and non-compact than larger crystals. The interfacial energy between crystal and fluid phase inferred from the measured critical sizes gave values similar to those found in macroscopic simulations.

Reversible Assembly of Iron Oxide Nanoparticles on Gold Nanorods for Magnetic Alignment and Plasmonic Control

Dr. Mehedi Rizvi, Dr. Ruosong Wang, Dr. Jonas Schubert, Mr. William Crumpler, Dr. Christian Rossner, Dr. Amy Oldenburg, Dr. Andreas Fery, **Dr. Joe Tracy**

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Overcoating gold nanorods (GNRs) with plasmonic or magnetic satellite nanoparticles (NPs) can modify the longitudinal and transverse surface plasmon resonances (LSPR and TSPR) through coupling with the satellite NPs. We report use of electrostatic interactions to reversibly assemble different types and amounts of satellite NPs on GNR cores, which allows coupling with and manipulation of the LSPR and TSPR of the GNR core. Cationic Fe_3O_4 NPs and spherical gold NPs (GNPs) functionalized with polyethylenimine (PEI) assemble on the surface of anionic GNRs functionalized with bovine serum albumin (BSA), yielding MagGNRs. The distinct extinction spectra of Fe_3O_4 NPs and GNRs make possible quantification of the loading of satellite NPs from optical extinction spectra. pH is a useful lever for controlling assembly and disassembly processes because the electrostatic properties of PEI- and BSA-functionalized NPs strongly depend on pH. Stable assemblies are obtained at pH between the isoelectric points of BSA (pI $\simeq$5) and PEI (pI $\simeq$11), because the core and satellite NPs have opposite charges within this window. At lower or higher pH, the core and satellite NPs have like charges, which inhibits assembly. Moreover, disassembly is possible by adjusting the pH to values outside of this range.

Magnetic alignment of MagGNRs arising from magnetic dipolar interactions on the anisotropic gold nanorod core is comprehensively characterized, including enhancement (suppression) of the LSPR and suppression (enhancement) of the TSPR for light polarized parallel (orthogonal) to the magnetic field. MagGNRs can also be driven in rotating magnetic fields to rotate at frequencies of at least 17 Hz. For suitably large gold nanorods (148 nm long) and Fe_3O_4 NPs (13.4 nm diameter), significant alignment is possible even in modest (<200 Oe) magnetic fields.

The effect of the glass transition temperature on the phase state of a colloidal system of oppositely charged latex particles

Dr. Sofia Morozova, Mr Albert Gevorkian, Dr Honghu Zhang, Dr. Weiqing Shi, Prof. Gilbert Walker, Prof. Oleg Gang, Prof. Eugenia Kumacheva

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Colloidal clusters and gels are of great interest in science and technologies as materials for sensors, cell scaffolds, precursors for absorbents and catalytic scaffolds. Particle softness strongly affects interparticle interactions and thus, on the state and properties of colloidal system. However, our understanding of the role of this factor in the properties of clusters and gels is only beginning to evolve. Understanding the relationship between particle softness and the formation of colloidal clusters and gels can benefit a broad range of technologies. Here we report the results of experimental studies of the impact of softness on network formation from the mixture of equally-sized oppositely charged polymer latex nanoparticles (NPs). Nanoparticle softness was controlled by performing experiments below or above the glass transition temperature (Tg) of the polymer, at which the interaction potential and adhesiveness of the NPs were significantly varied.

We demonstrated that in mixtures of oppositely charged polymer NPs with similar dimensions, symmetric opposite charges, at T<Tg hard contacts between NPs lead to their assemble in open clusters with hard-hard contacts, while at T>Tg soft-soft contacts between NPs results in in formation of dense precipitating aggregates and phase separation. Hard NPs formed H-H interparticle contacts, in which the NPs were not deformed. These NPs assembled in open clusters with

fractal dimension (Df) in the range of 1.5-1.9 (determined by image analysis, Static light scattering (SLS), Small angle X-Ray scattering (SAXS) and rheology experiments). Importantly, close correlation was observed between the results of SAXS and SLS for clusters NPs with more than six-fold difference in NP dimensions. Soft NPs undergo deformation during contacts which lead to partial coalescence and formation of aggregates with Df in the range of 2.5-2.9 (determined by image analysis, SLS and SAXS). Surprisingly, the addition of a small fraction of soft NPs to the mixture of oppositely charged hard NPs effectively triggered phase separation. We show that a transition from the colloidal gel to discrete precipitating aggregates occurs at a relatively small (20%) volume fraction of soft NPs in the stoichiometric mixture of oppositely charged NPs. These results were in agreement with adhesion interactions of NPs measured by atomic force microscopy. Clusters and network formation was qualitatively similar for oppositely charged NPs with dimensions in the range from 60 to 400 nm.
This result highlights the importance of hard-soft interactions with an intermediate value of the adhesive interparticle force. Our results shed light on the interactions of attractive hard and soft colloids before, during, and after the formation of hard-hard, hard-soft and soft-soft contacts. Moreover, since kinetically arrested colloidal gels have applications in many technologies, e.g., in food industry, personal care products, water purification, biotechnologies and as inks in extrusion-based 3D printing, our findings have far-reaching practical implications.

Theory of Entropy Driven Self-Assembly of Hard Particles

Mr. Isaac Spivack, Mr. Kristi Pepa, Mr. Trevor Teague, Dr. Domagoj Fijan, Dr. Sharon Glotzer

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Crystallization is a ubiquitous phenomenon that can arise across disparate length scales from diverse microscopic interactions. One fascinating example is the crystallization of hard particles, which interact solely via excluded volume and order to maximize entropy. Currently, the tools to enable an apples-to-apples comparison between hard particle crystals and crystals of other types (atomic, polymeric, etc.) do not exist. Towards this, we present a classical density functional theory that predicts the relative thermodynamic stabilities of colloidal crystals of hard particles. Uniquely, we treat hard shapes as fixed solute particles embedded in a solvent of fictitious pseudoparticles that distribute throughout the crystal according to an external potential arising from the positions and orientations of the hard shapes. We derive a free energy functional and minimize it to find the thermodynamically preferred pseudoparticle density distribution. We show that this pseudoparticle density distribution corresponds to the most probable crystal of the hard shape solute particles through comparison with simulations. In the future, we hope for this tool to enable direct comparisons between many classes of crystals, and lead to an enhanced understanding of crystallization in general.

Fluid Dynamics, Rheology

Angular Thresholds in Breaking Capillary Bridges

Mr. Samay Hulikal, Mengfei He, Marianna Marquardt, Hao Jiang, Anupam Pandey, Teng Zhang, Christian Santangelo, Joseph Paulsen

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Fluid droplets can be driven by the geometry of the underlying solid substrate. The modulation of liquid bridges impacts processes such as wet adhesion in insects and feeding mechanisms in shorebirds. Investigating the geometric parameters involved in the breakup of capillary bridges, we observe the existence of thresholds across which drastic changes in behavior occur. Notably, in the case of liquid bridges between angled supports, a critical angle emerges, resulting in a significant transition in post-breakup volumes. To understand this complex hydrodynamic process, we build a theoretical model and find that the seeds of the critical phenomena exist in the static liquid bridges. This understanding could provide fine-tuned fluid control and the potential for employing metamaterials in droplet manipulation.

Baseball gripping mechanics as a multiscale soft matter problem

Shravan Pradeep, Xiangyu Chen, Prof. Paulo Arratia, Prof. Douglas Jerolmack

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

A mysterious mud, named "Magic Mud", harvested from the Delaware river basin in New Jersey is the source for the gripping properties for Major League Baseball (MLB) for the past 90 years. Despite their extensive usage in baseballs, the mechanical basis for its lubrication and gripping properties on the baseball remains unknown. The mechanical properties of soil-based materials have optimized interparticle interactions from a mixture of cohesive agents (clay), natural stabilizers, geo/biopolymers, frictional particles (sand), and adequately distributed moisture. We posit that that the contribution of frictional and attractive components in the mud mixture controls the rheological (viscous dissipation) and tribological (frictional dissipation) properties. We investigate the mechanical properties of the baseball mud materials using macroscale rheology, microscale soft tribology, and nanoscale force characterizations to determine the grain-scale composition and its control on flow, frictional, and adhesive properties. At macroscale, rheological characterization of the mud showed that the baseball mud material is elastic (linear regime) and shear thinning (non-linear regime). In the microscale, soft tribology characterization of the mud-smeared baseball surfaces showed an increase in friction within the boundary regime. At nanoscale, the Atomic Force Microscopy (AFM) measurements showed that the baseball smeared with "Magic Mud" is twice as adhesive as that of the bare baseball surface. Our results suggest that the rheo-tribological properties of Magic Mud are controlled by two main components: (i) the micron-sized sand particles contribute to the frictional behavior, and thus the gripping properties of baseball mud, and (ii) the nanoscale clay particles that aid in material processing and nanoscale adhesive properties. We believe that the rheo-tribological framework developed in understanding the baseball mud can be extended towards developing sustainable earth-based lubricants and gripping agents.

Brittle-to-ductile rheology in composite hydrogels with a microfibrous network

Mr. Yug Chandra Saraswat, Dr Lilian Hsiao

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Recent studies have shown that the nonlinear and transient hydrodynamics of extracellular matrices in biological systems, such as increased stiffness, viscous dissipation, stress relaxation, and plasticity can substantially affect cell spreading, proliferation, and differentiation. Here, we report the strain stiffening and softening of composite 0.05 wt% agarose hydrogels composed of 0.038 wt% fluorescent dendritic chitosan microfibers dispersed in a water/glycerol solvent. A sol-gel transition occurs when the agarose is cooled below the gel point, during which the dendritic chitosan fibres self-assemble into a complex architecture within the agarose. The composite displays increased stiffness while still retaining high fracture strains. More interestingly, the presence of soft dendritic networks results in a complex softening-to-stiffening transition in response to various oscillatory and steady shear strains. The increased stiffness of the biopolymer composite is likely due to the formation of a dual network hydrogel in which chitosan microfibers form a sacrificial load-bearing network within the agarose matrix. The dendritic chitosan network might also suppress non-affine deformation within softer agarose matrix. At intermediate strains, re-distribution of internal stress occurs through temporary disruption in the chitosan network which could explain the observed softening properties. At higher strains, the background agarose matrix dominates the strain response as indicated by network stiffening until fracture. We use a confocal rheometer to visualize the heterogeneous yielding and breakdown of the inter-connected cluster network of chitosan microfibers within the strain softening regime to determine the microstructural mechanism responsible for strain softening. Findings from this study can help understand how cells might respond to the rheologically complex microenvironments that are abundantly found in nature.

Chemical species transport near sharp corners

Mr Mohamed Khattab, Dr CN Kaplan

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Mesenchymal cell migration is of particular interest for studying many mechanobiological phenomena including growth and cancer cell metastasis. The formation of cell protrusions during mesenchymal migration depends heavily on the interplay between multiple intracellular proteins including Rac and Rho GTPases, as well as the fluid-structure interactions between the cytosol and the cell membrane that develops kinks in the vicinity of the cell focal adhesion sites. Here we investigate how the advection and diffusion dynamics of a single chemical species are affected by Moffatt eddies, a low-Reynolds-number flow pattern emerging near a corner. To this end, we seek scale-free solutions to the 2D diffusion-advection equation to characterize the radial and angular dependence of the concentration field by using Moffatt's velocity profiles [1]. This will give us a basic understanding of the role of advection and diffusion in protrusion formation as a prerequisite to elucidating the efficiency of chemical signal transport inside the mesenchymal cell.

[1] Moffatt HK. Viscous and resistive eddies near a sharp corner. Journal of Fluid Mechanics. 1964;18(1):1-18.

Dissipative Active Motion of Colloidal Particles Rotating in Non-Newtonian Fluids

Mr. Abhirup Basu, Mr. Eric Buchsbaum, Dr. Orlin D. Velev

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

At the microscale regime, viscous forces dominate over inertial forces as Reynold's number << 1. Therefore, the locomotion of micromotors is based on breaking the flow-field symmetry around the particle. A common method of breaking the flow symmetry is by rotating the colloidal particles using a magnetic field near a substrate. As the particle rotates, it experiences higher hydrodynamic resistance in the lubrication layer between the particle and the substrate as compared to the resistance at the top of the particle. This difference in hydrodynamic dissipation rate results in the net translation of the particles. We report a new fascinating pattern of dissipative active motion of a new class of micro-scale colloidal rotators which rotate and translate in non-Newtonian fluids. These micro-scale rotators are synthesized by assembling iron oxide nanoparticles inside polydimethylsiloxane (PDMS) microdroplets, after which the host droplets are cured in the presence of a static magnetic field. Typically, in a Newtonian fluid such as water, these soft beads exhibit a net forward translation as they rotate clockwise, which is often referred to as rolling. Surprisingly, in shear-thinning fluids, such as xanthan gum in water, we encountered a new backward movement pattern of the microbeads, which we refer to as 'moonwalking.' In this new dynamic pattern, the translation is opposite to the one expected by the rotational clockwise direction of the microbeads. By changing the xanthan gum concentration in water, we demonstrated that these microbeads could switch from rolling to "moonwalking" due to the change in the fluid's rheological properties. Our COMSOL simulation results show that this anomalous motion results from the difference in the shear forces acting on the top and the bottom of the particles due to localized non-uniform shear thinning around the particle. We further exploited the light-adjustable rheological properties of a photo-rheological (PR) fluid to propel these particles along multiple directions upon UV exposure without the need to manipulate experimental conditions. The new moonwalking phenomenon has the potential to deepen our understanding of fundamental principles of transport of autonomous particles in soft viscoelastic media and may open the door to future applications of active rollers in advanced biomedical applications.

Dynamic thickening and dethickening of 3D dense suspensions of Quincke rotors

Navneet Singh, Anna R. Barth, Edward Y. X. Ong, Bulbul Chakraborty, James P. Sethna, Eric R. Dufresne, Itai Cohen

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Exploring the promising potential of synthetic active materials involves manipulating their macroscopic bulk properties through precise control of microscopic interactions among constituents. While past studies have been constrained by limitations in manufacturing scalability and the capacity to induce significant stresses, hindering investigations into 3D bulk properties, we present

imaging and rheological findings on dense suspensions of Quincke rotors that circumvent these barriers. Our experiments unveil that in the absence of shear, Quincke rotation activity gives rise to dynamically evolving percolating structures. Additionally, our experiments reveal an emergent viscosity that is controlled by both suspension volume fraction and the degree of Quincke rotation activity. Strikingly, we find that the system exhibits both dynamic thickening and dethickening, contingent upon the ratio of active stress to shear stress.

Fluctuating hydrodynamics of an autophoretic particle near a permeable interface

Dr. Günther Turk, Prof. Ronojoy Adhikari, Prof. Rajesh Singh, Prof. Howard Stone

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Artificial self-propelled systems, particularly micro-swimmers, have emerged as versatile models for simulating their biological counterparts and studying phenomena in systems far from thermal equilibrium. Catalytically covered phoretic particles, such as Janus swimmers, and active emulsions, such as droplets in surfactant solutions, serve as prime examples of artificial micro-swimmers. While phoretic colloidal particles typically exhibit autophoretic motion due to asymmetric chemical interactions, droplets can spontaneously self-propel through the non-linear interplay between surface osmotic flows and solute advection. In the limit where rapid diffusion of the solutes dominates their advection, spontaneous self-propulsion of isotropic particles can still be achieved near symmetry-breaking boundaries. Autophoresis near such boundaries is a focal point in the study of micro-fluidics, biophysics and surface science.

Here, using a naturally suited boundary domain integral description of both the chemical field and the fluid flow generated by the particles, we delve into analytically accessible results on such bounded motion. A particular focus point of our study lies on the combined effect of container boundary conditions beyond the well-studied no-slip wall and the resulting configuration dependent thermal fluctuations on the self-propelled dynamics. Our kinetic approach provides the Brownian motion of autophoretic particles near a boundary in terms of coupled roto-translational stochastic update equations containing mobility and propulsion tensors. The latter are found to arise from the active particles chemo-hydrodynamically coupling to the surrounding boundaries, with fluid and osmotic stresses finally inducing self-propulsion. We discuss our findings with the help of several examples relevant to current research in colloid and droplet dynamics. First, we analyse the Brownian dynamics of particles capable of complex motion in the bulk. We then introduce a chemically permeable planar surface of two immiscible liquids in the vicinity of the particle and provide explicit solutions to the chemo-hydrodynamics of this system. Finally, we study the case of an isotropically phoretic particle hovering above an interface as a function of interfacial solute permeability and viscosity contrast.

We hope that our analytical framework and stochastic analyses will provide valuable insights into the Brownian dynamics of autophoretic particles subjected to mechanical, chemical and hydrodynamic stresses and will thus contribute to the field of theoretical and applied soft matter science.

Growth and Coalescence of Nanoscopic Mesas in Stratifying Micellar Foam Films

Dr. Chenxian Xu, Dr. Yiran Zhang, Dr. Subinur I. Kemal, Dr. Vivek Sharma

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Freestanding films of soft matter exhibit stratification due to confinement-induced structuring and layering of supramolecular structures like micelles. Stratification in micellar films proceeds by the growth of thinner domains at the expense of surrounding thicker film, and local volume conservation leads to the formation of nanoscopic ridges at the moving front. The ridge often undergoes an instability leading to nucleation of nanoscopic mesas, that grow and coalesce over time along the moving front. The shape and size of ridges and mesas in stratifying films are visualized and analyzed using interferometry, digital imaging, and optical microscopy (IDIOM) protocols, with unprecedented high spatial (thickness < 100 nm, lateral ~500 nm) and temporal resolution (< 1 ms). In this contribution, we analyze the shape evolution and coalescence of mesas in an effort to develop a comprehensive understanding of drainage by stratification in micellar foam films, including the role played by the contribution of supramolecular oscillatory structural forces to disjoining pressure.

Low-cost optical plate for imaging shear sensitive liquid crystals

Christina Tang, Andrew Nguyen, Lenore Dougherty, Dawit Tekeste

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Rheological measurements with in situ visualization can be used to investigate the microstructural origin of complex flow behaviors of soft materials. In this work, we present a low-cost optical plate that costs approximately $50, is composed of 3D-printed and off-the-shelf components. The optical plate can be coupled with a digital camera such as a smart phone or GoPro to enable direct visualization of the flow. We examine design aspects such as materials selection, light placement, and camera properties. We then study the flow of a mechanochromic liquid crystal formulation. Specifically, strain sensitive liquid crystal formulations were achieved by blending ternary mixtures of cholesteryl chloride, cholesteryl pelargonate, and cholesteryl oleyl carbonate. The sensitivity of the color change using shear rate ramps is investigated. A blue shift was observed at ~30 Pa. The color change is dependent on the rate of change of the shear rate. We anticipate this will be a useful tool for applications in which macroscopic visualization of the flow is of interest.

Microactuators for Efficient Fluid Manipulation in Low Reynolds Environments

Ms. Viviana Londono-Calderon, Dr. Jacob Brooks, Dr. Jeremy Cribb, Dr. Richard Superfine

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

In this research, we present a novel approach to fabricate microactuators inspired by biological cilia, designed to effectively control and manipulate fluid flows within low Reynolds number environments. The so-called “scallop theorem” dictates that reciprocal one-dimensional actuators cannot generate directed fluid flow. However, phase-correlated hydrodynamically interacting actuators have not been studied at the microscale. Using lithography and molding techniques, we construct these microactuators with designed cross section and lattice parameters using polydimethylsiloxane (PDMS) with magnetic tips, enabling manipulation via external magnetic fields to induce beating patterns. Our design employs paired microactuators, each corresponding to a rectangular flap, wherein individual reciprocal movements collectively produce a non-reciprocal motion crucial for propelling fluids within low Reynolds number regimes. Through design strategies, we maximize microfluidic pumping and mixing, enhancing fluid manipulation capabilities. We fabricate high aspect ratio structures (1:20), with precise control over the magnetic filling process to maximize actuator bending. Each actuator exhibits a bending angle of approximately 27° when aligned with magnetic field lines. Demonstrating out-of-phase reciprocal actuation patterns, we showcase the ability to generate non-reciprocal beating patterns, crucial for driving fluid flow in low Reynolds number environments. Controlling these beating patterns is facilitated by an array of rotating permanent magnets, providing versatility in the actuation pattern of the microactuators. To visualize and study fluid propulsion, we employ fluorescent PDMS in actuator fabrication, enabling imaging of actuating structures and tracking of fluorescent beads as fluid flow indicators. Our platform serves as an experimental platform to test current models predicting that reciprocal actuators in close proximity can successfully drive flow in a low Reynolds number environment. By bridging biological inspiration with advanced fabrication techniques, our research contributes to the development of efficient microactuators for a wide range of applications, from microfluidics to biomedical devices.

Microscale hydrodynamic flows created by beating cilia

Mr. Rafał Błaszkiewicz

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Cilia play crucial roles in various microbiological contexts. In unicellular eukaryotes, they facilitate movement through coordinated motions. Cilia also cover coral surfaces, helping gather nutrients and remove waste. In humans, they move mucus in the respiratory system and transport egg cells through the fallopian tubes. While the steady flows generated by the collective movement of cilia are well-studied and understood, unsteady effects in the flow have received less attention. Although unsteady Stokes flows are less common, they occur in intriguing biological scenarios. In real-life situations, such unsteady flows can help organisms transport nutrients or evade threats. To understand the dynamics of these flows, we examine the beating of individual cilia and groups of cilia in the unsteady flow regime. The time-dependent Stokes equation, which remains linear, can be solved using time-dependent Green’s functions. These solutions involve a memory kernel with a known analytical form. Our study focuses on flow patterns created by time-varying forces that are constructed to model push of both a single cilium and a set of few cooperating cilia. Our research aims to establish the transport properties of these flows.
The poster presents simulations of flows generated by ciliary beats and the trajectories of advected particles, from which we can derive the system's transport properties. It also highlights the differences between stationary Stokes flow and the time-dependent regime we investigate.
This work has been conducted in collaboration with Arnold Mathijssen (UPenn, USA) and Maciej Lisicki (U. Warsaw, Poland).

Mutual information as a measure of mixing efficiency in viscous fluids

Ms. Yihong Shi, Prof. Ramin Golestanian, Dr. Andrej Vilfan

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Fluid mixing at the microscale is of paramount importance in biological organisms and in artificial systems. Examples range from the the uptake of oxygen, nutrients or chemical signals in aquatic organisms to microreactors and “lab on a chip” applications. In biology, mixing is frequently accomplished by cilia which drive long-range flows, but also localized regions of chaotic advection. A particular challenge to microscale mixing is posed by the time-reversibility of flows at low Reynolds numbers. Mixing therefore requires an interplay between advection (stirring) and diffusion. Here we introduce mutual information between particle positions before and after mixing as a measure of mixing efficiency. We demonstrate its application in a Couette flow in an annulus and show that the mixing efficiency depends in a non-trivial way on the time sequence of rotation. We show that under this measure, the mixing efficiency is symmetric upon time reversal of the actuation sequence. Among all sequences with the same rotation angle, the ones with optimal mixing consist of a fast rotation in the middle of the time interval, or in some cases two symmetrically arranged. We also determine mutual information from Brownian dynamics simulations using data compression algorithms and demonstrate that advanced neural network based compression algorithms can be applied to estimate mutual information to a high accuracy. Our results show that mutual information provides a universal and assumption-free measure of mixing efficiency in microscale flows. Furthermore, we expect that our formalism will also be applicable to more complex mixing situations, for example by active swimmers, natural or artificial cilia or in active materials. Our current work is to apply mutual information in studying mixing in active systems.

New Insights into Generating Monodispersed Drops with Glass Capillary Microfluidic Devices

Dr. Laura Adams, Dheeraj Sapkota

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

We report a new method for determining monodispersity in the microfluidic generation of water-in-oil single emulsions. The spacing between two consecutive emulsions during their generation is used to identify monodisperse and polydisperse regimes. A theoretical model accurately predicting our experimental findings for a variety of glass capillary microfluidic devices is also presented. Moreover, a phase diagram of drop diameter as a function of inner and outer fluid flow rates indicates optimal flow parameters for the production of monodispersed drops. Our findings emphasize the robustness of using droplet spacing as the parameter in determining monodispersity, despite geometric differences in microfluidic devices.

Quantifying chiral geometry with sedimenting helical ribbons

Dr. Greg Voth, Elias Huseby, Josephine Gissinger, Fabien Candelier, Nimish Pujara, Gautier Verhille, Bernhard Mehlig

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

We investigate the sedimentation of chiral particles in viscous fluid flow. We identify helical ribbons as simple particles with strong translation-rotation coupling whose symmetry ensures that the centers of mass, buoyancy, resistance, and mobility coincide. Experimental measurements of both
relevant mobility tensors show excellent agreement with simulations of ribbons made of interacting spheres. We observe quasi-periodic angular dynamics causing complex spatial trajectories. In tilt-spin phase space, orbits are closed due to time-reversal and reflection symmetry. Changing the helical ribbon length reveals a bifurcation at which the stable sedimentation orientations switch.

Rheology and 3D rotational dynamics of sheared dense colloidal suspensions

Mr. Austin Walker, Dr. Emanuela Del Gado, Dr. Jeffrey Urbach, Dr. Daniel Blair

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

In this talk, we will discuss our recent results on the rotational dynamics of dense colloidal suspensions that are subjected to externally applied shear. Using our custom confocal-rheology platform, we quantify the flowing state of these materials to observe the collective rotational behavior. Our in-house synthesized colloidal OCULI particles [1] have an offset core-shell construction, providing a real-space quantification of the rotational dynamics of each individual particle. This system allows us to simultaneously perform high resolution 3-D imaging in time, while performing bulk rheology. We track the particles within the dense colloidal dispersion when subjected to shear flow to link shear transformations to collective rotations within localized yielding events. We will demonstrate how varying the surface roughness of the OCULI results in different rheology and rotational dynamics.

This work is supported by NSF DMR 2226485

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The role of Hydrodynamic Interactions on the rheology of colloidal rods

Dr. Lucas Hildebrand Pires da Cunha, Dr. Paul Salipante, Dr. Steven Hudson

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Understanding the dynamics of rod-like particles under imposed flows is a fundamental problem in fluid mechanics with significant implications across various industrial sectors. The complex viscoelastic responses exhibited by colloidal rod suspension at semi-dilute concentrations are primarily governed by the flow-induced alignment of particles at the microscale. Despite extensive research on this topic since Jeffery's seminal work in 1922 on the dynamics of ellipsoidal particles in viscous fluids, the precise effects of hydrodynamic interactions (HI) between particles remain not well described. To address this gap, we employ numerical simulations based on the Brownian Dynamics method to explore the influence of HI on the rheology of semi-dilute colloidal rod suspensions. Our findings from this relatively simplistic model unveil a cascade effect wherein the tumbling of a single rod induces a disturbance in the flow, subsequently triggering the tumbling of neighboring particles and increasing the system's viscosity.

Topological DNA blends exhibit resonant deformation fields and strain propagation dynamics tuned by steric constraints

Dr. Rae Robertson-Anderson

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Understanding how polymers deform in response to local stresses and strains, and how strains propagate from a local disturbance, are grand challenges in wide-ranging fields from materials manufacturing to cell mechanics. These dynamics are particularly complex for blends of polymers of distinct topologies, for which several different species-dependent mechanisms may contribute. Here, we use OpTiDDM (Optical-Tweezers-integrating-Differential-Dynamic-Microscopy) to elucidate deformation fields and propagation dynamics of binary blends of linear, ring and supercoiled DNA of varying sizes. We reveal robust non-monotonic dependence of strain alignment and superdiffusive transport with strain rate. However, peak alignment and superdiffusivity are surprisingly decoupled, occurring at different strain rates resonant with the distinct relaxation rates of the different topologies. Despite this universal resonance, we find that strain propagation of ring-linear blends is dictated by entanglements while supercoiled-ring blends are governed by Rouse dynamics. Our approach captures critical subtleties in propagation and deformation dynamics of topological blends, shedding new light on the governing physics and offering a route towards decoupled tuning of response features. We anticipate our results to be broadly generalizable to mapping the deformation dynamics of polymer blends, with an eye towards bottom-up bespoke materials design.

Understanding fluid dynamics for all-aqueous printing of a viscoelastic droplet in yield-stress fluids

Ms. Xiaoxiao Ma, Mr. Jinchang Zhu, Dr. Liheng Cai

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

All-aqueous printing of viscoelastic droplets in yield-stress fluids is the foundational process of voxelated bioprinting, a technology using spherical bio-ink droplets as building blocks to create three-dimensional (3D) tissue mimics. However, the fundamental science of such a printing process is largely unknown. We develop a platform that allows for real-time visualization of both the side view and the vertical projection of a droplet when being printed in a yield-stress fluid made of granular hydrogels. Using Newtonian fluids with viscosity ranging by two orders of magnitude, we discover that, to form a round droplet with smooth surface, the ink should be of relatively high viscosity or extruded under relatively high shear rates. A similar observation applies to shear-thinning bio-inks. This behavior can be explained by a theory that the force associated with extruding the ink must be larger than the friction associated with the ink flowing through the porous granular hydrogel, such that the ink can mechanically displace the granular hydrogel to form a droplet of good fidelity. Further, for shear-thinning inks, the droplet roundness is determined by the ratio of droplet size to the nozzle diameter. Finally, using the yield stress of the supporting matrix and the shear stress associated with extrusion, we construct a two-parameter diagram-of-state to outline the conditions for printing droplets of good fidelity. Our results not only help establish the foundational knowledge of voxelated bioprinting but also provide the tools for engineering highly functional 3D tissues.

Unifying yielding mechanics in multiphase soft particulate matter systems

Shravan Pradeep, Prof. Paulo Arratia, Prof. Douglas Jerolmack

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Soft particulate suspensions are ubiquitous in nature. Their yielding and flow properties influence a wide array of materials, from consumer products to large scale geophysical flows. However, yielding mechanics in suspension rheology has traditionally been focused on two-phase mixtures: particles and the background solvent. Pure two-phase mixtures are rarely found in nature due to the variability in material type, size polydispersity, and diverse interparticle interactions. Here, we probe the mechanical failure of a multiphase particulate system, using model granular particles dispersed in a colloidal gel medium, thereby creating a system where the balance between frictional and cohesive interactions dictate the material failure and yielding properties. Using in-house assembled confocal rheoscope and granular rheometer with imaging capability, we extract microscopic signatures accompanying these yielding transitions. We find a transition from ductile to brittle failure, by varying the ratio of cohesive and frictional elements in the multiphase system. We propose a 3D rheological phase space that delineates three identified flow regimes: rate-independent plastic, rate-dependent plastic, and Newtonian, as a function of deformation rate, shear stress, and effective friction coefficient. We demonstrate that the mechanical framework proposed here is applicable to a model soil material: a multiphase suspension mixture of non-swelling kaolin clay and silica sand particles. Our approach provides a novel method to enhance hazard prediction models in multiphase soft particulate systems, such as geophysical flows.

Universal scaling of shear thickening suspensions under acoustic perturbation

Anna Barth, Navneet Singh, Edward Y.X. Ong, Meera Ramaswamy, Pranav Kakhandiki, Abhishek Shetty, James P. Sethna, Bulbul Chakraborty, Itai Cohen

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Nearly all dense suspensions undergo dramatic and abrupt thickening transitions in their flow behavior when sheared at high stresses. Such transitions occur when suspended particles come into frictional contact with each other to form structures that resist the flow. These frictional contacts can be disrupted with acoustic perturbations, thereby lowering the suspension's viscosity.

Acoustic perturbations offer a convenient way to control the suspension's shear thickening behavior in real time, as the suspension responds to the perturbation nearly instantaneously. Here, we fold these acoustic perturbations into a universal scaling framework for shear thickening, in which the viscosity is described by a crossover scaling function from the frictionless jamming point to a frictional shear jamming critical point. We test this theory on sheared suspensions with acoustic perturbations and find experimentally that the data for all shear stresses, volume fractions, and acoustic powers can be collapsed onto a single universal curve. Within this framework, a scaling parameter that is a function of stress, volume fraction and acoustic power determines the proximity of the system to the frictional shear jamming critical point and ultimately the viscosity. Our results demonstrate the broad applicability of the scaling framework, its utility for experimentally manipulating the system, and open the door to importing the vast theoretical machinery developed to understand equilibrium critical phenomena to elucidate fundamental physical aspects of the non-equilibrium shear thickening transition.

Using Vector Charge Electromagnetism to Examine Emergence of Gel Rigidity

Mr. Albert Countryman, Ms. H.A. Vinutha, Ms. Fabiola Doraly Diaz Ruiz, Dr. Bulbul Chakraborty, Dr. Xiaoming Mao, Dr. Emanuela Del Gado

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

We investigate the spatial correlations of microscopic stresses in soft particulate gels using 2D and 3D numerical simulations. We use a recently-developed theoretical framework predicting the analytical form of stress-stress correlations in amorphous assemblies of athermal grains that acquire rigidity under an external load via a mapping between the mechanical system and an emergent vector charge electromagnetism. These correlations exhibit a pinch-point singularity in Fourier space. This leads to long-range correlations and strong anisotropy in real space, which are at the origin of force chains in granular solids. Our analysis of the model particular gels at low particle volume fractions demonstrates that stress-stress correlations in these soft materials have characteristics very similar to granular solids and can be used to identify force chains. We show that the manner in which these systems adhere to and deviate from the predictions of the vector charge electromagnetic theory can inform upon the underlying physical properties of the gel system.

Variational formulation of physics-informed neural networks (vfPINN)
Chinmay Katke, C. Nadir Kaplan

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Physics-informed neural networks (PINNs) are deep neural networks that solve differential equations by minimizing a phenomenological loss function formed from these equations. The unknown variable is iteratively computed using backpropagation, finding solutions in a mesh-free setting. However, the involvement of higher-order derivatives in equations describing many physical systems results in high computational costs. Additionally, while solving coupled differential equations, PINNs introduce extra complexity due to ad hoc error weight factors that are either determined manually or via complex algorithms. We introduce a variational PINN (vfPINN) algorithm that optimizes functionals in integral form (e.g., Lagrangian, Hamiltonian, or Rayleighian) to overcome the aforementioned disadvantages: vfPINN naturally involves lower-order derivatives and replaces the ad hoc weight factors with rigorous physical scales. Our results from vfPINN show promising agreement with the known solutions to benchmark systems such as the Poisson's equation as well as other ordinary and partial differential equations. vfPINN achieves its accuracy through its ability to perform non-convex optimization of the functionals (when needed) by locating and excluding the singular points in the functional domain that cause non-convexity in the first place, known as conjugate points. Our ongoing research is focused on finding the conjugate points and in turn all solutions to non-linear partial differential equations that are known to have no unique solutions.

Glasses, Granular, Jamming

Can you hear a landslide coming (before it begins)?

Aditya Advani, Veronika Juylova, Richard Killburn, Clay Stoltenberg, Dr. Nakul Deshpande, Dr. Vashan Wright, Dr. Ted Brzinski, Dr. Karen Daniels

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

In disordered media, measurements of the vibrational Density of Modes (DoM) exhibit an excess number of low-frequency modes compared to Debye scaling and are associated with a loss of mechanical rigidity. We measure particle motion in earth materials, then compute the DoM using a method introduced in [1] and later extended to granular systems in [2]. We interrogate how low-frequency features in the DoM correlate with the packing structure, applied stress, and other characteristics of the sample. Changes in low-frequency features (like peaks) in the vibrational DoM before, during, and after perturbing the sample have previously been observed [3] to correlate with a loss of rigidity in granular structure. We aim to quantify these changes within idealized and soil-like samples to leverage existing geological monitoring infrastructure to understand better when conditions favor an earthquake or a landslide.

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[2] E. T. Owens and K. E. Daniels, Soft Matter 9, 1214 (2013)
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Coefficient of restitution of two colliding particles in experiment and simulation

Dr. Jeffrey Olafsen, Dr Kai Yang

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

We present a study of the coefficient of restitution of two particles free to collide in a vertically shaken channel both experimentally and via simulation. Multiple cases have been investigated with the driving frequencies, f, ranging from 23 to 32 Hz and the acceleration magnitudes, Γ, from 1.78 to 3.53 g. Both the experiment and simulation results suggest the coefficient of restitution is not simply a material constant, but rather depends strongly on the impact velocity. The dependence of the coefficient of restitution on the driving frequency and amplitude are also examined. The aim of the study is to understand the mechanism of super-elastic collisions, where the coefficient of restitution is measured to be greater than unity and suggests a gaining of translational kinetic energy after collision.

Compression-induced structural and mechanical transitions in disordered sticky-sphere systems

Dr. Michio Tateno, Dr. Wang Yinqiao, Prof. Hajime Tanaka

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Gels and attractive glasses, both non-equilibrium arrested states formed by sticky particles, appear in various soft matter systems, including colloids, emulsions, proteins, and wet granular materials. Previous research has uncovered intriguing similarities and differences in their structural, dynamic, vibrational, and mechanical properties. Nevertheless, the transition between gels and attractive glasses with increasing volume fraction and the clear distinction between the two remain ambiguous. Here, we address this issue by examining the continuous volume fraction variation during the uniaxial compression-induced gel collapse. Combining confocal microscopy observations with Brownian dynamics simulations, we identify a two-step structural transition in gels: from gels with space-spanning percolating voids to those with closed isolated voids, ultimately leading to attractive glasses without any voids. Notably, these first and second structural transitions exhibit a strong correlation with a rapid increase in normal stress and deviatoric stress, particularly evident at lower temperatures. This finding offers novel insights into the categorization and understanding of disordered non-equilibrium solids from a mechanical standpoint.

Glass Transition Behavior and Crystallization Kinetics of Celecoxib Carvedilol Co-Amorphous Formulations

Bret Tantorno, Dr. Gregory McKenna

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

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The majority of pharmaceuticals, approximately 60% to 70%[1], fall under Class II of the Biopharmaceutic Classification System, characterized by poor water solubility. This limitation often leads to reduced bioavailability and efficacy of active pharmaceutical ingredients (APIs). To address this issue, the use of APIs in the amorphous state has been explored, offering higher solubility compared to their crystalline counterparts[2]. However, the inherent instability of the amorphous state, prone to crystallization over time, poses a challenge in maintaining consistent bioavailability and dosages to patients overtime. In this study, we investigate the potential of co-amorphous formulations as a strategy to stabilize the amorphous state. Carvedilol (CAR) and celecoxib (CEL) were selected as model APIs due to blood pressure and anti-inflammatory medications being commonly prescribed together. Differential scanning calorimetry (DSC) analysis was performed on CAR/CEL mixtures, varying from pure CAR (1:0) to pure CEL (0:1) in 0.1 molar increments. The DSC results revealed notable findings during the heating cycles. The first heating revealed that the melting point of CAR (114˚C) remained consistent, whereas that of CEL (161˚C) decreased with increasing CAR content, due to an entropic difference between a pure crystal and its own melt versus a pure crystal and a mixture of CAR and CEL. Upon the second heating, it was observed that pure CAR formed a stable glass, whereas pure CEL exhibited a weak glass transition followed by cold crystallization and eventual melting. Notably, higher concentrations of CAR (0.2:0.8 to 1:0) in the mixtures suppressed cold crystallization in CEL, suggesting a stabilizing effect on the amorphous form of CEL. Furthermore, certain mixtures of CAR:CEL (0.6:0.4 to 0.8:0.2) exhibited a double glass transition, possibly attributed to phase separation at specific compositions. Lastly, the experimental glass transition data were fitted to the Gordon-Taylor (GT) equation, demonstrating a linear relationship between the mole fraction of CAR and the glass transition temperatures of the mixtures. Further research will focus on isothermal crystallization experiments to further understand the suppression of CEL crystallization by CAR, utilizing crystallization models such as the Johnson-Mehl-Avrami equation and classical nucleation theory. Additionally, phase diagrams of CAR/CEL mixtures will be constructed to explore potential phase separation phenomena. In conclusion, our study highlights the potential of co-amorphous formulations in providing stable and effective medications with tailored prescriptions.

We thank the National Science Foundation’s support under grant DMR 2105065, as well as the support from The Chemical and Biomolecular Engineering Department at NC State University.

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Granular active matter on approaching glassiness

Mr. Chetan Yadav

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

We are interested in understanding how the approach to the glassy regime will change with the introduction of activity in a fraction of particles in a system. In particular, we would like to know if the dynamics are merely sped up by activity or whether there is some qualitative change. To address these questions, we conduct experiments on a bidisperse mixture of discs in a plane, fluidized by vibration from a shaker. The discs are designed so that they can be chosen to have isotropic motions in the plane, or have a preferred polar mobility. We compare dynamics in 50:50 mixtures of large and small passive grains to 50:50 mixtures of large active and small passive grains as the total area fraction is increased. By studying the dynamic susceptibility, we see stronger heterogeneity in the active mixture, where dynamics is fastest along long-lived chains.

Locomotion of a scallop-like swimmer in granular media

Dr. Hongyi Xiao, Amir Nazemi, Dr. Achim Sack, Dr. Thorsten Poeschel

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Due to the soft and yielding nature of granular materials, simple swimming motions, which typically yield no locomotion in Newtonian liquids, can potentially generate propulsion in granular media. This study utilizes lab experiments and Discrete Element Method (DEM) simulations to examine the locomotion of a scallop-like swimmer with two flapping wings in granular materials. Results show that the swimmer could generate persistent locomotion by opening and closing its wings reciprocally. Analysis of particle trajectories and contact forces around the swimmer indicates that the observed swimming behavior is related to the swimmer selectively solidifying regions of surrounding particles via local shear jamming, which is non-reciprocal between the opening and closing stroke due to geometrical factors. We also discuss the role of friction, inertia, and flapping frequency via varying corresponding parameters in DEM simulations.

Metallic Glass Have More Rugged Potential Energy Landscape

Yue Fan, **Mr. Haoyu Li**

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Glass systems possess inherently disordered atomic packing and it is one of the unsolved problems to have an unambiguous structure-property relationship. Among different approaches, Potential Energy Landscape (PEL) provides a unique and intuitive aspect to probe the glass system behavior in hyperdimensional phase space. The current consensus on PEL in glassy systems is that it exhibits a two-scale mega-basin/sub-basin landscape corresponding to system level change, (e.g. glass transition) and cage-breaking atomic rearrangements (e.g., local plasticity events). In this classical picture, transitions corresponding to the sub-basin bottom of PEL (under low energy limits) are prohibited, which contradicts experimental observation and modeling studies. In this study, we seek to clarify this contradiction by a more complex image in the bottom of PEL in glass systems.

Here, we probe the smoothness of sub-basin bottoms in various glass models by imposing small cyclic mechanical perturbations. Glass models are prepared by quenching different interacting systems. Then they are given a shear and relaxation followed by a reverse strain and relaxation. Smoothness of the bottom of PEL is evaluated by measuring the net changes of atomic-level stress. We find that when a mechanical perturbation is applied, in pairwise-interacting systems (e.g., Lennard-Jones models, modified Johnson model, etc.) the changes of atomic-level stress exhibit sharp jumps only at cage-breaking critical strains, before which the stress level remains invariant. However, in many body-interacting system (metallic glass model), the atomic-level stress changes are much larger and exhibit a continuous variation even before the cage-breaking event happens, indicating additional ruggedness and complexity in the sub-basins of its PEL.

To further understand the details of sub-basin features in PEL, we also study the intra-cage surroundings of atoms in different systems by imposing single-atom perturbation, i.e., one atom is chosen and given a small displacement along different directions. By measuring the single-atom energy and system global energy change, we get an image of an atom's local environment. In single-atom perturbation study, we find that in pairwise-interacting systems, the variation of single-atom energy and global energy is always consistent, i.e., they always increase at the same time. Contrary to this, in many-body system, there are cases where single-atom energy decreases while global energy increases.

The results of cyclic perturbation indicate that many body-interacting glassy systems have a qualitatively different and more rugged bottom in the PEL from the pairwise ones, and the results of single-atom perturbation indicate that many body-interacting glass models have a more complicated local environment than the pairwise ones. These findings could supplement the classical picture of PEL with a focus on finer structures of sub-basin bottoms, and also reveal a profound connection between a system's bonding nature and its underlying PEL.

Non-affine motion in a quasi-2-dimensional granular matter under simple shear

Dr. Maniya Maleki, Mr. Mehran Erfanifam, Dr. Ralf Seemann, Dr. Reza Shaebani

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

In this experimental work, we study the dynamics of granular material in a quasi-2-dimensional setup, in dry and wet states. The setup applies simple shear to the grains through two rotating parallel walls at the sides and moving parallel narrow bars underneath the grains. The grains are hollow steel cylinders and are used in dry and wet states. In the wet state, we add a small amount of liquid to form liquid bridges and hence attractive interactions between the adjacent grains. We record the grains' movements using a camera and generate system velocity profiles for each experiment using a particle tracking method. We calculate the affine and non-affine motions of particles at different cell positions. Then we investigate the effect of packing fraction and fluid content on the affine and non-affine motions.

Relating the microscale to the macroscale in granular materials

Dr. Carmen Lee, Ephraim Bililign, Jonathan Barés, Emilien Azéma, Karen Daniels

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Granular materials, like soils and powders, play crucial roles in diverse applications from construction to agriculture to pharmaceuticals. Unlike continuous media, where strength can be determined by bulk material properties, the strength of granular materials is highly dependent on grain connectivity (fabric), force transmission, and frictional mobilization at the particle scale. Furthermore, these bulk properties are strongly dependent on the geometry and history of loading. It is well established that anisotropy in fabric and force transmission through a granular packing directly relates to the bulk scale strength of the packing. Although the relationship between particle-scale anisotropy and macroscale properties has been verified through simulated conditions, we have observed that it is valid for a broad variety of loading histories and geometries in experimental granular packings.

In this talk, I will present experiments conducted on a photoelastic granular system -- allowing us to measure individual interparticle contact forces -- subject to compressive and shear loading. By tracking both particle positions and interparticle contact force vectors, we map the anisotropy of the fabric and forces to the macroscale stress and strain. We find excellent agreement between the anisotropic particle-scale measures and the macroscale responses in experiments, independent of the loading geometry, showing that with knowledge of the forces and positions of the particles, one can predict the strength of the packing.

Solid Lubricants for Bio particles with Complex Shapes

Mr. Dhanush Udayashankara Jamadgni, Dr Paul Gregory, Dr Andrew Martin, Ms Alana Pauls, Mr Xiong Ye, Dr Paul Bogdan, Dr Nicholas Kotov, Dr Karen Daniels, Dr Martin Thuo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Bio-particle systems are complex granular systems. Their flow is affected by various factors such as friction, humidity, stress dissipation, etc. Seed systems in particular form complex networks due to their stochastic aspect ratio, size distribution, and surface texture which need to be continuously reorganized for the system to flow without piping, doming, or tunneling that leads to network jamming. Commercial seed lubricants are either toxic(asbestos) or lead to microplastic accumulation and pollution. In this work, we present the design and validation of bio-safe and cellulose-based network disruptors to Improve seed flow in agricultural planters.

Stokes-Einstein violations in models of dense cellular materials

Dr. Helen Ansell, Chengling Li, Prof. Daniel Sussman

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Vertex and Voronoi models are frequently used to model the glassy dynamics of densely packed cellular tissue. They are known to display anomalous glassy dynamics, such as sub-Arrhenius scaling of the dynamics with temperature [1,2]. Given this departure from the standard behavior of glassforming systems, we further investigate the low-temperature disordered dynamics of these models. Here we focus on the breakdown of the usual Stokes-Einstein coupling between viscosity and diffusivity in the Voronoi cell model of 2d confluent tissue as the temperature is varied. Further understanding of the unusual properties of these models will give insight into the scope of possible low-temperature disordered dynamics in other glassy materials as well as possible consequences for the glassy dynamics of biological tissues.

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Studies into the structural order of random pinning systems and their driven dynamics

Mr. Owen Tower, Mr. Jonah Eick, Ms. Lihy Buchbinder, Mr. Abdulai Gassama, Ms. Nehal Sharma, Dr. Robert Pelcovits, Dr. J. Michael Kosterlitz, Dr. Xinsheng Sean Ling

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The microscopic mechanisms by which materials change from liquids to solids without the usual crystallization process remains unknown. Whether window glass is a slowly aging liquid, or a true solid remains a longstanding unresolved question in condensed matter physics. Building on the recent research in two-dimensional (2D) colloidal crystals, we present theoretical and experimental studies regarding the nature of the glass transition. Our simulations were that of a 1D longe-range Ising model with a random external field in system sizes of 50 to 350 spins. The Metropolis algorithm was used to drive this system to equilibrium in a low-energy state (not necessarily ground state) in order to observe the possible existence of a phase transition. Some results of this theoretical study support the transition line between paramagnetic and ordered XY phases as predicted by Cardy and Ostlund. Ongoing experimental studies will probe the Cardy-Ostlund phase diagram even further. These experiments consist of 2D colloidal crystals, where a static, random substrate potential landscape is created, and the elastic behavior of the system near the deepinning threshold is explored. Previous studies regarding this system assumed inelastic behavior, and thus, the elasticity in systems near a depinning threshold was not studied. These results, combined with our computational efforts, aid in establishing a new paradigm in relating the structural order of random pinning systems to its driven dynamics.

The physics of sandcastles: Jammed granular columns with and without fluid.

Dr. Jeffrey Olafsen, Dr Oliver-Denzil S. Taylor, Dr Mihan H McKenna Taylor

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Understanding how porous structures become rigid and retain their strength or fail over variable saturation rates is crucial for designing materials with targeted performances under different processing conditions, the development of materials with time-dependent viscosities and the emerging science of manipulatable advanced geo-metamaterials. Nowhere are these issues more ubiquitous than in the physics of sandcastles. A wide variety of geotechnical, engineering, and physics studies have focused on the granular materials of different particle sizes and shapes for a variety of fluid saturations. These studies can be used to describe on a case-by-case basis the physical characteristics, such as shear wave and p-wave velocities, that are dominated by either the response of the granular material or the interstitial fluid matrix. What is lacking is a more universal description of the granular+fluid system, here in its jammed state, that can predict macroscopic parameters such as strength and stability. We present a low-dimensional "phase space" model that outlines the contributions to relative strength and stability of a jammed granular column at different fractional fluid saturations as determined from prior bulk studies. While the model does not include higher order effects (spatial or temporal dependence of the parameters), it allows a granular temperature to be defined which allows the strength and stability of the column to be distinguished for a full range of fluid saturations. The model's success can be shown for two drastically different granular media: fine, nearly monodisperse, smaller grains and coarse, more polydisperse, larger grains.

The transition from anelasticity to plasticity in amorphous solid: a molecular dynamics study

Dr. Baoshuang Shang

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Anelasticity, an inherent characteristic of amorphous solids, holds a significant role in comprehending how these materials relax and deform. Nevertheless, owing to the absence of long-range order in amorphous solids, unraveling the structural origins of anelasticity and distinguishing it from plasticity has remained a challenging task. In this research, we delve into the transition from anelasticity to plasticity within a two-dimensional model glass, making use of the frozen matrix method. Through manipulation of control parameters in the amorphous solid, we succeed in identifying three distinct mechanical behaviors: elasticity, anelasticity, and plasticity. Our exploration of how finite size influences these mechanical behaviors unravels a clear distinction between anelasticity and plasticity. Anelasticity acts as a crucial bridge, connecting the domains of elasticity and plasticity within amorphous materials. Moreover, our observations indicate that anelastic events remain localized, whereas plastic events exhibit subextensive characteristics. The transition from anelasticity to plasticity mirrors the entanglement of long-range interactions among element excitations. This study contributes valuable insights into the fundamental nature of anelasticity as an essential property of element excitations in amorphous solids.

Universal Scaling Solution for a Rigidity Transition: Renormalization Group Flows Near the Upper Critical Dimension

Mr. Stephen Thornton, Prof. James Sethna, Prof. Itai Cohen, Mr. Danilo Liarte

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Critical phenomena and universality in wide classes of statistical mechanical models close to their critical points have been well-understood through the lens of the renormalization group. Rigidity transitions induced by the formation of system-spanning disordered rigid clusters, like the jamming transition, can be well-described in most physically relevant dimensions by mean-field theories. However, we lack a theoretical description of these kinds of rigidity transitions that can detect an upper critical dimension and predict corrections to the theory in and below this upper critical dimension. Towards that end, we show that the critical exponents for a continuous isotropic rigidity transition predicted by a simple dynamical effective medium theory (the Coherent Potential Approximation, CPA) are not mean-field-like, dimension-independent quantities. We find that the theory has an upper critical dimension d=2, in which there are the usual logarithmic corrections and below which the critical exponents are modified. In doing so, we recapitulate Ken Wilson's phenomenology of the (4-ε)-dimensional Ising model, but with the upper critical dimension reduced to 2. We interpret this using normal form theory as a transcritical bifurcation in the RG flows, and posit their explicit forms, incorporating a dangerously irrelevant variable becoming marginal in d=2. We also derive universal scaling functions from the CPA sufficient to predict all linear response in randomly diluted isotropic elastic systems.

Interfaces, Surfaces, Membranes

Air bubbles entrapped during the coalescence of drops in a Hele-Shaw cell

Dr. Sangjin Ryu, Dr. Haipeng Zhang, Dr. Hua Tan

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

When initial contact occurs between two drops, a liquid bridge is formed between them and grows rapidly, which results in the surface-tension-driven coalescence of the drops. Drop coalescence occurs ubiquitously in various natural and engineering systems, and this surface-tension-driven phenomenon has been studied mostly for unconfined, free drops.

However, drop-to-drop interactions frequently occur while confined by no-slip surfaces of various properties in various real-world applications. Examples include inkjet printing, microfluidics, enhanced oil recovery (EOR) involving drop coalescence in underground pores, and the powder bed fusion (PBF) process for metal additive manufacturing that involves the coalescence of molten metal particles. Despite its importance, the effect of the confinements on drop coalescence remains poorly understood. To fill this knowledge gap, we experimentally and computationally investigated the coalescence of drops in a narrow confinement called the Hele-Shaw cell, which was formed by two parallel surfaces with controllable spacing.

For the Hele-Shaw cell, a straight microchannel of a small gap height was fabricated using polydimethylsiloxane (PDMS) and soft lithography. Glycerol was slowly injected into the Hele-Shaw cell to grow two drops. As the drops contacted each other, the growing liquid bridge between coalescing drops was captured using high-speed video microscopy. High-speed video microscopy experiments revealed that air bubbles were entrapped in the bridge connecting the two drops. It was found that these bubbles were created near the wall of the Hele-Shaw cell because of the stretching and following pinch-off of the air tube trapped between the growing bridge and the wall of the Hele-Shaw cell. As a result, air bubbles of various sizes were created in a nearly symmetric formation in the liquid bridge.
We confirmed our experimental observation using the numerical simulation. To model the dynamics of surface tension-induced multiphase flow, we employed an adaptive mesh refinement (AMR) approach within a finite volume framework, utilizing a Cartesian grid for computational efficiency. The volume-of-fluid (VOF) method was used to track the air-liquid interface. Our simulations accurately reproduced experimental observations, capturing key metrics such as liquid bridge length and the speed of coalescence front movement. Furthermore, our analysis unveiled the detailed evolution of the air-liquid interface during drop coalescence and elucidated the mechanism of the formation of air bubbles near solid boundaries.

Bifurcations of inflating balloons and interacting hysterons

Gentian Muhaxheri, Christian D. Santangelo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

While many materials exhibit a complex, hysteretic response to external driving, there has been a surge of interest in how the complex dynamics of internal materials states can be understood and designed to process and store information. We consider a system of connected rubber balloons that can be described by a Preisach model of non-interacting hysterons under pressure control, but for which the hysterons become coupled under volume control. We study this system by exploring the possible transition graphs, as well as by introducing a configuration space approach which tracks the volumes of each balloon. Changes in the transition graphs turn out to be related to changes in the topology of the configuration space of the balloons, providing a particularly geometric view of how transition graphs can be designed, as well as additional information on the existence of hidden metastable states. This class of systems is more general than just balloons.

Client competition regulates bulk and interface partitioning in biomolecular condensates

Dr. Teagan Bate, Dr. Kathryn Rosowski, Dr. Eric Dufresne

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The interfacial properties of biomolecular condensates have been emerging as critical to their behavior both in healthy and diseased cell physiology. The localization of clients to these interfaces, such as proteins and ribonucleic acids, may greatly impact this behavior. However, systematic, quantitative investigations of the mechanisms underlying interface partitioning of clients are not established. We use light microscopy to quantify partitioning of tubulin and RNA in FUS and Bik1 condensates. We find that tubulin and RNA compete to occupy the bulk and interface of these condensates. These data suggest that charge plays an important role.

Enhancing Solar Panel Efficiency through Nanostructured Coatings

Ms. Robin McDonald

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

A thin nano-structured coating applied to the top of solar cells has the potential to improve cell efficiency by increasing light trapping and reducing surface fouling. By substituting the conventional smooth encapsulation layer with a nanopatterned film or coating, we not only maintain low material usage but potentially reduce it further. By tuning the array of micro- and nanofeatures, we can enhance photon absorption by increasing the optical path length and suppressing the Fresnel reflection. The resulting patterned solar cells show an efficiency increase of about 2% at normal incidence and up to 30% for oblique angles. This translates to a daily power increase of about 3-10% depending on the panel tilt and latitude. We also incorporated conductive additives and nanoparticles into our UV-nanoimprint lithography (NIL) coating to mitigate the adhesion of light-blocking dust particles. Our coatings show a <1% drop in UV-Vis transmission upon the application of dust while conventional thermoset and thermoplastic imprinted polymers show about a 10% drop in transmission. In formulating our colloidal dust-mitigating NIL coating, we prioritized considerations including optical transmission, substrate adhesion, weatherability, and processability. Our work is compatible with high-throughput roll-to-roll processes, which enables a scalable approach for patterning both existing and future solar panels.

Experimental and Computational Investigation of nanoparticle ligand shell morphology

Ms. Xu Wang

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The incorporation of various types of ligands within the self-assembled monolayer on a nanoparticle (NP) can lead to a significant enhancement of desired characteristics. Currently, this lack of precise information on the atomic-level arrangement of ligands constrains our comprehension of how specific ligand combinations are linked to favorable properties. NPs with highly desirable properties can be produced by tuning the monolayer between stripe, patchy and Janus morphologies when a length mismatch is present between a pair of ligands with different end groups. We develop a novel method to reconstruct the ligand morphology on the NPs from Matrix Assisted Laser Desorption Ionization (MALDI) spectra using Configurational Bias Monte Carlo (CBMC). These studies will not only facilitate the prediction, but also the formulation of mixed-ligand monolayer NPs with desired functionalities.

Exploding drops on lubricated surfaces

Dr. Daniel Daniel, Dr Marcus Lin, Dr Peng Zhang

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Traditionally, investigations of Coulomb explosions have focused on charged microdrops levitated using quadrupole electric fields, i.e., a Paul trap. In a surprising twist, our work introduces a simple method to observe Coulomb explosions, with no drop levitation and no external electric field. Instead, we generate a charged water drop using a conventional micropipette, which we then deposit on a plastic petri dish lubricated with a thin oil film. As the droplet evaporates, its radius shrinks until it reaches the Rayleigh limit at which point we observe multiple, highly periodic Coulomb explosions (> 60 events over 20 mins)—the first time Coulomb explosions have been reported for a sessile drop on a surface. Each event produces a finely ejected liquid jet, which disintegrate into microdroplets explosively within microseconds. Our Coulomb explosions span diverse length scales (from micron to millimetres) and time scales (from microseconds to minutes), with potentially wide-ranging applications from nanoscopic material fabrication to electrospray ionization.

Exploring Nanostructured Biomimetic Surfaces: Measuring Hydrophobic Properties via Free Energy Barrier using Coarse-Grained Molecular simulation

Mr. Fan Meng

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Wettability stands as a fundamental physicochemical property characterizing solid surfaces, with surfaces exhibiting unique wettability patterns proving particularly captivating. Such surfaces play pivotal roles across diverse domains including energy utilization, environmental protection, healthcare, sustainable development, and factory manufacturing.

On the other hand, drawing inspiration from nature's ingenuity, bio-inspired materials have emerged as a frontier of scientific inquiry, offering boundless possibilities across various disciplines. For instance, mosquitoes possess the ability to prevent fog condensation on their compound eyes in humid environments, lotus leaves exhibit self-cleaning attributes owing to their slender downy hairs, water striders navigate surfaces at high speeds due to their super-draining structure, and fish evade sticking to oil underwater. Even butterfly wings remain unsoaked amidst the rain. Nature presents an array of templates featuring superhydrophobic structures, showcasing remarkable hydrophobic properties.

This research aims to investigate the hydrophobic characteristics of biomimetics surface via free energy barrier using coarse-grained molecular simulation. By utilizing the free energy barrier evaluation system, we explore the intricate relationship between biomaterial surface structures and hydrophobicity. We investigate the butterfly wings and mosquito eyes model, we seek to develop a comprehensive evaluation system that considers surface parameters' influence on the free energy barrier. Through rigorous simulation and analysis of biomimetic material surfaces, we aim to validate and enhance the reliability of the free energy barrier assessment method. These consecutive study not only advances our understanding of hydrophobicity across diverse biomaterials but also facilitates the optimization of biomaterial properties for various applications.

In the course of our investigation, we shed light on the elusive intermediate state, a departure from the typical Cassie or Wenzel state. This newfound insight enriches our theoretical framework for surfaces with distinctive properties.

This research contributes to the development of biomimetic materials with enhanced hydrophobic characteristics and innovative fabrication processes. Beyond the confines of academia, the implications extend broadly, promising advancements in environmental conservation, medicine, and beyond.

Fundamental principles of flexible solids

Dr. Zeb Rocklin

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Flexible solids such as membranes, polymers and mechanical metamaterials are capable of undergoing myriad soft, nonlinear deformations along certain modes while also supporting substantial stress under certain loading conditions. This sharp contrast between different types of deformation leads to rich behavior, including buckling, wrinkling, memory, and complex functional response. In this presentation, I will explore rationally designed flexible solids that are capable of prescribed deformations, such as uniform dilations. Such a simple designed mode necessarily leads to a family of deformations that dominate over standard elastic response. Analytic theories based on this insight can strongly predict the nonlinear deformation of these flexible solids and even achieve multiple target shapes with a single structure.

Hydration Forces, Hydration Solids, and The Hygroelastic Theory

Dr. Ozgur Sahin, Christina McBean, Saima Sumaiya, Leonardo Ruiz-Ortega, Brunvens Sejour, Adedayo Ogunlana

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

A large fraction of biological matter on Earth exhibits hygroscopic behavior. Found in plants, bacteria, fungi, and animals, these water-responsive materials have diverse chemical compositions, but they also share common physical characteristics. Based on the hydration force, we recently developed the hygroelastic theory that provides a unified microscopic physical basis for the equilibrium and non-equilibrium mechanical behaviors of hygroscopic biological matter (1). Further, the theory helped discover unusual equilibrium and non-equilibrium phenomena originating from the hydration force (1). Originally obtained on the hygroscopic spores of a common soil bacterium, these earlier results indicate a previously unrecognized class of matter that we termed “hydration solids”. We predict that many types of biological matter could belong to this distinct class of solid matter. Here we present thorough evidence of hydration solid behavior in a cellulose-based material. Despite having a chemical composition substantially different from that of bacterial spores, our results confirm the predicted equilibrium and non-equilibrium phenomena in the cellulose-based material. Furthermore, quantitative predictions of theory are also confirmed by the results. These findings increase the possibility that hydration solids represent a major class of matter in Nature.

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Hydrophobic Interactions in Unstable Wetting Films

Dr. Roe-hoan Yoon, **Dr. Mohit Gupta**

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Flotation is a major separation process in which air bubbles selectively collect hydrophobic particles from the aqueous phase. Practically all metals humans use are produced using this simple process in the minerals industry. When a mineral particle approaches an air bubble, a thin liquid film (TLF) of water (or wetting film) is formed between the two macroscopic surfaces. Initially, the film is thinned by the capillary forces created by the changes in bubble curvature. As the film thins further to ~250-300 nm, the film thinning is controlled by the surface forces, i.e., electrical double-layer (EDL), van der Waals (vdW), and hydrophobic (HP) forces, in the film. The first two forces are usually repulsive, while the latter is attractive. It is, therefore, necessary to create a stronger hydrophobic force that can overcome the repulsive force (or energy) barrier so that the disjoining pressure (Π) of the films becomes negative, which is a prerequisite for the wetting film to rupture and form a finite contact angle (θr) at the three-phase contact line. In general, the more negative the disjoining pressure is, the higher the kinetics of film thinning and, hence, the rate of bubble-particle attachment and flotation (Huang and Yoon, 2020).

In the present work, a series of surface force measurements were conducted while slowly approaching an air bubble toward a gold surface hydrophobized by thiol (CnSH) coating. In this method, an air bubble was used effectively as a force sensor. The measurements were conducted at different temperatures to obtain Gibbs free energy changes (ΔG) using the Frumkin-Derjaguin isotherm (1938, 1940), followed by determining the entropy changes (ΔS) from the temperature coefficients of free energy changes, and subsequently the enthalpy changes (ΔH). The results showed that bubble-particle interactions entail decreases in both enthalpy and entropy, but

|ΔH|>|TΔS|, indicating that the process is driven by enthalpy changes involving significant enthalpy and entropy compensations. Based on these findings, a flotation model has been developed from first principles. It can be used to predict the performance of a flotation process and to design full-scale flotation plants.

By

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Interfacial and Bulk Damage quantification of thin films on soft substrate

Akash SIngh, **Costantino Creton**, Roberto Santoprete, Gustavo Luengo, Matteo Ciccotti

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Thin films on soft substrates are a subject of interest in several applications such as cosmetics and flexible electronics (OLED). Understanding damage to the film or debonding from the substrate can be crucial for the functionality, aesthetics, and lifetime of such films. However, understanding remains limited due to the large deformation of the soft substrate compared to investigations for rigid substrates[1], evidence of mixed-mode interfacial fracture and sliding at the interface[2], and due to the inelastic behavior of the film. We show a robust methodology to characterize damage and adhesion and more generally, the durability of thin films on a soft substrate. Results can then be extended to different substrates. The method involves macroscopic mechanical measurements and simultaneous local optical imaging using camera and confocal microscopy to characterize the different features of the deformed film and the mechanisms by which thin coatings accumulate damage due to the stretching of the substrate. After extracting the local deformation field in both the film and at the interface [3] (using fluorescent markers embedded near the surface of the substrate), we derive suitable algorithms (DIC, particle tracking) to extract local deformation mismatches due to phenomena such as debonding, slippage and plasticity. These quantifications can be used to obtain the desired interfacial adhesion and cohesive energy of the film. Measurements using this methodology are performed on standard elastic SBR films on soft elastomeric substrate and can be compared to standard method such as notch and peel tests to validate the methodology.

References

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[2]. Newby, Z et al, Langmuir 13, 1805–1809 (1997)

[3]. W. Style, R. et al, Soft Matter 10, 4047–4055 (2014)

Modeling Electrolytes at Charged Mineral Interfaces Using Classical Density Functional Theory

Dr. Thomas Petersen

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The organization of water molecules and ions between charged mineral surfaces determines the stability of colloidal suspensions and the strength of phase-separated particulate gels. In this research, we assemble a density functional that measures the free energy due to the interaction of water molecules and ions in electric double layers. The model accounts for the finite size of the particles using fundamental measure theory, hydrogen-bonding between water molecules using Wertheim's statistical association theory, long-range dispersion interactions using Barker and Henderson's high-temperature expansion, electrostatic correlations using a functionalized mean-spherical approximation, and Coulomb forces through the Poisson equation. These contributions are shown to produce highly correlated structures, aptly rendering the layering of counterions and co-ions at highly charged surfaces and permitting the solvation of ions and surfaces to be measured by a combination of short-range associations and long-ranged attractions. The model is tested in a planar geometry near soft, charged surfaces to reproduce the structure of water near graphene and mica. For mica surfaces, explicitly representing the density of the outer oxygen layer of the exposed silica tetrahedra allows water molecules to hydrogen-bond to the solid. When electrostatic interactions are included, water molecules assume a hybrid character, being accounted for implicitly in the dielectric constant but explicitly otherwise. The disjoining pressure between approaching like-charged surfaces is calculated, demonstrating the model's ability to probe pressure oscillations that arise during the expulsion of ions and water layers from the interfacial gap and predict strong inter-attractive stresses that form at narrow interfacial spacing when the surface charge is overscreened. This inter-attractive stress arises not due to in-plane correlations under strong electrostatic coupling but due to the out-of-plane structuring of associating ions and water molecules.

Multiphysics interactions between electret fibers and airborne particles and droplets

Dr. Amit Kumar, Dr. Sashank Gautam, Dr. Hooman Tafreshi, Dr. Behnam Pourdeyhimi

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

In this work, we present a series of numerical simulations devised to improve our understanding of how electrostatically charged fibers in a N95 mask capture airborne particles and droplets. Various scenarios of clean fiber, fiber loaded with solid particles (neutral or charged), and fiber loaded with neutral droplets were considered. Especial attention was paid to the impact of fiber dipole orientation on the rate of particle capture. The contributions of the Coulomb and dielectrophoretic forces in capturing particles of different charge polarities were predicted and compared with one another. Coulomb force comes into play when both the particle and fiber carry some charges, while the polarization force manifests even when only one entity is charged. Our simulations further revealed that Coulomb force strength depends on the particle's charge-to-mass ratio and the magnitude of the electrostatic force, contingent upon the charge polarity of both particles and fibers. Conversely, polarization force strength is proportional to the cube of the particle diameter and the gradient of the electrostatic field, independent of particle and fiber charge polarity. Our simulations also revealed that particle deposition can improve the capture efficiency of a bipolar fiber when exposed to small particles (e.g., 400 nm or smaller), regardless of the charge polarity of the airborne or deposited particles. However, this trend was not consistently observed for larger particles, as their trajectory, influenced by aerodynamic effects and polarization force (the capture mechanism for large particles), was affected by the electrostatic shielding effect. For the case of airborne droplets, our simulations revealed that droplet deposition always reduces the capture efficiency of an electret fiber. Notably, the surface charge density of the fiber and the permittivity of the droplets emerged as the most influential parameters contributing to this reduction in capture efficiency. This is due to the higher permittivity of droplets leading to increased electrostatic shielding, while a decrease in the surface charge density of the fiber results in a reduction of the electrostatic field.

Nano-porous Surfaces and Associated Interfacial Forces

Mr. Michał Góra, Dr. Paula Navascués, Mr. Urs Schütz, Dr. Dirk Hegemann, Prof. Dr. Manfred Heuberger

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Nano-porous materials have become an important focus in materials research because of their outstanding chemical and physical properties, leading to a wide range of applications including energy capture, -conversion and -storage [1], liquid-fluid separation [2] or antimicrobial use [3]. The presence of holes creates an additional internal surface area and extra volume at the interface, which is expected to give room for extra kinetic effects. The broad interest in such systems is associated with the process of fluid imbibition or selective solute interdiffusion into the porous structure, particularly following alterations in interfacial solution properties or involving contact with a second surface. Porous surface forces are thus expected to significantly deviate in terms of strength, range and dynamics compared to their planar counterparts.

Systematic fundamental examination of nano-porous surfaces demands different porous model systems covering various pore and depth dimensions, while maintaining minimal surface roughness between individual pores. In this work, we introduce three primary methods to fabricate such porous surfaces. The focused ion beam (FIB) technique and reactive ion etching (RIE), utilizing anodized aluminum oxide films as the etching mask, are used to create precise nano-porous surfaces with controlled pore diameters ranging from few nanometers up to several hundreds of na-nometers. In contrast, plasma-enhanced chemical vapor deposition (PECVD) is used for the fabrication of hydrophobic and randomly structured nano-porous plasma polymer films, featuring pore diameters below two nanometer.

Using three direct force measurement techniques, namely atomic force microscope (AFM), colloidal probe microscope (CPM) and extended Surface Force Apparatus (eSFA), we investigate porous surface forces at different time- and length scales. Depending on the amount of intentionally added porosity, the interaction of fluid molecules within the enhanced pore surface leads to specific alterations in molecular arrangements and thermodynamic behaviors compared to the situation of bulk liquids interfacing plain surfaces.

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Phase lines in mean-field models with nonuniform external forces

Dr. Yoav Tsori, Roni Kroll

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

We look at the influence of external fields on systems described by generic free energy functional of the order parameter. The external force may have arbitrary spatial dependence, and the order parameter coupling may also be arbitrary. The treatment generalizes seemingly disparate phenomena occurring in, e.g., pure fluids, liquid and polymer mixtures, lipid monolayers, colloidal suspensions in electric fields, fluids, and nematics in gravity, solutions in an ultracentrifuge, and magnetic dipoles in magnetic fields. The phase lines and thermodynamic behavior are calculated at the mean-field level. We find a first-order transition line, similar to prewetting transitions. The bulk critical point becomes a line of second-order transition. The first- and second-order lines meet at a ``surface'' critical point that is shifted to higher or lower temperatures than the bulk critical point. The second-order line depends on the spatial dependence of the force, while the first-order line is universal.
The susceptibility may diverge at a finite location ${\bf r}$. Several analytical expressions are given in the limit where a Landau expansion of the free energy is valid.

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J. Chem. Phys. vol 157, 231103 (2022).

Physics of Multiphase Droplet Adhesion to a Fiber

Dr. Hooman Tafreshi

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

This talk presents an overview of our research on the use of magnetic fields in studying droplet adhesion to curved surfaces, e.g., a fiber. The presentation starts by discussing ways to quantify the force required to detach a droplet from a fiber, for its industrial applications, but then continues to take a deeper dive into the fluid mechanics of compound droplets, droplets comprised of

two immiscible liquids. In particular, a new approach of measuring the force of adhesion between compound droplets and fibers of different interfacial properties will be discussed using atomistic and continuum-level numerical simulations accompanied by dedicated experimental measurements. The presentation will also include discussions on ways to reduce, and perhaps control, the liquid residue left on a surface after droplet detachment.

Plateau-Rayleigh instability of a soft layer coated on a rigid cylinder

Dr. Tak Shing Chan, Dr. Bharti Bharti, Prof. Andreas Carlson

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

We study the Plateau-Rayleigh instability of a viscoelastic soft solid layer coated on a rigid cylinder i.e., a soft fibre with a rigid core. The onset of instability is examined using a linear stability analysis. We find that increasing the rigid cylinder radius or the stiffness of the layer reduces the growth rate of the fastest growing mode. For each rigid cylinder radius, a critical elastocapillary number is found below which all wavelengths of disturbances are stable. The critical value for a soft fibre with a thick rigid cylindrical core can be several orders of magnitudes larger than that for a totally soft fibre (no rigid core), which highlights the strong stabilizing effect of the rigid core on the system. Increasing the relaxation timescale of the viscoelastic material also slows down the growth of disturbance, but has no effect on the critical elastocapillary number. Interestingly, the wavelength of the fastest growing mode is independent of the rigid cylinder radius for the purely elastic case.

Predicting Emergence of Nanoscale Order in Surfaces Oxides through Preferential Interactivity Parameter

Dr. Andrew Martin, Prof. Martin Thuo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Diffusion and surface oxidation are critical, and necessary processes in metal alloy designs and use. Surface oxide provides unique opportunities to improve material properties or performance beyond bulk alterations. Surface oxidation is, however, often oversimplified into a classical diffusion process. Passivating oxide surfaces are also thought to be lacking in complexity or critical information. A closer look, however, shows inherent complexity with kinetics-driven competition between the elements in the process leading to redox-speciation across a very small (nm) thickness. Questions that remain to be answered for a comprehensive understanding of surface oxides are diverse and call for interdisciplinary approaches. By using thermodynamics-based Preferential Interactivity Parameter (PIP) alongside kinetic consideration, we show how complexity in these oxides can be predicted under different compositional, phase and thermal conditions allowing us to tailor these thin films.

Shaping a Soft Future with Liquid Metals

Dr. Michael Dickey

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Gallium-based liquid metals have remarkable properties: melting points below room temperature, metallic thermal and electrical conductivity, water-like viscosity, low-toxicity, and effectively zero vapor pressure (they do not evaporate). They also have, by far, the largest interfacial tension of any liquid at room temperature. Normally small volumes of liquids with large tension form spherical or hemi-spherical structures to minimize surface energy. Yet, these liquid metals can be patterned into non-spherical shapes (cones, wires, antennas, or films for thermal interfaces) due to a thin, oxide skin that forms rapidly on its surface. In addition, the metal can be rendered into a 'gel' or 'paste' by incorporating other materials into the metal, such as oxide flakes or metal particles. Doing so changes the rheology of the metal and thus, the way it flows as it dispenses from a nozzle. This talk will describe efforts in our research group to pattern and manipulate metal into useful shapes—such as circuits or as thermal interface contacts—that take advantage of the properties of liquid metal. It is possible to pattern liquid metal in unique ways, such as injection or direct-write 3D printing at room temperature to form ultra-stretchable wires, self-healing circuits, and stretchable barrier materials. Perhaps the most fascinating aspect of liquid metals it the ability to use interfacial electrochemistry chemistry to remove / deposit the oxide to manipulate the surface tension of the metal over unprecedented ranges (from the largest tension of any known liquid to near zero!). This allows manipulating the shape and position of the metal for shape reconfigurable devices. This work has implications for thermal interface materials as well as soft and stretchable electronics; that is, devices with desirable mechanical properties for human-machine interfacing, soft robotics, and wearable electronics.

Stereo-Structural Fine Tuning of Chromaticity

Ms. Alana Pauls, Dhanush U. Jamadgni, Dr. John Gitua, Dr. Martin Thuo

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Lanthanoid carboxylates were synthesized and in situ self-assembled to illustrate temperature-driven evolution in chromaticity. Evolution in structure (crystallinity), composition, luminosity, and chromaticity were investigated revealing the coupled role of divergence in order/structure (spatial organization), and composition in tuning observed color. Loss of crystallinity or increase in residual carbon leads to decrease in luminosity even with increase in hue. Comparing Ho and Er congeners shows that the density of accessible transition states relates to shifts in low and high wavelength components of color. This work demonstrates that, just as interface dipoles can lead to change in semiconductor bandgap, structure and composition can analogously alter observed color.

Strong and Functional Hierarchical Biofoam Structures

Dr. Juha Koivisto, Isaac Miranda-Valdez, Kourosh Mobredi, Aref Ghaemi, Tero Mäkinen, Mikko Alava

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Hierarchical biofoams consist of tuned micron-scale films made by self-assembling cellulose fibers. The films create anisotropic elliptical bubbles that are extruded into rod-like structures and further into macroscopic beam-like assemblies of foam. Extremely strong structures per weight are created by manipulating the orientation of the fibers in the bubble film. The tunable yield stress of the foam can be up to 48 times larger in the strong direction than in the perpendicular soft direction. Similar anisotropy can be observed in thermal and hygroscopic behavior. The natural swelling or expansion response of biomaterials to changes in ambient conditions such as humidity or temperature enables directed motion. Coupling the expansion to a designed hierarchical structure performs simple tasks like opening and closing a valve, leading to passive dynamics: motion without traditional energy supplies such as batteries or fuel. These kinds of novel programmable forest-based materials contribute to several sustainable development goals by replacing high-embodied-energy materials in the construction sector.

Study of the interface between liquid polymers and viscoelastic polymers in dynamic and static states.

Mr. Brahim El-khalil Remini, Pr Ralf Seemann

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Applying liquid polymers dewetting from viscoelastic substrates, we study the interface between a liquid and a soft solid in both dynamic and equilibrium situations; i.e. dewetting holes and sessile droplets.
Using optical and atomic force microscopy we studied droplets ranging from a hundred nanometer to a few micrometers in radius and explored their 3d shape on viscoelastic polydimethylsiloxane substrates with shear module ranging from 1 kPa to 500 kPa. Bridging these droplet sizes and elasticities, we move from the elasticity-dominated regime to the capillary-dominated regime.
In the elasticity-dominated regime, deviations from Young contact angles were observed while in limit of the capillary-dominated regime, the liquid-solid interface shows a similar deformation as the liquid-liquid deformation where the surface tensions are balanced according to the Neumann construction. For the dynamic regime, rim profiles of the dewetting holes were studied with a special focus around the three phase contact line and dewetting contact angles could be measured with a good precision.
Taking advantage of the nanoscopic resolution of the AFM, phase separation at the three phase contact line and cloaking could also be observed.

The Biomechanical Influence of Polysaccharides Found in Anti-Wrinkle Formulations on Human Skin

Mr. Sebastian Hendrickx-Rodriguez, Mrs. Ashley David, Mr. Kuan Liu, Dr. Reinhold Dauskardt

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Human skin acts as the main barrier between us and the outside world, simultaneously protecting against external threats and transducing external stimuli into sensations. Modulation of this interface can affect both how we perceive, and how we are perceived. The topmost layer of skin, known as the stratum corneum (SC), is particularly susceptible to changes because of its direct proximity with the outside environment. For example, the application of tightening polymer films—frequently found in cosmetic formulations—onto the skin surface affects the SC's appearance, diffusional properties, and stress state. Therefore, in this work we relate the chemical structure of several polysaccharides to their biomechanical influence on the SC, and then use this knowledge to explain the function of polysaccharides in anti-wrinkle formulations.

To investigate the biomechanical response of the SC to polysaccharide film formers, ex vivo SC samples were used to measure the evolution of skin stress using classical thin film techniques. As the polysaccharide film forms and shrinks on the surface of the skin, it induces compressive stresses on the SC. We relate these biomechanical stresses to the polymer's crystallinity measured using X-ray diffraction (XRD). We then use digital microscopy to characterize the microroughness of the skin surface and correlate changes in the microtopography to induced compressive stresses from the polysaccharide.

We found polysaccharides with a higher degree of crystallinity generally lead to larger increases in SC stresses, likely due to their higher stiffness. Interestingly, if the polysaccharide induces stresses larger than a critical value, the SC buckles out of plane leading to the formation of small microwrinkles that diffusely scatter light and hide larger mm-sized wrinkles. This action mechanism for anti-wrinkle formulations has not been reported before, and can serve as the basis for the smarter design of cosmetic products. For example, the induced stresses from polymer film shrinkage deforms the underlying skin tissue where a system of cutaneous mechanoreceptors transduce strains into electro-chemical signals that we perceive as skin tightness. By incorporating additional ingredients into anti-wrinkle formulations, such as moisturizers and humectants, we can relieve this uncomfortable sensation.

Through this research, we envision engineering the molecular composition of a cosmetic formulation containing polysaccharides, surfactants, and moisturizing components to deliver a controlled sensorial experience to the consumer via careful consideration of how these ingredients affect the biomechanical function and properties of human skin. This requires insight from various soft matter fields including polymer physics, biology, cosmetic chemistry, and material science at interfaces and surfaces.

Thermodynamics of morphological transitions in growing membranes

Dr. Jordan Shivers

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The growth of lipid membranes at sub-micron scales plays an important role in many essential cellular processes, such as the formation and organization of vital cellular organelles. However, describing the underlying physics of this growth remains an ongoing challenge. This challenge stems from the fact that, at these scales, membrane growth reflects a delicate interplay of material exchange, bending deformation, apparent variation in material properties, and, crucially, in-plane viscous flow that often cannot be neglected. To address this challenge, we consider the nonequilibrium growth dynamics of a minimal model of fluid membranes, in which sufficiently large driving forces produce a striking morphological transition marked by out-of-plane buckling, in-plane flow, and dramatic changes in the growth rate. To understand this behavior, we first construct a continuum description of growing membranes using tools from differential geometry and linear irreversible thermodynamics. This yields expressions relating the nonequilibrium driving to the rate of growth, size fluctuations, and effective material properties. We then validate these predictions via coarse-grained simulations of fluid vesicles. Next, we demonstrate that one can derive analogous relationships using ideas from stochastic thermodynamics, including the recently derived thermodynamic uncertainty relations. These allow us to establish rigorous constraints on the parameters required for growth-driven morphological changes, which we validate in simulations. Our results suggest a multifaceted approach for understanding and constraining the effects of active driving forces on the mechanics and morphology of biological matter.

Liquid Crystals

Catching the wave: particle transport by a moving phase boundary

Dr. Timothy Atherton, Dr. Linda Hirst, Mr Tom Shneer, Ms Jocelyn Ochoa, Ms Alauna Wheeler, Dr Chaitanya Joshi, Mr Emmanuel Flores, Dr Benjamin Stokes

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Non-equilibrium particle transport in liquid crystals can be exploited to create a variety of complex composites by cooling the system through a phase transition. Despite a wide variety of possible morphologies, the mechanisms behind structure selection are poorly understood. We construct a fundamental model of nanoparticle transport by moving LC phase boundaries and find a suprising analogy with chemotactic assembly. Solutions of our model show two transport regimes where particles either surf on, or are swept up by the moving phase boundary. Results successfully predict experimental observations, enriching our understanding of phase transition-driven structure formation.

Collective action and entanglement of magnetically active liquid crystal elastomer ribbons

Dr. Asaf Dana, Dr. Mustafa Abdelrahman, Dr. Taylor Ware

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Systems in which individual components convert free energy into mechanical work are commonly referred to as active matter. Physically entangled active matter is an emerging area of both living and man-made systems, where mechano-functionality of the collective emerges through physical interaction of individual elements. Liquid crystal elastomers (LCEs) are a class of stimuli responsive polymers that undergo large, reversible, anisotropic shape change in response to different stimuli, including heat and light, making them ideal candidates for many applications, especially as deployable devices. LCE films fabricated using surface-alignment techniques with prescribed director rotation along the thickness (twisted nematic) exhibit three-dimensional conformations in response to variations in temperature. The addition of magnetic particles enables motion of the individual units under a rotating magnetic field. The combination of the induced motion from the magnetic field along with the temperature-induced bending facilitates ribbon entanglement into a macroscopic multifunctional solid that is capable of assembly and disassembly on command. Namely, single ribbon motion was found to exhibit a significant transition across a temperature range of approximately 100 degrees from a simple oscillatory motion to complex trajectories that visit larger amounts of positions in the field. Tuning of the nematic twisting angles (between 0 and 90 degrees) and the offset angles relative to the axes of the surface director (between 0 and 20 degrees) allowed for tuning the critical temperatures for entanglement along with the mechanical properties of the structure. The resulting systems exhibit two different regimes that facilitate assembly or disassembly based on the amount of kinetic energy transferred to the units at different rotation speeds of the magnetic field. The outcomes of this project are expected to open the way for new active matter systems composed of dynamic elements, where rich material functionality can be uncovered and applied towards the development of a variety of unique autonomous devices.

Flow-Induced Structures in Lyotropic Chromonic Liquid Crystals

Ms. Delace Jia, Dr. Qing Zhang, Professor Irmgard Bischofberger

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Lyotropic chromonic liquid crystals (LCLCs) are materials of interest for their biocompatibility and unique structural properties compared to traditional thermotropic liquid crystals. Their response to shear, however, remains largely unknown. We show that nematic LCLC solutions arrange into intriguing large-scale structures at high flow rates when pushed out of equilibrium by a pressure-driven flow in a microfluidic cell. We align a LCLC solution perpendicular to the flow direction. At low flow rates, the liquid crystal solution remains in this alignment adopting a log-rolling state. At a range of higher flow rates, transient horizontal stripes appear along the flow direction; these stripes subsequently break up into subunits that self-assemble into steady-state vertical band structures. We present scaling arguments for the characteristic length scale of the vertical bands that account for the independence of the selected length scale on flow velocity and the dependence on the microfluidic cell geometry. We further discuss the director field that underlies the structure of the vertical bands.

Morpho---A programmable environment for shape optimization and shapeshifting problems

Dr. Timothy Atherton

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

An emerging theme across many domains of science and engineering is materials that change shape, often dramatically. Determining their structure involves solving an optimization problem where a given energy functional that promotes shape deformation is minimized with respect to the shape of the domain and auxiliary fields describing the structure. Such problems are very challenging to solve and there is a lack of suitable simulation tools that are both readily accessible and general purpose. To address this gap, we present \textit{Morpho}, an open-source programmable environment, and demonstrate its versatility by showcasing a range of applications from different areas of soft matter physics: swelling hydrogels, complex fluids that form aspherical droplets, soap films and membranes, and filaments.

Shape Morphing of Twisted Nematic Elastomer Shells

Ms. Alexia Chatzitheodorou, Mr Christian Santangelo

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Liquid Crystal Elastomers have been explored as materials capable of emulating movements of human muscles. We study the geometry of Twisted Nematic Liquid Crystal Elastomers (TNLCEs) by modeling a layered TNLCE with a varying nematic director. We introduce a mathematical framework based on elasticity theory wherein we identify a novel term that results from the interplay between the orientational order and elasticity. This emergent term plays a significant role, dominating traditional bending contributions yet it is weaker than the stretching contributions. Additionally, we perform a linear stability analysis and examine the stress distribution within a specific geometry. We also explore the shape morphing of more complex geometries, which is driven by the emergent elasticity, using numerical methods.

Measuring, Characterization

BOTTS: 500% Faster Viscoelastic Master Curves via Broadband Chirps

Dr. Richard Sheridan

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The Time-Temperature Superposition (TTS) principle has been used to create master curves that represent the viscoelastic behavior of soft materials across timescales that would be otherwise inaccessible to experiments. However, the time to collect these master curves can span several hours, representing a barrier to large-scale data generation. The standard direct frequency sweep (DFS) strategy of complex modulus measurement at each temperature is not time-optimal, and recent work has shown that broadband chirps can accurately measure complex modulus over a defined frequency range in a minimal amount of time. Our new technique, Broadband-Optimized Time-Temperature Superposition (BOTTS) utilizes this efficiency to speed up the acquisition of master curve data by a factor of 5 on commercially available dynamic mechanical analyzers. This practically eliminates the data collection bottleneck of the instrument data collection step and paves the way for rapid curation of master curves from a broad class of soft materials.

Data-Driven Rheology: A Direct Link Between Complex Moduli and Predictions

Dr. (Amir)Hossein Salahshoor

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The prevailing classical framework of modeling material systems has been to calibrate empirical material models using observational data, and then use the calibrated model in calculations. An alternative paradigm is data-driven mechanics, which, in turn, aims to directly utilize the material data to find solutions of suitably-formulated boundary-value problems. In this talk, I will present a novel data-driven viscoelasticity (DDV) framework for predicting the steady state dynamic response of a viscoelastic solid from dynamic viscoelasticity data including data from Dynamic Mechanical Analysis (DMA), nano-indentation, Dynamic Shear Testing (DST) and Magnetic Resonance Elastography (MRE), without the need for regression or material modeling. The main advantage of this new physics-based paradigm is that it makes direct use of all the data. In particular, no loss of information is incurred with respect to the material data set, no modeling biases or errors are introduced, and no ad hoc choices need to be made regarding the functional form of the viscoelastic material model. This has many applications in mechanics of soft materials and biomechanics.

I will demonstrate how DDV reformulates the steady state wave propagation problem in viscoelastic domains to an optimization problem. We operate in the Fourier representation of the phase space of stresses and strains, where harmonic histories of stresses and strains will be represented as sums of Dirac measures. With recourse to the optimal transport theory, we define Flat norm as a notion of distance that accounts for distances between both amplitudes of measures and the underlying frequencies. The main advantage of the flat norm is that it allows the response of the system at one frequency to be inferred from data at nearby frequencies. Endowing the phase space with a flat norm topology, DDV then aims to minimize a distance between physically admissible histories of stress and strain, in the sense of compatibility and equilibrium, and representations of the dynamic viscoelasticity data. By showcasing this paradigm in different example, we demonstrate the corresponding Data-Driven scheme and within conventional commercial codes and its robust convergence properties, both with respect to the solver and the data. I will end my talk by discussing future directions of this framework, as well as some of the applications of DDV in soft materials and biomedical engineering, and how it can enable new paradigms of patient specific modeling in computational medicine.

Serial flow cytometry as a method to measure membrane elasticity

Leroy Jia, Sydney Lee, Matthew DiSalvo, Paul Patrone, Gregory Cooksey

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Flow cytometry, in which cells or other kinds of particles are flowed through a microchannel and measurements of attached fluorescent biomarkers are made, has been used to detect, count, and sort particles with extremely high accuracy and repeatability. We built upon this technology and invented a robust method to measure the elasticity of cell membranes. High-speed neuromorphic cameras were used to accurately image the deformations of membranes as they traveled through the instrument. An asymptotic theory based on perturbing coupled Stokes equations allows us to calculate the deformations in terms of spherical harmonics and determine the focusing positions of particles. We demonstrate that this information allows us to determine the elasticity and other physical properties of the cell with controlled uncertainty.

Networks & Gels

Activating physical crosslinking in synthetic extracellular matrices by switch peptides

Nitsan Eliraz, Michael Tetteh, Professor John B. Matson, Professor Ronit Bitton

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The native extracellular matrix (ECM) integrates many dynamic chemical and physical signals to influence cell behavior. Among those, cryptic sites (matricryptins) are short signaling peptides buried within ECM proteins; These sites remain inaccessible to cells until enzymatic cleavage triggers the protein's rearrangement, making them accessible.

Recently, we demonstrated that depsipeptides ("switch peptides") can undergo enzyme-triggered changes in their primary sequence, with proof-of-principle studies showing how trypsin-triggered primary sequence rearrangement forms the bioadhesive pentapeptide YIGSR. The engineered cryptic sites-mimetic were integrated into alginate-based synthetic ECM hydrogels that experienced a cell-initiated gain of bioactivity.

The dynamic mechanical properties of ECM, also known as viscoelasticity (time-dependent stress response), have recently been shown to significantly influence aspects of cellular behavior and function such as migration, growth, and proliferation.

The overall aim of our research is to develop hydrogels that will retain macroscopic stability while modeling the microscopic dynamics of native ECM. To that end, we aim to construct a double network hydrogel composed of a primary network of chemically crosslinked polymer chains decorated with self-assembling switch peptides. These switch peptides will form a secondary physically crosslinked network only after a specific enzyme triggers a rearrangement that changes the hydrogel's viscoelasticity.

This class of switch peptides are depsipeptides that contain polyaminoacid linked via an ester bond to Serine residue that has a protecting sequence on its N-terminal. Upon enzymatic cleavage of the protecting group, oxygen to nitrogen (O → N) acyl shift turns the primary sequence into a linear peptide capable of self-assembling to create nanofibers.

Here, we present three switch peptides that, upon enzymatic activation, form the linear sequence Ac-FFXXSGK (X= Ala, Gly, or Val). Using EDC chemistry, these peptides were conjugated to oxidized alginate chains that were then chemically crosslinked by adipic dihydrazide to create acyl hydrazone bonds.

SAXS and cryoTEM measurements show that the primary switch peptides are not self-assembled while the post-cleavage sequence forms β-sheets that self-assemble to nanofibers.

Rheology measurements show that the viscoelasticity of hydrogels with various crosslinking degrees can be tuned by changing the peptide sequence (pre- and post-enzymatic cleavage), the peptide-to-polymer ratio, etc.

Capillary-Induced Deformation and Solvent Transport in Hydrogels

Mr. Boxue Zheng, Dr Tak Shing Chan, Prof Harald van Brummelen, Prof Jacco H Snoeijer

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Capillary forces induced by droplets can deform a soft substrate. When the soft substrate is made of poroelastic materials such as hydrogels which consist of polymer networks that can be swollen by solvent, the deformation is coupled with the transportation of the solvent. We implement a finite deformation model to investigate this coupled dynamic process. We formulate the total free energy of the system that includes the stretching of the polymer network and the mixing of the network with small molecules. Our aim is to shed light on the intricate relationship between capillary forces, substrate deformation, and solvent diffusion.

Controlling the complexation between polyanionic microgels and cationic peptides to create self-defensive antimicrobial surfaces

Yunhua Guo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

We have been exploiting directed self-assembly to modify the surfaces of tissue-contacting biomaterials to render them self-defensive against bacterial colonization. These surfaces release antimicrobials only if, when, and where bacteria contact the surface. Otherwise, the antimicrobial remains sequestered. Our approach uses polyanionic microgels with typical hydrated diameters of ~5-10 µm. Much of our work has used poly(acrylic acid) (PAA) microgels synthesized by membrane emulsification of an aqueous precursor solution dispersed in paraffin oil followed by thermal polymerization. These microgels are electrostatically deposited onto surfaces (e.g., glass or polycaprolactone (PCL)) primed by poly(allylamine hydrochloride)(PAH). The microgels form a discontinuous sub-monolayer coating. There are four key steps in rendering such surfaces self-defensive: (1) antimicrobial loading; (2) antimicrobial sequestration; (3) triggered antimicrobial release; and (4) surface cytocompatibility. Many small-molecule cationic antimicrobials will load by electrostatic complexation into the microgels when microgel-modified surfaces are exposed to low-ionic-strength antimicrobial solutions. Complexation causes the microgels to deswell, and we follow the microgel diameter by in situ optical microscopy to assess the loading state. We have studied FDA-approved antibiotics (e.g., colistin) and antimicrobial peptides (AMPs, e.g., Sub5), among other macro-cations (e.g., peptoids). Sequestration of the antimicrobial within the microgels under physiological pH (7.4) and ionic strength (0.14 M) is a critical constraint for downstream translation. Increasing [Na+] from 0.01 M to 0.14 M causes a burst release of colistin from PAA whereas Sub5 remains stably sequestered at [Na+] as high as 0.5 M. Consistent with this experimental finding, coarse-grained molecular dynamics (CGMD) simulations indicate that Sub5/PAA complexation is stronger than colistin/PAA complexation. All-atom molecular dynamics simulations furthermore show that Sub5 self-assembles into dimers and trimers while colistin remains in monomeric form. Such bundling enhances complexation strength in part because of a greater entropic change associated with counterion release upon antimicrobial/microgel complexation. Using an in vitro model of hematogenous contamination, challenging Sub5-loaded microgel-modified surfaces with S. aureus suspended in DMEM culture medium shows a 90% reduction in colonization relative to unmodified control surfaces. CGMD simulations indicate that complexation between Sub5 and the S. aureus cell membrane is more stable than that between Sub5 and PAA. Hence, there is a thermodynamic driving force for Sub5 to transfer from PAA to S. Aureus, and its release can be triggered by the close proximity of the challenging bacteria to the microgel-modified surface. In contrast, mammalian cells do not trigger Sub5 release. As one indicator of cytocompatibility, we find that mesenchymal stem cells spread and proliferate more rapidly on microgel-modified surfaces than on unmodified controls. Overall, we have developed a microgel-modified surface that enables stem-cell proliferation while self-defensively preventing bacterial colonization.

Developing Simulations to Guide Design of Biotic-Abiotic Machines

Jonathan Michel, Lauren Melcher, Qiaopeng Chen, Jennifer Ross, Michael Rust, Megan Valentine, Rae Robertson-Anderson, Moumita Das

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

I will discuss ongoing computational work to support efforts to build a biotic-abiotic actuator driven by actomyosin. In the cortices of many cells, the ratchet motion of nonmuscular myosin II minifilaments along actin filaments is the mechanism of force generation. The actomyosin cortex enables robust cell behaviors such as furrow constriction during cell division and migration over surfaces. We aim to harness this system to create soft machines, in which a bulk gel of biotin-tagged actin filaments driven by myosin II adheres to PEG-DA hydrogel slabs that are surface functionalized with neutravidin and deforms them by exerting active stresses upon their boundaries. The large design space of experiments demands efficient computational tools to aid in protocol refinement. We simulate actomyosin using an agent-based model in which actin filaments are modeled as wormlike chains made of series of rigid rods coupled by bending potentials. Actin is crosslinked and subjected to dipolar active forces by myosin minifilaments and evolved in time using constrained Brownian dynamics. Gel slabs are modeled using large-amplitude, continuum elasticity theory. Gel slabs are partitioned into tetrahedral finite elements, with surface facets bearing sticky sites that allow actin to bind to and exert stresses upon hydrogel slabs. Our approach offers predictions of stresses upon, and deflection of, gel slabs, as well as the structure and dynamics of the actomyosin phase. This offers an avenue for model validation by quantitative comparison with an experimental ground truth and subsequent guidance of experiments.

Dynamics of Active Relaxing Networks

Dr. Tuhin Chakrabortty, Xiangting Lei, Dr. Saad Bhamla

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Most contractile protein network structures in intra-cellular systems utilize ATP-driven motor proteins to generate active contraction. Recently, there has been a growing interest in protein structures that generate ultrafast contraction without motor proteins in single cellular systems such as Spirostomum and Tetrahymena. Instead of using ATP for contraction, these protein networks use ATP to generate active relaxation. While a significant amount of work is dedicated to understanding the mechanisms of active contractile networks, not much is known about the working principles of these active relaxing networks. In this work, we present a network model to systematically study the dynamics of active relaxing protein networks. We find that the active relaxing networks can exhibit phase transitions from a local protein cluster to a global contractile network. We validate our model prediction with an in-vitro model system composed of cortical proteins from ciliates of Tetrahymena species which generate a visco-elastic network capable of contracting and relaxing with binding and unbinding of Ca2+ ions. We demonstrate the applicability of active relaxing networks in designing synthetic cells as a simplified alternative for motor-based contractile networks.

Elastic microphase separation: the role of network parameters beyond elastic modulus

Ms. Harsha Koganti, Senthilkumar Duraivel[Department of Materials Science and Engineering, Cornell University Department of Physics, Cornell University], Dr. Nan Xue, Eric Dufresne

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The molecular weight of polymer chains affects the elasticity of elastomers inversely for the one-to-one ratio of reactive groups on polymer and crosslinker. However, our recent experiments involving vinyl-terminated polydimethylsiloxane and an octa-functional crosslinker found that changing the crosslinker ratio to the polymer almost nullifies the effect of molecular weight on the elastic modulus. This variation can be observed in the experimental data obtained from uniaxial tensile and indentation tests. Swelling experiments of the elastomer in ethyl acetate were carried out, and the data supports the above result. Swelling, a function of the molecular weight of polymer chains, tends to have the same value for different lengths of chains, suggesting a similar network topology with an increase in the crosslinker reactive groups ratio. This indicates an increase in linear chains in low molecular weight polymers, increasing the molecular weight of chains between effective crosslinks mimicking the network structure in high molecular weight polymers.

Fracturing and Controlled Cracking Path in Topological Maxwell Lattice

Dr. Xinyu Wang, Dr. Siddhartha Sarkar, Prof. Stefano Gonella, Prof. Xiaoming Mao

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We show fracturing analysis of topologically polarized Maxwell lattices upon external stretching. Topological mechanics led to the discovery of topologically protected floppy modes and states of self-stress at the edges and the domain walls of Maxwell lattice. To put Maxwell lattice into practical fabrication, we need realistic structural lattices characterized by non-ideal, finite-thickness hinges. Recent progress has shown that in both ideal and realistic lattices, when topological Maxwell lattices are being stretched, stress focuses on states of self-stress domain walls, and bond-breaking events start at these domain walls, even in the presence of cracks, implying the robustness of topological polarization in the Maxwell lattice. In this work, we stretch the lattices to the failure stress of the material and observe non-trivial cracking paths in the topological materials. We use simulations, theory and experiments to understand the cracking behaviors, and we further show how to use defects, material properties, and topological decay rate to control and program the failure patterns and meta-material properties.

Freezing hydrogels reveals a simple, power-law behavior of their osmotic pressure

Ms. Yanxia Feng, Dr. Dominic Gerber, Dr. Stefanie Heyden, Dr. Martin Kroger, Dr. Eric Dufresne, Dr. Lucio Isa, Dr. Robert Style

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Hydrogels are particularly versatile materials that are found across a wide range of natural and industrial applications. One key reason for this versatility is their high water content, which lets them dramatically change their volume and many of their material properties – often by orders of magnitude – as they swell and dry out. To understand hydrogel behavior, we need techniques to characterize how these properties change across a range of different water contents. Here, we show that one approach is to use Gel-Freezing Osmometry (GelFrO), an extension of freezing-point osmometry(FPO), which is commonly used to characterize aqueous solutions. We re-imagine FPO to apply to hydrogels by tracking the shrinkage of a gel layer in contact with ice. We demonstrate GelFrO for several different hydrogels, by measuring their mechanical response to compression and their osmotic pressure as a function of polymer content. We use the results to derive a new, broadly applicable constitutive model for hydrogel mechanical behavior. Moreover, we compare the results with classical gel-swelling theoretical predictions, and do not find good agreement. Instead our data is well-described by simple power-law expressions. We interpret this as a hallmark of a microscopic fractal structure of the gel's polymer network, and propose a simple way to connect the gel's fractal dimension to its mechanical properties. GelFrO offers many advantages over current approaches, including the ability to work with small samples, the need for only relatively short equilibration times, and the fact that it gives access to a wide range of gel compressions. This technique helps us understand mechanical and osmotic pressure behaviour of hydrogels.

From gels to 3-D networks: Creating multifunctional hybrid polymer-metal oxide nanofiber based aerogels

Tahira Pirzada, Muhammed Ziauddin Ahmad Ebrahim, Vahid Rahmanian, **Dr. Saad Khan**

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Gels containing water or solvents abound in applications with considerable efforts being made to fabricate new ones with enhanced functionalities. An area that remains less explored is the creation of aerogels by replacing the liquid matrix of gels with air. Can we preserve the structure of these systems on liquid removal and can we create materials that are just as versatile by doing so? This work investigates the development of novel fibrous aerogels with advanced functionalities through solvent replacement from a fibrous dispersion in a non-solvent. While traditional gels find numerous applications, aerogels, their air-filled counterparts, remain less explored mainly because of lack of mechanical robustness and shapeability. We present a facile and sustainable approach utilizing solid templating and sol-gel electrospinning to fabricate highly porous, flexible fibrous aerogels (NFA) from composite nanofibers of 1) cellulose acetate (CDA) and silica, 2) polyvinylpyrrolidone (PVP)-titania (TiO2) and 3) polyacrylonitrile (PAN) and PVP. Scanning electron microscopy (SEM) reveals hierarchical architectures: large secondary pores (30-50 µm) interconnected by a network of entangled nanofibers with primary pores of 2-5 µm. X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared spectroscopy (FTIR) studies demonstrate the nature of binding between the components of the hybrid fibers. With low bulk density (~10 mg/cm^3) and high porosity (>98%), these NFAs exhibit enhanced mechanical flexibility and multifunctionality based on the architecture and composition of the hybrid nanofibers. The PVP-TiO2 NFA exhibits a low thermal conductivity (0.062 W m−1 K−1) together with considerable mechanical flexibility up to strains of 50% with >90% recovery, without the need for post-processing. These NFA exhibits antibacterial properties upon UV exposure and sorb common volatile organic components (VOCs) or oil which decompose on exposure to UV radiation showing promising attributes as viable candidates for a diverse range of applications. Superhydrophobic nature and high oleophilicity of the CDA-silica hybrid aerogels enable them to be ideal candidates for oil spill cleaning, while their low thermal conductivity and flame retardancy can be explored in various applications requiring stability at high temperatures. Going one step further, we explore multiple innovative approaches for synthesizing materials metal-organic frameworks (MOFs) - with three-dimensional network structure and exceptionally high surface area and pore volume on the NFAs as a sustainable and scalable material platform. We compare MOFs grown using different pathways of introducing the metal-oxide precursor notably through atomic layer deposition (ALD), in-situ introduction in the nanofibers through electrospinning and by the growth of metal-oxide nanorods on the NFAs. The resulting 3D structure exhibits elasticity, low density (~10 mg/cm 3), and hierarchical porosity. Mechanical compressibility tests confirm the durability and resilience of the MOF-NFAs, making them suitable for mechanically stressful environments. Incorporating MOFs into the aerogel structure maximizes surface area and exposes active sites within the micropores of ZIF-8, facilitating efficient CO2 molecule adsorption(4.04 mmol/g) and heavy metals removal specifically Cu(II) ions (>99%). In short, the combination of these functional features with facile processing approaches positions our hybrid NFAs as promising candidates for diverse applications, potentially surpassing their liquid-based counterparts in functionality and applications.

Linear and nonlinear viscoelasticity in physical gels made with polycations, polyanions, and their mixtures; rheology and microrheology approach

Mr. Ricky Frank López-Santiago, Dr. Prof. Rolando Castillo

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

For different physical gels made from polysaccharides (alginate, chitosan, and mixtures), we have investigated their linear and nonlinear viscoelastic behavior and their relationship with the mesoscopic structure. Different physical mechanisms form all gels. The alginate gel was formed

by complexation between alginate chains and Ca2+. The chitosan gel was formed by modification of the hydrophobicity of the medium, and the alginate/chitosan gel was formed by slow electrostatic interaction between the chains.
The Chambon & Winter criteria show a similar critical exponent near the gel point for all gels n ~ 0.6, demonstrating that, regardless of the physical mechanism of gelation, the percolation threshold associated with gel network formation is the same. In previous work, we obtained a similar critical exponent for physical gelatin gels [1], supporting our observation of the similarity of polymeric critical physical gels. We also investigated the strain-hardening behavior of the matured gels using the LAOS protocol; the BST scaling model was used to interpret the results in mesoscopic terms, such as the fractal dimension (df). We also obtained the Lissajous-Bowditch (LB) curves. For alginate gels, df ~ 1.25 - 1.33, and its value depends on Ca2+ concentration; as Ca2+ concentration increases, the fractal dimension decreases, showing a difference in their network structure due to the formation of different forms of complexation between Ca2+ and alginate chains. For chitosan gels, df ~ 1.33 – 1.49, and their value depends on the rate at which the modification of the hydrophobicity of the medium; at a high rate, df decreases. The alginate/chitosan mixture forms a microgel, which was confirmed by the nonlinear viscoelasticity spectrum and micrographs obtained by AFM. The fractal dimension was impossible to obtain in this system due to BST-scaling model limitations. The LB curves are different for all gels in the region of nonlinear viscoelasticity; they serve as a fingerprint.
Additionally, we employed diffusion wave spectroscopy micro-rheology to measure the mean square displacements (MSD) of the microspheres embedded in the precursor solution to study the kinetics of gelation. In a kinetic study, we observed that the MSD decreased according to the formation of the network, and the shape of MSD is different according to the physical gelation mechanism. The MSD data can be used to obtain the viscoelastic spectra at high frequencies, allowing us to observe the different relaxation modes of the chains in the network.

[1] López-Santiago, R. F., Delgado, J., & Castillo, R. (2024). Competition among physical, chemical, and hybrid gelation mechanisms in biopolymers. Soft Matter, 20(11), 2518-2531.

Manufacturing Techniques of Disordered Metamaterials Using Laser and Electron Beam Powder Bed Fusion

Katherine Moody, Molly Li, Phuonganh Pham, Dr. Ryan Hurley, Dr. Katie Newhall, Dr. Mason A. Porter, Dr. Karen E. Daniels, Dr. Christopher Rock

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Three-dimensional open geometries which originate from non-traditional manufacturing sources such as point clouds, sphere packings, and code-based Standard Tessellation Language (STL) file generation can be challenging to manufacture when the structures are very complex. In the current study, we created rigid 3D structures by connecting nearby points or grain centers with rods to fabricate an open-frame disordered metamaterial geometry for testing. This approach produced multiple connecting rod angles ranging from 0 to 90 degrees relative to the build plate. The geometries were successfully manufactured as prototypes using polymer additive manufacturing processes. However, prototyping using laser powder-bed fusion was challenging for the

low-angle connecting rods due to heat-transfer differences of printing on powder compared with a solid substrate. We performed a systematic study to emulate the complex rod angles by printing cylinders ranging from 0.5 mm to 5 mm in diameter and angles ranging from 0 to 90 degrees relative to the build plate. Unsupported cylinders tended to lose geometric integrity at angles under 30 degrees and typically failed at 10 degrees, resulting in geometric deviation and rough surfaces on the downskin of the rod. However, varying input energies, scan strategies, and selective support strategies mitigated the geometric deviation to successfully fabricate 3D disordered components with limited and removable supports. Electron beam powder bed fusion also successfully produced geometries with fidelity, but structures had noticeable surface roughness.

Measurement of vibrational modes in disordered metamaterials fabricated by laser powder bed fusion.

Sidharth Gat, Dr. Christopher Rock, Dr Karen Daniels

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Hyperuniformity can be found in quasicrystalline materials, epithelial cells, the large-scale structures of the universe, granular materials, soap bubble rafts, chicken eyes, emulsions, and more. We aim to quantify the relationship between the driving frequency and the spatial distribution of vibrations in disordered metamaterials, and compare them with predictions from the jamming literature. In this study, we focus on Lloyd’s algorithm for producing a series of disordered structures, iterations of which produce hyperuniform structures in the limit of large iterations. We use open metamaterials generated from the Delaunay triangulations generated after 1, 10, 30, and 100 iterations of Lloyd's algorithm. Each sample is a quasi-2D structure printed from 17-4PH powdered steel using laser powder bed fusion. Using a scanning laser Doppler velocimeter (SLDV), we apply sinusoidal perturbations and measure the spatial patterns of the resulting vibrational modes. Because the SLDV measures the instantaneous velocity via the Doppler shift in laser frequency, we are able to assign a vibration amplitude to each edge of the network under both constant-frequency driving and ambient noise conditions.

Modeling Phase Stability of Concentrated Suspensions of Compressible Microgels

Mr. Oreoluwa Alade, Prof. Alan Denton

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Microgels are soft colloidal particles, made of crosslinked polymer gels, that can swell by absorbing a good solvent. Internal degrees of freedom allow microgels to respond to external stimuli by changing size. Sensitive responses to variations in temperature and concentration inspire many practical applications, e.g., to drug delivery, biosensing, filtration, and photonic crystals. At sufficiently high concentrations, mutual crowding can drive microgels to form facets or interpenetrate [1]. To explore the influence of particle softness and compressibility on thermodynamic phase stability, we adapt a coarse-grained model in which spherical microgels interact via the Hertz elastic pair potential and can both deswell, interpenetrate and facet, as governed by the

Flory-Rehner theory of polymer networks. In our model, faceting reduces the volume available for swelling, while interpenetration reduces polymer-solvent mixing entropy. By performing Monte Carlo simulations that incorporate novel trial changes in particle size [2], we compute Lindemann parameters to determine the liquid-solid phase stability boundary over a range of particle softness, tuned by varying crosslink fraction. To assess under what conditions faceting or interpenetrating conformations are favored, we compare free energies computed via thermodynamic integration using the Frenkel-Ladd method [3]. We further compute structural properties of bulk suspensions, including radial distribution functions and static structure factors. In contrast to the phase behavior of incompressible hertzian spheres [4], we find that suspensions of compressible microgels crystallize at significantly lower volume fractions, when accounting for free energy costs of faceting and interpenetrating. Our results extend previous studies of microgel phase behavior and can help to interpret experimental observations.

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Supported by the National Science Foundation (DMR-1928073).

Modeling the Response of Compressible Microgels to Crowding by Nanoparticles

Mr. Mahesh Aryal, Prof. Alan Denton

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Microgels are soft, compressible, colloidal-sized particles, composed of crosslinked polymer networks. Their internal degrees of freedom enable microgels to swell or deswell, in response to changes in environment, by absorbing or expelling solvent in solution. The presence of other molecular species (e.g., cosolvents or nanoparticles) can enrich the swelling response, facilitating applications of these “smart” colloidal particles, e.g., as drug delivery vehicles and biosensors. We adopt a coarse-grained model based on the mean-field Flory-Rehner theory of polymer networks, which attributes the swelling of microgels to a competition between polymer-solvent mixing and chain conformational entropies. We extend the Flory-Rehner theory to ternary mixtures by incorporating, as a third implicit species, “nanoparticles” that can perturb the polymer network through volume exclusion. In practice, the nanoparticles could represent macromolecules, such as biopolymers, drug or dye molecules. The penetration of a polymer network by nanoparticles is described by polymer field theory, which predicts a free energy cost of penetration that scales with the ratio of polymer chain to nanoparticle size. Within our computationally efficient coarse-grained approach, we perform Monte Carlo simulations, including novel trial moves [1] that allow microgels to change size and nanoparticles to penetrate microgels. We investigate how single-microgel properties (e.g., crosslink density) and solution properties (e.g., nanoparticle concentration, solvent quality) influence swelling of microgels and nanoparticle partitioning inside and outside of microgels. For bulk suspensions of microgels interacting via the Hertz elastic pair potential, we further compute structural properties, namely, radial distribution functions and static structure factors. We find that nanoparticle crowding promotes microgel deswelling, weakening interparticle correlations, and that with increasing nanoparticle concentration in the solution, microgels reach a maximum loading capacity dependent on nanoparticle size and polymer crosslink fraction. Our results can help interpret experiments and guide the design of novel soft materials by providing insights into how the response of microgels to external stimuli can be tuned by adding nanoparticles.

[1] M. Urich and A. R. Denton, Soft Matter 12, 9086 (2016).

Supported by the National Science Foundation (DMR-1928073).

Mucin-derived adhesive hydrogels

Dr. George Degen, Dr. Corey Stevens, Dr. Gerardo Cárcamo-Oyarce, Dr. Jake Song, Dr. Katharina Ribbeck, Dr. Gareth McKinley

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Every wet epithelial surface of the body is coated in a layer of mucus that hydrates, lubricates, and prevents infection of the underlying tissue. These properties result from a family of glycosylated proteins called mucins, which assemble into viscoelastic networks by disulfide bonding and noncovalent interactions. The biological functions of mucin proteins have motivated research on mucin-based materials for biomedical applications. However, many applications require robust gelation and adhesion, beyond the transient crosslinking and non-covalent adsorption of native mucins. Here, I demonstrate that catechol-functionalized polymers crosslink mucin proteins into adhesive hydrogels. Gelation is shown to primarily result from covalent bonding between catechols and cysteine thiols, with gelation dynamics and adhesion tuned by the concentration and architecture of the polymer constituents. I then present potential applications of the hydrogels as antifouling coatings and tissue adhesives. Collectively, the results suggest the promise of catechol-based crosslinking of thiolated polymers for achieving adhesive hydrogels for biomedical applications.

Network-Network Interactions in Multi-Component Gels

Mauro Mugnai, Emanuela Del Gado

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Multi-component gels are common in biology and display striking material properties.
Indeed, the extra-cellular matrix features a combination of various proteins and sugars, including collagen, elastin, and glycosaminoglycans, and engineered double network (DN) hydrogels exhibit remarkable toughness.
Understanding and controlling the properties of these networks at a molecular level requires knowledge of the way in which network-network interactions affect morphology and rheology of the combined gel.
In order to predict properties of DNs, we designed a series of rheological tests performed on in-silico self-assembled multi-component gels.

The model includes two-body interactions, which drive self-assembly, and three-body terms that create filamentous networks.
We systematically changed the strength of network-network interactions that control the mechanical coupling between the two components and generated a remarkable variety of topologies and mechanical responses.
Our results underscore the richness of DN hydrogels, illustrate how to control their properties, and set the stage for comparison with experiments.

Nonlocal Intrinsic fracture energy of polymer networks

Shu Wang

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The fracture of polymer networks is inherently linked to the scission of network chains, yet their quantitative connection remains elusive. The classical perspective on the intrinsic fracture energy of polymer networks originates from the Lake-Thomas model, which posits that energy dissipation occurs within the scale of broken bridging chains at the crack tip. However, recent advances in polymer mechanochemistry and single-molecule force spectroscopy have suggested that the assumption of such a limited energy dissipation length scale by the Lake-Thomas model may underestimate experimental observations by one to two orders of magnitude. We introduce a conceptual framework that considers the non-local intrinsic fracture energy of polymer networks. This model encompasses not only the energy released from the scission of bridging chains but also the subsequent energy dissipation from the network continuum. The scission of a bridging chain releases crosslinks and opens the corresponding topological loop. The released crosslinks are to be captured by the opened loop and the load is transferred to the next bridging chain. The amount of energy released and dissipated in the network continuum is controlled by the stretchability of the opened loop. Based on this loop-opening process, we propose that the intrinsic fracture energy per broken chain approximately scales with the product of the fracture force and the contour length of the opened loop. This model provides predictions of intrinsic fracture energy that align well with various experimental data on the fracture of polymer networks.

Novel Volumetric mapping of 3D Nanomechanical Heterogeneities in Gelatin, Collagen, and Polypeptide Hydrogels and Films

Kevin Grassie, Bryan Huey, Yusuf Khan, Yao Lin, Jianan Mao, **Fei Wang**

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Porous and fibrous hydrogels and films are promising scaffolds for tissue engineering and drug delivery. To assess their nanovolumetric mechanical properties, far-field longitudinal ultrasonic excitation and simultaneous 3D optical mapping are employed to detect down to picometer scale displacement vectors throughout a uniformly loaded gel or film using up to thousands of fluorescent markers as beacons. This allows local distortions within the hydrogel, and even incorporated cells, to be volumetrically mapped and the force distribution to even be back-calculated. Results are reported for a range of gelatin, collagen, and polypeptide compositions, as well as applied acoustic power and load duration, and compared to macroscopic storage and loss moduli determined by rheology. Spatial variations in local magnitudes and vectorial directionality, as well as elastic recovery, are also visualized and statistically analyzed by specimen and depth. Collectively, this approach reveals 3D nanomechanical heterogeneities resulting from local differences in hydrogel cross-linking, density, hydration, and/or cellular mechanical structures and active adhesion.

Organic Phosphate Degradation via Functionalized PA-6 Fabrics

Mr. Nate Brown, Owen Duckworth, Kirill Efimenko Efimenko, Jan Genzer

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Organic phosphates are invaluable as agricultural fertilizers due to their stability and ease of application. However, the overuse and run-off of such fertilizers can result in detrimental environmental impacts such as algal blooms and contaminated water sources. In addition to agriculture applications, the limited sources of phosphorous have incentivized much research effort into reducing, reusing, or capturing phosphorous-containing compounds. Here, we propose the application of hydroxamic acid functional gel coatings to Nylon 6 fabrics (PA-6 HA) as a means of organic phosphate hydrolysis, yielding inorganic phosphates necessary for crop growth. Such conversion enables the reduced use of phosphate fertilizers via improved efficiency of inorganic phosphorous uptake by plants. PA-6 HA fabrics demonstrate degradation dependence on crosslinking content with 5 mol% concentrations yielding 87.95% conversion over 48 hours. Conversion decreased with increasing organic phosphate concentration, indicating a low content of non-catalytic hydroxamic acid moieties within the bulk gel coating. With sub 150 nm coatings, phosphorous uptake by PA-6 HA was minimal compared to metal organic framework UIO-66 but displayed initial noticeable absorption with films approaching micron scales. Thus, hydroxylamine functionalized gel coatings of PA-6 demonstrate viable organic phosphate behavior while exploring the potential of functionalized thin gel coatings.

Peptide self-assembly orchestrates structure transition of in-vitro actin bundle networks

Kengo Nishi, Stephen Klawa, Tengyue Jian, Yuan Gao, Qunzhao Wang, Prof Ronit Freeman

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The mechanical properties of cells are finely regulated by the actin cytoskeleton. In this process, endogenous protein crosslinkers play a pivotal role in regulating hierarchical structures of actin networks, essential for various cellular processes including cell migration, division, and shape changes. The ability to synthetically regulate their network architecture is essential for engineering novel biomaterials with tunable mechanics. Here, we introduce peptide nanotechnology to synthetically regulate the architecture of actin bundle networks. We discovered that our fibrous peptide assemblies architect actin bundle networks, mimicking natural actin crosslinkers and regulating their transition from straight to branched bundles by controlling the nanostructures of peptide assembly. We further encapsulate these structural hierarchies and control their spatial localization within cell-size droplets to engineer new synthetic cells and tissues.

Pristine Carbon Nanotubes as Supramolecular Linkers to Crosslink Microgels into Macroscopic Hydrogel Composites for Versatile Advanced Applications

Dr. Yunxiang Gao, Mohammad Islam, Promise Otuokere, Favour Ezeogu, Victoria Robinson

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Pristine Carbon Nanotubes (CNTs), known for their hydrophobic nature, have traditionally been dispersed in aqueous solutions using amphiphilic small-molecular surfactants, 1-D linear polymers, or single-strand DNAs. In this study, we present the novel finding that pristine CNTs can also be effectively dispersed in aqueous solutions using 3-D microgels. Under specific conditions, pristine CNTs can function either as flocculants, precipitating microgels, or as nanobridges, crosslinking microgels into macroscopic hydrogel-composites. The resulting hydrogel composites exhibit high conductivity with a minimal CNT dosage. By employing pristine CNTs as supramolecular linkers, the resulting hydrogel composites show potential applications in low-cost water purification, multi-functional soil amendment for sustainable agriculture, writable-circuit inks, versatile moisture, environmental and heath sensors, as well as tissue engineering scaffolds. This study expands the understanding of CNT dispersion in aqueous solutions and introduces a versatile method for creating macroscopic hydrogel composites from crosslinking microgels, with significant practical applications in sustainability, agriculture, electronics, and biotechnology.

Programming rigidity transitions and multifunctionality in disordered underconstrained spring networks

Tyler Hain, M. Lisa Manning, Chris Santangelo

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Our goal is to design multifunctional materials that are tuned to be near a rigidity transition and exhibit other desired behaviors. We focus on underconstrained central force networks near a second-order rigidity transition. Unlike the jamming transition seen in granular systems, which is governed by first-order perturbations and constraint counting, a second-order rigidity transition occurs when geometric incompatibility drives the system to a critical configuration that possesses a state of self-stress. The space of all critical configurations forms a hypersurface in configuration space -- the critical manifold. If a network is strained, it will eventually intersect this critical manifold, but the resulting self-stress is an emergent property. To program features into the self-stress, we describe a parameterization that treats the self-stresses as the degrees of freedom to develop an expression for all configurations on the critical manifold. With this parameterization we can calculate derivatives of any objective function with respect to the self-stresses on this manifold. This allows the critical manifold to be leveraged as a design space through gradient descent on a cost landscape. We compare features of random disordered networks that have been strained to the rigidity transition to those in networks that have been optimized to possess various structural or elastic response properties.

Revealing the mechanism of kinetic arrest in suspensions of rod-like cellulose nanocrystals using angle-resolved optical spectroscopy

Dr. Thomas Parton, Dr Bruno Frka-Petesic, Dr Richard Parker, Professor Silvia Vignolini

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Cellulose nanocrystals (CNCs) are rod-like nanoparticles whose chiral self-assembly into photonic films has been promoted as a sustainable source of coloration. Upon drying, an aqueous CNC suspension passes through two regimes: first, a liquid phase, where the CNCs self-organize into a cholesteric liquid crystal, followed by a kinetically-arrested phase, where the helicoidal structure compresses upon loss of solvent, resulting in a solid film with vibrant structural color. The transition between these two regimes plays an important role in the visual appearance of CNC films, but details on when and how kinetic arrest occurs have remained elusive.

In this study, we combined angle-resolved optical spectroscopy of structurally-colored films (approx. 100 vol% CNC) with a model for compressed helicoidal structures to retrieve the suspension conditions during kinetic arrest (approx. 10 vol% CNC). This analysis indicates a shift in the mechanism of kinetic arrest from a glass transition at lower ionic strength to gelation at higher ionic strength, consistent with rheological studies. In contrast, neutral additives (glucose, poly(ethylene glycol)) appear to primarily reduce the compression upon drying without affecting cholesteric behavior, as supported by a general analytical model. These findings deepen our understanding of CNC co-assembly with various commonly-used additives, enabling better control over the production of multifunctional structurally colored materials.

Parton, T.G. et al., Soft Matter, (2024). DOI: 10.1039/D4SM00155A

Frka-Petesic B. et al, Phys Rev. Mater., (2019). DOI: 10.1103/PhysRevMaterials.3.045601

Size dependent, stress driven transport in poroelastic media at the microscale

Mr. Alexander Marshall

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Heterogenous multiphase materials are found in contexts ranging from geological to biological. In the latter context, tissues and individual cells are poroelastic – they consist of a background matrix that is suffused by a solvent carrying solutes with a distribution of sizes. These materials, within their physiological context, undergo dynamic stresses at a variety of time and length scales, and these stresses cause deformations that necessarily induce advection. These flows induce redistributions of solutes with potentially significant complexities emerging from the size dependent transport in porous media. Within biological contexts, strain mediated transport is understood to induce metabolite transport in tissues, with this concept applied to the design of tissue engineering constructs and processing methodologies. Within model systems, there is a limited set of controlled studies. Remarkably, these macroscale experiments have demonstrated concentration enhancements in cyclically strained centimeter-scale hydrogel specimens. While the implications of this strain dependent transport have been appreciated in tissue physiology and engineering, there is a dearth of studies at the microscale. It is at the microscale that we can study phenomena at the size of individual cells, and access the competition between molecular scale, pore size, and stress gradients that are at play in biological contexts. We employ thin films of polyacrylamide as a model poroelastic system with tunable size-dependent transport, with atomic force microscopy to apply precise microscale stresses. We study the size dependent particle transport using light sheet microscopy to follow concentration maps and apply single particle tracking to follow individual particle motion during material strain.

Supramolecular Templation of Entanglements and Their Spectroscopic Detection in Polymer Elastomers and Gels

Dr. Fu-Sheng Wang, Erin Krist, Ben Kruse, John Dickenson, Prof. Aleksandr Zhukhovitskiy

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Trapped entanglements in polymer networks are essential for the material's mechanical properties, such as stiffness and toughness. However, the quantitative correlation between mechanical properties and the number or topology of entanglements remains unclear. The challenge lies in the lack of experimental methods to install trapped entanglements quantitatively with defined topology. Herein, we present a supramolecular templation strategy—based on phenanthroline-copper coordination chemistry—to introduce trapped entanglements into gels or elastomers. The topology of the templated entanglements is controlled by the geometry of the complexes. Using the templates, we can bring the phenanthroline pairs spatially close to each other in the materials, as evidenced by the formation of the phenanthroline exciplex. In terms of mechanical properties, the polymer networks with the templated entanglements showed a stiffness increase of up to 100% compared to the control materials without sacrificing the toughness. Moreover, we show that the entanglement modulus of the materials increases linearly with the amount of the templated entanglements introduced. These observations suggest the successful installation of trapped entanglements using the supramolecular templates.
TEM study on hydrogel network formation via free-radical polymerization

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Mr. Masahiro Yoshida, Dr. Ryuji Kiyama, Dr. Jian Ping Gong

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Hydrogels are composed of polymer networks and water, and show unique properties such as low friction, biocompatibility and material retension/permeability. These distinctive characteristics have led to the utilization of hydrogels in various fields. In order to enhance the properties of hydrogels or develope novel types of hydrogels, it is essential to study the process of hydrogel network formation. This process plays a crutial role in determining the network structure, which in turn influences the properties of the hydrogel.

Due to its significance, formation of gels has been studied for more than 80 years through both theoretical and experimental approaches. However, despite the compelling information obtained, microscopic approaches have not been extensively utilized until now. This is primarily due to the difficulty microscopes face in capturing the thermal fluctuations and low electron density of polymers and networks.

Very recently, our group successfully developed a microscopy method for hydrogel networks. This method effectively addresses the challenges posed by the thermal fluctuations and low electron density by introducing a skeleton network and mineral staining, respectively. Using transmission electron microscopy (TEM), this method enables us to observe the network structures at the nanoscale in real-space at room temperature.

This time, using the aforementioned method, we investigated the polymer network formation of hydrogel prepared by free radical polymerization. Timelapse observation appeared to be an ideal strategy, albeit challenging, as the TEM observation method could not facilitate in-situ observations during the polymerization. However, based on scattering research, timelapse observation can be approximated by observing the end structure of gels prepared with various monomer concentrations. Therefore, we followed previous research and observed end structures with altered monomer concentrations.

The hydrogel networks were synthesized by free-radical co-polymerization of vinyl and divinyl monomers. Specifically, 2-acrylamido-2-methylpropane sulfonic acid sodium salt (NaAMPS) was employed as the vinyl monomer, while N,N'-Methylenebisacrylamide (MBAA) served as the divinyl monomer. The concentrations of NaAMPS and MBAA were varied within a range that allowed the polymerization product to cover the sol-gel transition.

Overall, as the NaAMPS concentration was increased from 0.04 M to 0.4 M, with a fixed MBAA concentrationof 16 mol% relative to NaAMPS, a structural change from isolated clusters (sol phase) to percolated network (gel phase) was observed. This result was consistent with a model suggested by previous scattering results. In detail, ring-like clusters were observed at 0.06 M NaAMP, while a percolated network with significant mesh-size heterogeneity ranging from 10 nm to 1 μm was observed at 0.08 M NaAMP. In both concentrations, a characterisic trunk-like structrue with a thickness of approximately 100 nm was observed. This trunk-like structure is composed of 10 nm-scale network. This similarity suggests that a samilar polymerization process took place in both monomer concentrations.

During the presentation, we will delve into the mechanism of network formation in further detail.

Toughening of poly(ionic liquid) gels with nanomaterials having different shapes

Dr. Takaichi Watanabe, Ms. Yuna Mizutani, Dr. Carlos G. Lopez, Ms. Yume Tao, Dr. Tsutomu Ono

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Ionic-liquid gels, which are known as ion gels, have attracted considerable attention due to their high ionic conductivity and CO_2 absorption capacity. However, their low mechanical strength has been a major obstacle to their practical applications. One of the promising ways to overcome this challenge is the incorporation of nanomaterials, such as silica nanoparticles, TiO_2 nanoparticles, and metal-organic frameworks (MOFs) into ion gels. In this study, we explored how different shapes of alumina particles influence the mechanical characteristics of alumina/poly(ionic liquid) (PIL) double-network (DN) ion gels. These gels consist of either spherical or rod-shaped clustered alumina nanoparticles embedded within a chemically crosslinked poly[1-ethyl-3-vinylimidazolium bis(trifluoromethanesulfonyl)imide] (PC_2im-TFSI, PIL) network. Our findings revealed that alumina/PIL DN ion gels exhibit superior mechanical strength compared to PIL single-network ion gels without particles. Specifically, rod-shaped alumina/PIL DN ion gels demonstrated fracture energies approximately 2.6 times higher than their spherical counterparts. The spherical alumina consistently enhanced mechanical properties across various concentrations, while the rod-shaped alumina led to a stiffer ion gel and demonstrated a threshold for toughness improvement with diminishing returns beyond a specific concentration owing to the formation of large aggregates. Cyclic tensile tests suggested that the improved mechanical properties stem from the efficient dissipation of loading energy through the destruction of the alumina network. TEM observation indicated that the variation in the mechanical strength depending on the shape can be attributed to differences in the aggregation structure of the alumina particles. Our study underscores the intricate relationship between nanomaterial shape and the macroscopic properties of ion gels, offering insights for designing ion gels with optimized mechanical properties.

Universality in Strain Stiffened Articular Cartilage

Mr. Japheth Omonira, Mr. Stephen Thornton, Prof. Itai Cohen

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Articular cartilage is the soft tissue that coats the long bones in our bodies and provides smooth function of our joints. The tissue mechanics are primarily governed by its extracellular network comprised of collagen fiber network supported by a secondary network of aggrecan molecules. Though mechanical trauma to articular cartilage is a known cause of osteoarthritis, little is known about how the tissue transitions from a physiological regime to a strain-stiffened, injurious regime. Here, we give a theory of the shear modulus in terms of a universal crossover scaling function from an unstrained state to a strain-stiffened state associated with network alignment. Experimentally, we find the local shear moduli at various extracellular matrix constituent concentrations can be collapsed onto a single universal scaling curve. This collapse shows two different scaling regimes, one associated with an isotropic network, the other associated with a strain stiffened network characterized by different critical exponents. This discovery invites the developed understanding of critical phenomena to elucidate the physical aspects of strain stiffening in this biologically important tissue with the potential to elucidate its function in health and disease.

Water two liquids, anyway?

Joan Montes De Oca

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Since Speedy and Angel discovered the anomalous behavior of water's thermodynamic functions upon supercooling, the scientific community has expended significant effort to explain those observations. We have finally reached a consensus on the existence of a liquid-liquid phase transition after many important contributions presented evidence to this effect, and particularly after Debenedetti and Sciortino proved that water LLCP fits within the 3D Ising's universality class. However, despite this consensus, many articles discussing thermodynamic anomalies of water still treat water as a mixing of "two liquids" that undergo phase separation upon cooling. Although the "two-liquid" approach successfully predicts water's behavior, it is often deemed a cartoonish vision because it is unclear what those two liquids represent in pure homogenous water. In this presentation, I'll show that, although not the most intuitive way to understand the liquid-liquid phase transition, liquid water can be understood as the mixture of three, tetra, and penta coordinated molecules. Furthermore, by analyzing partial radial distribution functions and the corresponding structure factors, I'll show that molecules with three or five hydrogen bonds separate from molecules with four hydrogen bonds upon supercooling. This observation not only sheds new light on the molecular mechanism behind the liquid-liquid phase transition but also opens up opportunities for innovative molecular design techniques in aqueous solutions.

Polymers

Additive manufacturing of high-resolution architected copper by controlled shrinkage of highly swollen, infused bottlebrush hydrogel scaffolds for enhanced catalysis.

Mr. Emmanuel Oduro, Dr. Daniel A. Rau, Mr. Baiqiang Huang, Mrs. Yulu Zhang, Dr. Sen Zhang, Dr. Li-Heng Cai

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Additive manufacturing (AM) of metals via hydrogel infusion emerges as a general approach to creating advanced architected metallic materials. However, existing resins are limited to highly crosslinked organogels, which have a limited swelling ratio and must undergo solvent exchange with water before being infused with a metal salt solution. Here, we report a process of AM of high-resolution architected metals without solvent exchange. We develop a highly swellable hydrogel resin for stereolithography (SLA) printing by exploiting foldable poly (ethylene glycol) (PEG) bottlebrush polymers as network strands. At a dry state, the backbone of the bottlebrush polymer collapses; upon exposure to water, the hydrophilic PEG chains absorb water and extend the bottlebrush backbone, resulting in >10 times swelling in volume. We develop a process for controllable shrinkage of three-dimensional (3D) hydrogel scaffolds infused with a copper salt solution, which are calcined and reduced to create high-resolution architected copper. We demonstrate that the copper scaffolds exhibit enhanced catalytic performance attributed to their unique morphology and multiscale structure. Our discovery paves the way to create architected multiscale metals for high-performance catalysis.

Bottlebrush polyethylene glycol nanocarriers translocate across human airway epithelium via molecular architecture enhanced endocytosis

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Mr. Baiqiang Huang, Dr. Zhijian He, Dr. Liheng Cai

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Pulmonary drug delivery is critical to the treatment of respiratory diseases. However, the human airway surface presents multiscale barriers to efficient drug delivery. Here we report a bottle-brush polyethylene glycol (PEG-BB) nanocarrier that can translocate across all barriers within the human airway surface. Guided by the molecular theory, we design a PEG-BB molecule consisting of a linear backbone densely grafted by many (~1,000) low molecular weight (~1000 g/mol) PEG chains; this results in a highly anisotropic, wormlike nanocarrier featuring a contour length of ~250 nm, a cross-section of ~20 nm, and a hydrodynamic diameter of ~40 nm. Using the classic air-liquid-interface culture system to recapitulate essential biological features of the human airway surface, we show that PEG-BB rapidly penetrates through endogenous airway mucus and periciliary brush layer (mesh size of 20-40 nm) to be internalized by cells across the whole epithelium. By quantifying the cellular uptake of polymeric carriers of various molecular architectures and manipulating cell proliferation and endocytosis pathways, we show that the translocation of PEG-BB across the epithelium is driven by bottlebrush architecture enhanced endocytosis. Our results demonstrate that large, wormlike bottlebrush PEG polymers, if properly designed, can be used as a novel carrier for pulmonary and mucosal drug delivery.

Bound Layer in Hydrophilic Polymer Thin Films: Effect of Annealing

Mr. Sonam Zangpo Bhutia, Dr. Sivasurender Chandran, Dr. Sathish K. Sukumaran, Dr. Dillip K. Satapathy

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The conformation of polymer chains is strongly affected in the vicinity of a solid, impenetrable surface. Near an attractive surface, chains adsorbed to the surface form a distinct polymer layer. This “bound layer” is known to significantly influence the structural and dynamical properties of polymer films. Recently, we proposed a novel method to accurately determine the thickness and the density of this bound layer by analyzing the swelling behavior of polymer thin films when exposed to solvent vapor. In this study, we explored the properties of the bound layer in unannealed and annealed Poly(vinyl alcohol) (PVA) films by varying the duration and temperature of annealing. The thickness of the bound layer, ds, was determined using two independent methods:

analysis of the swelling kinetics and Guiselin's approach, which involved rinsing off the unadsorbed chains with a good solvent. We measured the swelling kinetics of PVA thin films exposed to water vapor using in-situ spectroscopic ellipsometry and X-ray reflectivity. Interestingly, the ds values obtained from both swelling kinetics and Guiselin's approach were found to be essentially independent of the initial film thickness. For annealed PVA films, the ds determined using Guiselin's approach were slightly larger than those determined using the swelling kinetics. This suggested that the thickness of the “adsorbed layer” determined using Guiselin's approach may include contributions from the polymer chain ends (tails) that protrude above the bound layer, in addition to the contribution from the bound layer itself. Further investigation revealed that unlike the bound layer, the adsorbed layer underwent swelling upon exposure to water vapor. In summary, we will present a detailed analysis of the effect of thermal annealing on the bound layer characteristics and the swelling behavior of the adsorbed layer.

Charge Regulation Triggers Condensation of Short Oligopeptides to Polyelectrolytes.

Mr. Sebastian Pineda Pineda, Dr. Pablo Miguel Blanco, Mr. Roman Staňo, Dr. Peter Košovan

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Electrostatic interactions between charged macromolecules are ubiquitous in biological systems, and they are also important in materials design. Attraction between oppositely charged molecules is often interpreted as if the molecules had a fixed charge, which is not affected by their interaction. Less commonly, charge regulation is invoked to interpret such interactions, i.e., a change of the charge state in response to a change of the local environment. Although some theoretical and simulation studies suggest that charge regulation plays an important role in intermolecular interactions, experimental evidence supporting such a view is very scarce. In the current study, we used a model system, composed of a long polyanion interacting with cationic oligolysines, containing up to 8 lysine residues. We demonstrated, using both constant pH Monte Carlo simulations [1] and NMR and potentiometric titration experiments, that while these lysines are only weakly charged in the absence of the polyanion, they become charged and condense on the polyanion if the pH is close to the pKa of the lysine side chains. We show that the lysines can coexist in two distinct populations within the same solution: (1) practically nonionized and free in solution; (2) highly ionized and condensed on the polyanion [2]. Using this model system, we demonstrate under what conditions charge regulation plays a significant role in the interactions of oppositely charged macromolecules and generalize our findings beyond the specific system used here.

Keywords: charge regulation; counterion condensation; polyelectrolyte complexes; electrostatic association; constant pH Monte Carlo; potentiometric titration; NMR titration; pKa.

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Combination therapy of microporous hydrogel scaffolds displaying supramolecular peptide assemblies to enhance wound healing

Mr. Pablo Cordero Alvarado

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Dysregulation of the overlapping immune processes during wound healing may result in overactivation of inflammatory pathways and elevated secretion of pro-inflammatory molecules, ultimately resulting in delayed and poor wound healing. Supramolecular peptide nanofibers and Microporous Annealed Particle (MAP) scaffolds are promising strategies to modulate local immune activity for the safe and rapid treatment of inflammation without the need for additional immunostimulatory factors or recurrent administrations. Additionally, MAP scaffolds allow for rapid wound closure and significant regeneration to cutaneous wounds, including augmented regeneration of skin appendages, and increased tissue tensile strength. As a dual-arm strategy to modulate immune pathways during wound healing, we have designed an immunotherapy utilizing MAP scaffolds and the peptide nanofiber Coil29. Our MAP+Coil29 material elicits robust epitope-specific Th2-biased humoral and cellular immune responses, while also enabling rapid tissue regeneration following a single application at the wound site. Our work aims to modulate inflammation via local application of MAP+Coil29 scaffolds at the injury site of a murine wound healing excisional model. We hypothesize that in addition to a local Th2-biased response favoring regeneration, materials raising autologous antibody responses against inflammatory molecules will result in further enhanced regeneration of cutaneous wounds, with longer lasting efficacy compared with current passive blockade technologies.

Competing addition processes give distinct growth regimes in the assembly of 1D filaments

Tyler Brown, **Dr. Ashif Akram**

We present a simple model to describe the concentration-dependent growth of protein filaments. Our model contains two states, a low entropy/high affinity ordered state and a high entropy/low affinity disordered state. Consistent with experiments, our model shows a diffusion-limited linear growth regime at low concentration, followed by a concentration independent plateau at intermediate concentrations, and a rapid disordered precipitation at the highest concentrations. We show that growth in the linear and plateau regions is the result of two processes that compete amid the rapid binding and unbinding of non-specific states. The first process is the addition of ordered molecules during the periods where the end of the filament is free of incorrectly bound molecules. The second process is the capture of defects, which occurs when consecutive ordered additions occur on top of incorrectly bound molecules. We show that a key molecular property is the probability that a diffusional collision results in a correctly bound state. Small values of this probability suppress the defect capture growth mode, resulting in a plateau in the growth rate when incorrectly bound molecules become common enough to poison ordered growth. We show that conditions that non-specifically suppress or enhance intermolecular interactions, such as the addition of depletants or osmolytes, have opposite effects on the growth rate in the linear and plateau regimes. In the linear regime stronger interactions promote growth by reducing dissolution events, but in the plateau regime stronger interactions inhibit growth by stabilizing incorrectly bound molecules.

Design of Composite Polymer Brushes for Adsorption of Contaminants from Water

Sergei Rigin, Jan Genzer, Yaroslava Yingling

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Polymer brushes designed for environmental clean-up have emerged as a promising solution for addressing water contamination. Key design considerations include optimizing the brush density and thickness to maximize surface area and adsorption capacity, as well as the careful selection of functional groups and embedded adsorbent materials tailored to target specific contaminants. The embedding of external adsorbent media (e.g., metal and metal oxide nanoparticles) within the brush is influenced by the configurations of both the brush and the particles, making the final structure prediction challenging. In this work, we employ coarse-grained molecular dynamics simulations with the MARTINI Force Field to explore the impact of the brush grafting density and degree of polymerization on its thickness and swelling dynamics, as well as the effects of nanoparticle ligands, particle size, and brush-particle interactions on diffusion of nanoparticles within the brush. We systemize the conformational changes of dry polyethylene glycol (PEG) brushes and the resulting surface patterns, highlighting favorable chain lengths (within the range of 100-500 monomers) and grafting densities (up to 1 chain/nm^2) required for a desired surface coverage. Furthermore, by controlling nanoparticle diffusion into hydrated brushes through the tuning of particle size, ligand length, ligand grafting density, and mimicking different ligand chemistries by adjusting the strength of polymer-ligand interactions, we establish suitable configurations for each of the three interaction regimes: repulsion, surface rolling, and mixing. These findings lay the foundation for a novel class of adsorptive materials designed to capture harmful pollutants from aqueous environments, thereby contributing to environmental sustainability.

Formation of ultrasoft, stretchable, and biodegradable films from plasticized agarose for sustainable electronics

Mr. Mesbah Ahmad, Dr. Yuxuan Liu, Dr. Yong Zhu, Dr. Orlin Velev

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Agarose, a naturally occurring biodegradable biopolymer, can emerge as a potential substitute for non-biodegradable fossil fuel-based substrates in soft electronics. However, one needs to find means to adjust and control its stretchability and flexibility. We report and analyze the formation of ultrasoft stretchable films of agarose plasticized with glycerol. Glycerol molecules interrupt the intramolecular hydrogen bonds among the agarose chains by forming intermolecular hydrogen bonds with them. This results in an increase in the free volume allowing the chains to gain higher mobility. Agarose and glycerol dissolved in hot water yield a transparent viscous solution. Below the gelation temperature of agarose (38□C), the viscous solution forms a gel and can be molded. After the excess water evaporates, a thin agarose film is obtained. The stretchability of the films increased by over 60% with increasing glycerol content, while the maximum tensile stress notably decreased to the order of magnitude of human skin. Swelling and weight loss properties resulting from water absorption and glycerol leaching were also assessed to understand molecular interactions within the dried hydrogel matrix. This study demonstrates that plasticizing the agarose biopolymer radically reduces stiffness and enhances stretchability, rendering it suitable for soft electronic substrates. The utilization of sustainable and biodegradable substrates for soft electronics offers an effective solution to mitigate e-waste. To showcase the suitability of agarose film as a substrate, silver nanowires (AgNWs) were printed onto the films for soft electronic circuit fabrication. The biodegradability of such plasticized agarose films and the recyclability of AgNWs, point toward solutions for sustainable and eco-friendly soft electronics development.

Halogen-bonded shape memory liquid crystal polymer

Mr. Hongshuang Guo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Stimuli-Responsive Liquid Crystalline Elastomers (LCEs) are a class of materials that can undergo significant changes in their properties and shape in response to external stimuli. In particular, harnessing the power of halogen bonding (XB), a non-covalent interaction between an electron-deficient halogen atom and a Lewis base, holds great potential for developing advanced LCEs with unique functionalities. In our study, we present a novel approach utilizing a liquid crystalline network comprising both permanent covalent crosslinks and dynamic halogen bond crosslinks. By incorporating XB into the LCE matrix, we achieve a reversible thermo-responsive shape memory behavior. The I···N halogen bond, a widely studied motif in crystal engineering, plays a pivotal role in enabling temporary shape fixation at room temperature and subsequent shape recovery when exposed to human body temperature. Notably, our research showcases the remarkable versatility of shape programming in these halogen-bonded LCE networks through simple human-hand operation. Additionally, we propose a micro-robotic injection model that allows for complex 1D to 3D shape morphing in aqueous media at 37 °C. Through meticulous structure-property-performance studies, we establish the indispensable contribution of the I···N crosslinks in driving the shape memory effect observed in our halogen-bonded LCEs. The introduction of halogen bonding expands the toolbox for designing smart supramolecular constructs with tailored mechanical properties and thermoresponsive behavior, opening up exciting possibilities for future medical devices and other advanced applications.[1,2]

Acknowledgements: Academy of Finland, European Research Council and Academy Postdoctoral Researcher projects.

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Hydrolytic Crack Growth and Embrittlement in Poly(ethylene terephthalate)

Atte Kadoma, Dr. Quan Jiao, Dr. Joost Vlassak, Dr. Zhigang Suo

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Poly(ethylene terephthalate) (PET) is a thermoplastic of high-volume applications, and is identified as Number 1 in the Resin Identification Code on single-use packages. The ester bonds in the polymer chains are prone to hydrolysis, but the rate of hydrolysis is extremely low at room temperature. Here we show that hydrolysis causes PET to grow cracks even at room temperature and under low loads. The hydrolytic cracks greatly outrun erosion. When PET is submerged in water and subjected to a fixed load, the crack velocity increases with pH. At high loads, the crack grows rapidly, and hydrolysis is negligible, so that the crack grows with substantial plastic deformation and the fracture surface is rough. At low loads, the crack grows slowly and hydrolysis is fast enough, so that the crack grows with negligible plastic deformation and the fracture surface is smooth. These observations show that hydrolysis embrittles PET. Under development for sustainability and healthcare are biodegradable and biomass-derived polymers, many of which have hydrolysable groups in the main chains or crosslinks. They are all potentially susceptible to hydrolytic crack growth and embrittlement. It is hoped that this study will aid the development and applications of these polymers.

Liquid-Liquid Phase Separation In Multicomponent Polymer System

Ms. Tahmida Iqbal, Dr. Edward Van Keuren, Dr. Eleni Hughes

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

This study highlights experiments to understand the effect of additives on liquid-liquid phase separations (LLPS) in polymer solutions. In LLPS, distinct domains with different polymer concentrations form within a polymer solution at specific concentrations and temperatures. One well-known example of LLPS is in polyethylene glycol (PEG) and dextran (DEX) aqueous two-phase systems (ATPS), where- it has been observed that at specific concentrations, a PEG-DEX solution will phase separate into PEG-rich and DEX-rich domains near room temperature. While this phenomenon is understood, there has been less work on the effect of additional components on the kinetics and thermodynamics of the separation. We will present work on the effect of adding small amounts of biological compounds such as urea, tryptophan, and histidine on the LLPS of PEG-DEX. Our initial studies show that the phase transition temperature is generally reduced, even with low concentrations of additives. Phase contrast imaging is done on samples to observe and analyze the phase separation, with Fourier analysis of the images yielding characteristics length scales vs. time and temperature. Moreover, differential dynamic microscopy (DDM) is used to detect the fluctuations near the transition temperature to track pre- spinodal fluctuations and their effect on the final morphology of the system.

Mechanochemically self-amplified HF release and polymer deconstruction

Yixin Hu

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Hydrogen fluoride (HF) is a versatile reagent for transforming materials, playing a siginificant role in self-immolative polymers, remodeling siloxanes, and degradable polymers.Therefore, the ability to produce HF within materials on-demand presents opportunities for developing adaptive materials. In this work, we introduce the production of HF through mechanical activation on alkoxy-gem-difluorocyclopropane (alkoxy-gDFC) mechanophore by adding difluorocarbene to enol ethers. After the mechanochemical activation, one fluorine atom on alkoxy-gDFC migrates to form α-fluoro allyl ether which is able to be hydrolyzed and release HF. The conversion to HF is acid catalyzed reaction, therefore, the HF generation is self-amplified. The generated HF is detectable by fluoride indicators and is used for breaking down polybutadiene containing HF-sensitive silyl ethers. As a result, the alkoxy-gDFC mechanophore offers a method for mechanically controlled HF release, adding a new dimension to polymer modification strategies that previously relied on heat.

Modeling the emergence of collective nascent chain behavior and its implications for the sequences and aggregates of step-grown copolymers.

Dr. Kateri DuBay, Dr. Ryan Hamblin, Dr. Nhu Nguyen, Wenxin Xu, Dr. Zhongmin Zhang

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The sequential ordering of different monomers within synthetic copolymers is remarkably difficult to control. Our understanding of the determinants of and variations within copolymer sequences, even in simple step-growth reactions, remains limited. Here, we perform simulations on a generic model of an irreversible step-growth copolymerization between two types of monomers, A and B, in solution. Our results demonstrate that attractions among the nascent oligomers can exert considerable influence over the sequential arrangement of monomers in the final set of copolymers and any assemblies they form. The observed effects cannot be fully accounted for within conventional polymerization theories but can be readily explained by a phase separation between A-rich and B-rich segments that emerges from and is limited by the copolymerization process itself. In addition, we investigate the interplay between differing non-bonded attractions and activation energies as well as the influence of chain stiffness, selective solvent conditions, and sequence seeding on the resulting co-oligomer sequences and their aggregates.

Osmolyte-induced Conformational Stabilization of a Hydrophobic Polymer

Ms. Pooja Nanavare, Mr. Abhijit Bijay Jena, Dr. Soham Sarkar, Prof. Rajarshi Chakrabarti

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Elucidating the role of osmolytes on conformations of hydrophobic macromolecules is the stepping stone towards understanding the effect of osmolytes on proteins. Therefore, we use all-atom molecular dynamics simulations and umbrella sampling techniques to dissect the mechanism of osmolyte-induced conformational stability of a 32-C hydrocarbon chain. Our conformational analysis reveals that in presence of 4 M choline chloride (ChCl), the polymer has even more compact structure than in water. On the other hand, 8 M urea stabilizes the extended state. Interestingly, polymer adopts an intermediate hairpin-like conformation in a mixed osmolyte solution of 4 M ChCl and 8 M urea due to interplay of interactions between ChCl and urea. We find relative accumulation of water and the hydrophilic part of choline, preferential binding of urea near the collapsed and the extended states of the polymer, respectively. Analyses split out enthalpic and entropic contributions to free energy. This decides the enthalpic or entropic contribution to the stabilization of preferred conformation in the osmolytes solution chosen. Our simulations show in the aqueous solution of ChCl, the hairpin state is stabilized by entropy gain. In contrast, the enthalpic contribution stabilizes the hairpin state in mixed environments. However, collapsed state is energetically not favored in the presence of urea. In brief, via employing an in silico approach, we provide the importance of osmolytes in stabilizing the conformational states of hydrophobic polymer.

Overcoming premature fracture: Reduction of stress concentration effects in additively manufactured lattices using three-dimensional grading of soft material interfaces

Mr. Jacob Peloquin, Mr. Dimitrios Owen, Dr. Ken Gall

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Additive manufacturing (AM) has enabled researchers to print complex geometries that provide combinations of properties previously unachievable. In particular, sheet-based and strut-based lattice structures have been incorporated into applications where high strength, lightweight materials are needed. However, fabrication of these lattices through AM creates inherent surface defects that give rise to stress concentrations, which for rigid plastics often result in premature, unpredictable failure. Recent developments in AM technology such as material jetting (MJ) have enabled multi-material fabrication, with MJ specifically allowing tailorable material distribution down to the voxel scale. In this work, we utilized the capabilities of MJ technology to design multi-material lattice structures with soft-rigid material interfaces functionally graded in three dimensions. Rigid polymer (RP) lattice structures were printed fully encased within a soft polymer (SP) shell, and the interface between the two materials was functionally graded from RP to SP along the surface normal of the RP lattice. The rate of spatial variation and the thickness of the SP shell were varied, and all lattices were subjected to uniaxial tension and compression loading to determine their mechanical performance relative to the control RP-only lattice. Fracture mechanisms were investigated using scanning electron microscopy (SEM) to compare the stress-shielding ability of the different variations in SP shells. Ultimately, a graded interface mitigates the effects of stress concentrations to improve mechanical performance of the lattice by integrating the brittle surface of RP with the soft, energy absorbent SP material. This study provides foundational knowledge of the design considerations, mechanical performance, and fracture mechanisms of multi-material rigid polymer AM lattice structures with soft polymer shells and three-dimensional interfacial grading.

Quasi-active transport of tracer particles in flowing semidilute polymer solutions

Neha Tyagi, Dejuante Walker, Charlie D Young, Charles E Sing

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The flow driven control of particles and molecules in polymer solutions has broad implications in many areas of material science, providing insights into colloidal dynamics in polymer coatings, polymer processing of nanocomposites, charge transport dynamics in flow batteries, and transportation of drug-delivering particles. In most practical situations, these polymer solutions are semidilute, such that the polymer chains are interpenetrating. The emergent length scale of concentration fluctuations, known as the mesh size, is typically sufficiently large to have minimal impact on the penetrant diffusion. However, recent computational(1) and single-molecule research(2) has demonstrated that strong applied flows can lead to significant polymer stretching, which in turn leads to strong local flows caused by hydrodynamic interactions. In this talk, I will use Brownian dynamics simulations to show that these hydrodynamic effects can have a strong effect on the diffusive motion of a tracer particle in semidilute solutions. Upon varying polymer concentration and flow rate, molecular diffusion can be shown to be enhanced by more than an order of magnitude due to the non-equilibrium dynamics of the surrounding polymer matrix(3). We show that these particles exhibit diffusive behaviors analogous to active Brownian motion, due to the flow-driven transport of nearby stretching polymer chains. This has implications for the transport of small molecular weight species in flowing polymer solutions, even at polymer concentrations where diffusion is otherwise unhindered.

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Reproducing Viscoelastic Behaviours of End-linked Polymer Networks using Simulations

Mr. Tim Bernhard

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Molecular simulations of polymer networks allow for otherwise impossible insights into the relationship between the microscopic structure and the macroscopic properties of materials. Current simulation studies are limited to relatively small systems and/or short time scale, making accurate predictions of macroscopic viscoelastic properties difficult. This is especially true for highly fluctuating systems such as damping elastomers or near-critical polymer networks (networks that just passed the solution-gel transition). Understanding the influence of the microscopic structure on the macroscopic properties would be of special interest for such network systems, as they could serve important applications for example in medicine and health technology. Here we assess the current possibilities, limitations and computational requirement needed to reproduce experimental data of storage and loss moduli of such end-linked network systems using classical Kremer-Grest Molecular Dynamics simulations and Dissipative Particle Dynamics simulations with slip-springs.

The Crystallization and Rigid Fraction of PLLA

Logan Williams

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Semicrystalline polymers such as poly(L-lactic acid) (PLLA) are known to consist of 3 phases, the mobile amorphous phase (MAF), the rigid phase (RF), and the crystal phase. Fast scanning calorimetry (Flash DSC) is used as a model polymer to study the crystallization and concomitant RF of a model polymer, PLLA. Contrary to recent studies, the α' and α polymorph of PLLA form with an associated RAF content of ~20%. Kinetic modeling is used to gain insight into the development of both the crystallization and the growth of RF.

The Data-Driven Organic Materials Lab

Martin Seifrid

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Self-Driving Labs (SDLs), which combine machine learning (ML) with automated experiments, offer a transformative approach to research. They empower scientists to shift from a focus on individual experiments to discerning trends within large datasets. ML-guided experiment selection, a hallmark of SDLs, boasts superior sample efficiency, time savings, and resource optimization when contrasted with traditional one-factor-at-a-time, combinatorial, or design of experiment approaches. Moreover, automated experiments conducted by SDLs yield data that is more precise, repeatable, and reproducible. My ultimate vision for SDLs is that, akin to NMR spectroscopy, mass spectrometry, HPLC, peptide synthesis, and PCR, they will evolve from specialist tools into indispensable methods, routinely accelerating scientific advancement.

Toward this end, we are interested in advancing SDL technologies for the design of organic mixed conducting materials with precise structural control. Through an in-depth examination of these materials, we will contribute to enhancing SDL technologies, particularly for thin film organic materials research. Furthermore, incorporating synthesis and film fabrication within the SDL framework enables the concurrent optimization of molecular structure and processing—a long-standing aspiration in organic materials research.

In this poster, I will present efforts in ML-guided automated synthesis, processing and characterization, as well as informatics methods relevant to organic mixed conductors as well as polymer science and engineering more broadly.

The Particle Geometry Effect on Polymer Chain Scaling Behaviors

Dr. Xiangyu Zhang, Kireeti Akkunuri, Dr. Thi Vo

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The emergence of advanced functional materials with heterogeneous monomer structures necessitates accounting for particle anisotropy, which can be represented by various geometries in coarse-grained models. Therefore, an important question arises: How does the scaling behavior change when the "random walker" is a cube, octahedron, or other shapes? A multi-faceted approach, combining theory, molecular dynamics and Monte Carlo simulations, is employed to investigate geometry effects on polymer scaling. Four geometric shapes - patched spheres, tetrahedron, octahedron, and cubes - with two connection methods - face-to-face and vertex-to-vertex - are examined. In each case, three different bond lengths, corresponding to closely-connected, mid-range-connected and distantly-connected systems, are studied. The findings show that in distantly-connected and mid-range-connected systems, the scaling exponent exhibits weak dependence on particle shape, as they resemble ideal random walk and self-avoiding random walk behaviors, respectively. However, significant differences emerge for closely-connected systems due to varying degrees of rotational constraints imposed by different shapes. This is further verified by entropic bonding theory, yielding similar results. Molecular dynamics simulations are applied to investigate scaling behaviors in polymer melts, revealing consistent trends. This study provides fundamental understanding for the complex relationship between particle geometry and polymer scaling behavior.

The subdiffusive motion of sticky dendrimers in an associative polymer network

Ms Silpa Mariya, Prof. Jeremy J. Barr, Prof. P. Sunthar, Prof. Ravi Prakash Jagadeeshan

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Understanding the motion of bacteriophages in the mucosal layer between the external environment and internal tissue is important for infection prevention and therapy. Experiments have demonstrated that the motion of a T4 phage within the mucus layer is subdiffusive, with the subdiffusive behaviour attributed to the adherence of proteins on the phage to the glycans on the mucin network, thereby giving it greater residence time and increasing its efficiency in infecting its bacterial host [1]. The aim of this work is to understand the subdiffusive behaviour of the phages in the mucus layer by modelling phages as “sticky” dendrimers diffusing in a “sticky” associating polymer network with the help of Brownian Dynamics simulations. Essentially, the dendrimers interact with the network of linear polymers through associative interactions. We have shown recently that even non-associating dendrimers exhibit subdiffusive motion in semidilute polymer solutions and their diffusivity can be collapsed onto a master plot when the data is interpreted in terms of appropriately scaled variables [2]. Here, we examine the effect of including stickers at the ends of dendrimer arms that are capable of associating with complimentary stickers on a network of linear polymers. A multi-particle Brownian Dynamics simulation algorithm based on the GPU-accelerated Python package HOOMD-Blue has been employed. Hydrodynamic and excluded volume interactions are taken into account. The effect of polymer concentration, number of stickers and sticker strength on the dynamics of dendrimers has been analysed. The sticky dendrimers exhibit subdiffusion even when their size is smaller than the “mesh size” of the network, while the non-sticky dendrimers remain diffusive. The origin of subdiffusive behaviour is shown to be related to the time scale of sticker binding, the number of stickers and the radius of gyration of the dendrimer. The diffusion coefficient decreases for both the sticky and non-sticky dendrimers with increasing concentration. This trend is analogous to the observed behaviour of the adherent and non-adherent phages in varying mucin concentrations [1].

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Understanding Polymer Biodegradation Under Different Environmental Conditions

Anicah Smith O'Brien, Dr. Morton A. Barlaz, Dr. Saad A. Khan

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The environmental devastation caused by single-use plastics necessitates the advancement of sustainable materials. Thus, materials that meet both in-use requirements and provide a viable alternative for sustainable disposal must be developed. Biodegradable plastics are a promising solution, as they can undergo biological recycling, where valuable products such as compost and biogas are produced upon disposal. (Poly)-lactic acid, or PLA, a polyester derived from renewable biomass, is a promising biodegradable polymer with potential to be widely implemented into consumer products. PLA is certified as compostable at thermophilic temperatures, but current research is predominantly focused on unmodified PLA. However, before integration into consumables, PLA requires modification to overcome its hydrophobicity and brittleness. Yet, the impact of common modifications including surface coatings, additives, and blending on PLA biodegradation remains elusive. In this study, we aim to unravel the impact of surfactant coatings on PLA biodegradation in relation to temperature, oxygen presence, and structure. PLA films and fibers were fabricated and coated with sorbitan monolaurate or polysorbate 20, chosen for their typical use as wetting agents in consumer products. Characterization of the materials included contact-angle measurements to assess the coating's impact on wettability and Quartz-Crystal Microbalance to examine adsorption kinetics. Both aerobic and anaerobic biodegradability were studied as a function of temperature, as the material could be treated by composting (aerobic) or disposed of in a landfill or anaerobic digester (anaerobic) at the end-of-life. Carbon dioxide and methane generation were used to quantify aerobic and anaerobic biodegradation, respectively. Additional indicators of biodegradation were also measured throughout the duration of the experiments, including molecular weight, crystallinity, and biofilm thickness. The insights gained from this work will aid in the development of sustainable materials with functional moieties for various applications including disposable medical devices, single-use packaging, and hygiene products.

Self-Assembly

Biophysical characterization of hard/soft nanoparticles for surface activity of pulmonary surfactants in the treatment of infant respiratory distress syndrome

Dr. Pinchu Xavier

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Pulmonary surfactant (PS) is a lipid-protein film lining the whole alveolar surface of the lungs which plays a key role in lowering the surface tension almost to 0 mN/m, avoiding alveolar collapse and reducing work during the respiration cycles [1]. PS is composed of roughly 80-90% (by mass) phospholipids, 8-10% neutral lipids such as cholesterol, and 5-10% surfactant proteins with specialised functional roles. Dipalmitoyl phosphatidylcholine (DPPC) (40%) forms a closely packed monolayer at the air-water interface and is principally responsible for lowering surface tension [2]. Furthermore, additional unsaturated phosphatidylcholines (POPC, 25%), anionic phosphatidylglycerol (POPG, 8-10%), and cholesterol (8-10%) keep the film fluid, which is important for surfactant dynamics. Surfactant proteins (SP-A, SP-B, SP-C and SP-D) is responsible for the formation of surface associated reservoir formation during expiration (at lower surface tension) and for the efficient respreading during inhalation [3]. Though the structure, mechanism and morphology of PS film are not well understood, its dysfunction is known to cause severe respiratory distress syndrome (RDS) [4]. The quaternary PS model DPPC:POPC:POPG:cholesterol (6:2:1:1 by mol) and their interactions with hard/soft nanoparticles (NP) is studied using a Langmuir trough containing a 150-mM NaCl subphase to mimicking the physiological environment, along with reflectivity techniques such as Brewster angle microscopy, ellipsometry and neutron reflectometry. Our results indicate the role of cholesterol and surfactant proteins associated with the formation of extended structures in the highly compressed films (~0 mN/m). We found that the presence of cholesterol affects the lower surface tension values of PS film, as it will not squeeze out rapidly. Cationic silica NPs (20 nm) interacts with negatively charged POPG which leads to aggregate formation inhibiting to reach a higher surface pressure whereas anionic NPs forming complex with lipids (DPPC) increase the compressibility of film. For the case of PS with core-shell nano gels of NIPAM-poly(N-isopropylacrylamide), at larger area of the trough, predominant behaviour of nanogels and a near zero surface tension observed at lower concentration of NIPAM. Our findings highlighting the physiological function of various constituents of the PS film and their interactions with NPs may contribute to relevant pharmaceutical developments for RDS.

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Colloidal deposits with unique reflection symmetry to fractal patterns: effect of confinement

Mr. Sanjib Majumder, Dr. Madivala Basavaraja, Dr. Dillip Satapathy

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Drying of a particle-laden drop on a substrate leaves behind a particulate deposit whose morphology depends on a multitude of factors, including inter-particle interaction, substrate wettability, particle-solvent interaction, substrate temperature, etc. During the evaporation of a drop, capillary force, Marangoni force, and drop dynamics affect the final deposit pattern. Generally, when the particle-laden drop dries in sessile or pendant mode, the gradient in evaporative flux along the interface is parallel to the substrate which helps the drop to remain pinned assisted by the Capillary force. Upon confining the dispersion drop between two substrates not only changes the drop shape but also the gradient in evaporative flux along the interface becomes perpendicular to substrate which usually results in discrete deposit patterns due to stick-slip motion of the drop.

In this investigation, we will elucidate how it is possible to generate intriguing continuous deposit patterns from drying microgel-laden aqueous droplets by confining the droplet between two plates. A comprehensive analysis of how the morphology of the deposit obtained by drying microgel-laden aqueous droplets can be modulated by meticulously adjusting the spacing between the plates and particle concentration will be presented in detail.

Deep Inverse Design of Patchy Polygons for Mesoscale Assembly of 2D Superlattices

Mr. Po-An Lin, Dr. Simiao Ren, Jonathan Piland, Dr. Leslie Collins, Dr. Yonggang Ke, Dr. Stefan Zauscher, Dr. Gaurav Arya

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

A major objective of materials discovery is engineering precise and complex molecular building blocks whose self-assembly leads to equally complex hierarchical architecture. Supramolecular assembly of DNA origami building blocks provides a highly promising approach due to their ability to be designed into arbitrary nanoscale shape with precise chemical functionalization. Inspired by the self-assembly of patchy colloidal particles, researchers have recently begun to introduce patches of mutually attractive chemical moieties at designated sites on DNA origami to assemble them into higher-order architectures. Here, we use a coarse-grained patchy particle model of DNA origami polygons grafted with sticky brushes to explore the range of 2D assembly patterns achievable using these building blocks. We find that these building blocks can self-assemble into a range of highly intriguing superlattices, including Kagome and checkerboard lattices. However, designing such functionalized DNA origamis to target specific assembly structures is highly challenging because the underlying relationship between the building block design and the resulting assembly structure is very complex; the factorial scaling of design space with user-controlled parameters like the shape of building block, protrusion ratio, and patch size renders brute-force search impractical. Deep learning has emerged as a powerful tool for addressing such inverse-design tasks. We employ a neural adjoint method, a neural network model specialized in inverse-design tasks, to discover building block designs that produce periodic tiling patterns as they assemble. The neural adjoint model, trained on design parameters and a scale-invariant and symmetry-informed representation of the assembly structure, successfully identified building block designs that closely resemble the desired target structure across multiple length scales. We then derived general design rules for patchy polygons from the model's output to create complex tiling patterns. We envision that our approach can be generalized to more complex designs and used to tailor structural and topological properties to expand the application space of 2D materials.

Designing athermal disordered solids with automatic differentiation

Dr. Mengjie Zu, Dr Carl Goodrich

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Inverse design, which aims to form desired organised structures and function materials, is increasingly important in nanotechnology and material science. However, the principles of inverse self-assembly of multiple-component systems, particularly disordered solids, are unveiled. Discovering the role of interactions between constituent particles in their emergent mechanics is essential to understand the self-assembly process, as well as to manipulate it to obtain functional materials. We propose a novel numerical approach, which directly connects interactions with their effect on emergent elastic properties, to study the self-assembly of disordered solids. In this project, we build and optimize objective functions regarding to desired properties with elementary parameters such as particle sizes and interacting parameters. By central on Poisson's ratio, we show how the validations of optimized parameters for ensemble and individual systems. We further show that, with multiple desired properties, including structural and mechanical properties, our approach efficiently searches the optimized parameters for certain properties. This approach is highly robust, transferable, and scalable. It provides a new perspective to discover the relationship between composed building blocks and their emergent behaviours.

Direct observation of non-classical crystallization pathways in binary colloidal systems

Shihao Zang, Sanjib Paul, Cheuk Wai Leung, Theodore Hueckel, Glen Hocky, Stefano Sacanna

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Crystallization is a key self-assembly process where basic units form ordered structures. Traditional views describe this as a step-by-step addition of units, but recent findings reveal more complex pathways. In our study, we use index-matched fluorescently-labeled fluorinated colloids[1] or density-matched polystyrene colloids with opposite charges in water to show the formation of ionic crystals via polymer-attenuated Coulombic self-assembly (PACS)[2], controllable by particle size and salt levels. With confocal microscopy, we directly observe these particles forming crystals, tracking defect motion and crystal behavior over time. Our results uncover a two-step nucleation process: first, amorphous clusters form and then transform into crystal nuclei. These nuclei grow through direct addition of monomers, incorporation of clusters, and merging with other crystals. Experiments and simulations reveal varied crystal forms, including CsCl-like with rhombic dodecahedral shapes and Thorium Phosphide-like structures with Triakis tetrahedral shapes. In addition, we have identified a novel crystal structure with L_3S_4 stoichiometry, which exhibited rod-like crystal habit. This work opens new avenues in understanding crystal formation, with implications for designing materials with specific properties.

[1] Zang, S., Hauser, A.M., Paul, S., Hocky, G.M., Sacanna, S. Crystal clear: enabling 3D real space analysis of ionic colloidal crystallization. Nature Materials. Accepted
[2] Hueckel, T., Hocky, G.M., Palacci, J., Sacanna, S. Ionic solids from common colloids. Nature 580, 487–490 (2020).

DNA assemblies with emergent functions

Dr. Gaurav Arya, Dr. Marcello DeLuca, Dr. Sebastian Sensale

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

DNA nanotechnology is a promising approach for creating soft robotic nanomaterials due to its ability to create nanostructures of unprecedented geometric complexity and high programmability. While recent advances have led to dynamic DNA devices capable of undergoing complex motions, the size and functionality of these structures remains limited [1]. In this talk, I will describe our recent efforts in designing and modeling complex multicomponent DNA nanomaterials with tailored or emergent dynamic behaviors characteristic of smart robotic systems. I will begin by discussing a software we developed that uses feedback from coarse-grained molecular dynamics simulations to automate the design of freeform 3D DNA nanostructures and their assemblies [2]. I will then show how we used this framework along with mesoscopic models, simulations, and statistical mechanics to create 1D arrays of sterically interacting DNA origami structures that can communicate mechanical signals along the array [3,4] and 2D arrays of interacting DNA rotors that can undergo intriguing order-disorder transitions akin to, and beyond, the Ising lattice [5]. Such systems capable of exhibiting complex dynamic, organizational behavior could be harnessed for applications in sensing, soft robotics, optics, and energy harvesting.

[1] DeLuca, M., Shi, Z., Castro, C.E. and Arya, G., 2020. Dynamic DNA nanotechnology: toward functional
nanoscale devices. Nanoscale Horizons, 5:182-201.

[2] Pfeifer, W., Huang, C.M., Poirier, M.G., Arya, G. and Castro, C., 2023. Versatile Computer Aided Design of Freeform DNA Nanostructures and Assemblies. Science Advances 9, eadi0697.

[3] Wang, Y., Sensale, S., Pedrozo, M., Huang, C.-M., Poirier, M.G., Arya, G., and Castro, C.E., 2023. Steric Communication between Dynamic Components on DNA Nanodevices. ACS Nano 17:8271-8280.

[4] Sensale, S., Sharma, P. and Arya, G., 2022. Binding kinetics of harmonically confined random walkers. Physical Review E, 105:044136.

[5] DeLuca, M., Pfeifer, W.G., Randoing, B., Huang, C.-M., Poirier, M.G., Castro, C.E. and Arya, G., 2023. Thermally reversible pattern formation in arrays of molecular rotors. Nanoscale, 15:8356-8365.

Efficient Monte Carlo Framework for Simulating Self-Assembly of Faceted

Nanoparticles

Mr. Safak Callioglu, Mr. Quanpeng Yang, Mr. Yuanchuan Shao, Mr. Joseph Laforet Jr., Mr. Brian H. Lee, Prof. Gaurav Arya

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Faceted nanoparticles exhibit useful catalytic and plasmonic properties, due to their sharp edges and flat surfaces. We recently introduced a novel rod-surface discretization approach to derive accurate analytical potentials for describing the orientation-dependent van der Waals interactions between faceted nanoparticles [1]. Here, we present an efficient Monte Carlo simulation framework that utilizes these analytical potentials to simulate the self-assembly behavior of faceted nanoparticles such as nanocubes. We implement efficient virtual cluster moves [2] in this framework to avoid unphysical energy traps during assembly and capture their correct size-dependent diffusive behavior. The results show that our approach can simulate the self-assembly of nanocubes many orders of magnitude faster than atomistic models and predict assembly morphologies very similar to atomistic models. On the other hand, coarse-grained models of nanocubes are unable to capture the expected self-assembly behavior and morphology.

[1] Lee, B. H.; Arya, G. Analytical van der Waals interaction potential for faceted nanoparticles. Nanoscale Horiz. 2020, 5, 1628–1642.
[2] Whitelam, S.; Geissler, P. L. Avoiding unphysical kinetic traps in Monte Carlo simulations of strongly attractive particles. J. Chem. Phys. 2007, 127, 154101.

Enabling Asymmetrical Assembly of Supramolecular Peptide Nanofibers

Ms. Helena Freire Haddad, Ms. Kat Lazar, Mr. Vinicius Xie Fu, Ms. Lauren Kenselaar, Dr. Joel Collier

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Self-assembling fibrillar peptide materials have gained traction in biological applications such as scaffolds for tissue repair, immunotherapies, and depots for drug delivery. Their high aspect ratio and large surface area allows for a highly multivalent display of antigens, proteins, or small molecules, while the modular nature of these platforms enables co-assembly of different components at precise ratios. However, peptide assemblies are dynamic and polydisperse in nature, making it challenging to precisely control their organization. We have previously described a capping system to control the lengthwise assembly of alpha helical peptide nanofibers useful in immunoengineering applications, in order to control nanofiber size and transport through lymphatic tissues and cells. This previous work was based on the Coil29 peptide, in which alpha helices stack into ladder-like structures via coiled coil folding. In the work described here, we sought to construct nanofibers with asymmetric poles. Such structures could incorporate multiple large antigens in discrete regions of the nanofiber or exhibit directional motility through biologic media.
We investigated two different strategies for the formation of asymmetric nanofibers. The first strategy utilized a “passive” capping system previously developed. Briefly, one of two capping peptides containing one hydrophobic face of the coiled coil was co-assembled with the Coil29 backbone peptide, resulting in nanofibers with one terminus capped to further elongation. These

were then combined to form polarized, bifunctional nanofibers. Fluorescently labeled peptides were utilized to investigate the spatial distribution of the various nanofiber components, and we found that this method could produce nanofiber batches with 5-30% demonstrating bifunctionality. To further enhance the assembly of bifunctional nanofibers, we developed a "click cap" system by modifying each alanine residue in the central RAYAR sequence, which is responsible for the vertical stacking of peptides with either an azide-containing amino acid (RXYAR) or a cysteine for conjugation with maleimide-PEG4-DBCO (RAYCR). These click-chemistry moieties stop assembly with the normal Coil29 backbone on one end of the nanofiber via steric hindrance, and preferentially bind together via a click chemistry azide-DBCO reaction. Nanofiber size and morphology were confirmed via atomic force microscopy imaging. Circular dichroism measurements were performed to confirm the alpha helical structure of the nanofibers was preserved after coassembly with click caps. Confocal imaging analysis showed an increase in bifunctional nanofiber frequency was observed compared to half-capped fibers combined at either room temperature or annealed, with up to 50% of particles being polarized. Together, this work highlights a thermodynamic and a chemical approach to assemble fibrillar, peptide based materials asymmetrically for biological applications.

Enzyme-triggered peptide fibrillation in a synthetic droplet

Dr. Naresh Dhanasekar, Mr Quincy Snyder, Mr Stephen Klawa, Miss Margaret Daly, Prof. Ronit Freeman

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The underlying process in creation of a complete and functional synthetic cell remains one of the greatest challenges of the current century. In doing so, one of the key components involved in decorating a synthetic cell is the functional cytoskeletal filamental networks, which are inherently designed to perform various motor and cellular functions. Although, natural cytoskeletal architects have been encapsulated in a synthetic droplet, polymerization, and assembly of such constructs under in vitro conditions prove extremely challenging. Hence, the construction of synthetic components is vital, and building artificial systems using such components could create a milestone in understanding the living system under in vitro conditions. Here we used the advantage of supramolecular chemistry for the fruitful self-assembly of a short peptide via the enzymatic morphological conversion of a phosphorylated peptide (Fmoc-FF-pS) in a synthetic droplet. Interestingly, we observed significant changes in the self-assembly process of the phosphorylated peptide between the bulk medium and the reaction carried out in the aqueous droplet, which we hypothesize due to the interface effect. Furthermore, varied enzyme doses were used to test the degree of polymerization in the aqueous droplet as opposed to the aqueous medium. Finally, we used molecular crowding agents to stimulate the growth of peptide bundles from filaments. This study provides molecular insights of peptide fibrillar production in a synthetic droplet, which significantly contributes for effective biomimetics of cytoskeletal like structures.

Exploring Geometric Frustration in Self Assembly of Mechanical Metamaterial Using a Generalized Elasticity Theory

Mr. Sourav Roy, Dr. Michael Wang, Dr. Gregory Grason, Dr. Christian Santangelo

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Mechanical metamaterials have been studied extensively to explore their unusual properties owing to instabilities arising from their micro-structures. Our simple continuum framework for the mechanics of a metamaterial thin sheet shows that in the Föppl–von Kármán limit, the elasticity of the sheet screens the curvature induced stress through soft deformation modes. We use this approach to explore the characteristic shapes of a geometrically-frustrated metamaterial with an incompatibility between in-plane and and out-of-plane strain. We uncover new dimensionless numbers which, in concert with the Foppl-von Karman number dictate how the soft modes affect this competition and give rise to anomalous equilibrium shapes.

Failure in the working curve: Determining interlayer adhesion in stereolithography printing via photorheology

Ms. Zoe Benton, Dr. Daniel Rau, Mrs. Myoeum Kim, Dr. Liheng Cai

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The working curve that guides stereolithography (SLA) Additive Manufacturing (AM) determines the optimal parameters for successful printing by relating UV Exposure to Cure Depth. However, this curve often predicts an exposure time appreciably lower than what is required for successful bottom-up SLA AM. This discrepancy is, in part, because for successful printing, the cured layer's adhesion to the build window must be less than that layer's adhesion to the previously cured layer, factors not considered by the traditional working curve. We introduce a new technique that mimics the SLA printing process and measures the adhesion forces during a simulated recoating process. We find that accounting for the adhesion forces versus exposure time creates a more robust working curve for predicting optimal printing parameters with a higher degree of success. Our results provide a better understanding of processing physics and thus facilitate the advancement of SLA printing.

Geometric frustration meets mechanical metamaterials

Dr. Michael Wang, Sourav Roy, Christian Santangelo, Gregory Grason

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Geometric frustration occurs when the local preferred ordering of a system cannot be realized on a global scale. There has been recent interest in engineering frustration into the assembly of soft materials through the intentional design of misfitting building blocks as a way of controlling the sizes and morphologies of assemblies. As a frustrated assembly grows, the accumulation of stresses from misfits competes with the attractions between building blocks leading to so-called self-limiting assembly. Understanding and controlling the stress accumulation is key to assembling structures with well-controlled sizes much larger than that of a single building block. Mechanical metamaterials, due to their unique structural transformations, have a remarkable property of absorbing stresses through soft modes. We here merge these two concepts to study how the stress-absorbing properties of dilational mechanical metamaterials can be harnessed to control the self-limiting sizes of frustrated assemblies. By introducing a simple building block model to combine both frustration and dilations, we show that the incorporation of a soft dilational mode into frustrated structures (e.g. via a square-twist or Kagome mechanism) can significantly enhance their self-limiting sizes. In addition, we briefly discuss how frustration can stiffen an otherwise soft or floppy dilational metamaterial.

Geometrically frustrated self-assembly of hyperbolic crystals from icosahedral nanoparticles

Mr. Nan Cheng, Dr. Kai Sun, Dr. Xiaoming Mao

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Geometric frustration is a fundamental concept in various areas of physics, and its role in self-assembly processes has recently been recognized as a source of intricate self-limited structures. Here we present an analytic theory of the geometrically frustrated self-assembly of regular icosahedral nanoparticle based on the non-Euclidean crystal $\{3,5,3\}$ formed by icosahedra in hyperbolic space. By considering the minimization of elastic and repulsion energies, we characterize prestressed morphologies in this self-assembly system. Notably, the morphology exhibits a transition that is controlled by the size of the assembled cluster, leading to the spontaneous breaking of rotational symmetry.

Harnessing Liquid Crystal Disclinations for Next-Generation Architected Materials

Mr. Jeremy Money, Dr. Jose Adrian Martinez-Gonzalez, Dr. Andrew Gross, Dr. Monirosadat Sadati

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Architected cellular materials encompass a broad range of material systems, from open celled foams to sheet based lattices. Comprised of unit cells of varying geometries and tessellation patterns, these materials give rise to unique properties attributed primarily to the geometric arrangement of their constituent elements. Enabled by additive manufacturing technologies, architected cellular materials are increasingly making their way into commercial design and production, offering solutions to many challenges faced by industries such as biomedicine and personal protective equipment. However, additional barriers to ubiquity such as resolution limits (Unit cell size < 500 nm), and the mutually exclusive stiffness/toughness tradeoff of lattice-based architectures, present opportunities for the development of novel unit cell geometries with extremal properties and alternate fabrication routes. Current areas of design inspiration are drawn from the intricate patterns displayed by nature or solid atomistic crystals. However, the opportunity for novel approaches to unit cell design presents a frontier ripe for exploration.

One such approach exists in the study of the behavior of thermotropic liquid crystals and their interpenetrating networks of defects, or disclination lines. These systems possess the long range orientational ordering of solid crystals while retaining fluid-like properties of liquids. When exposed to temperature fields and varying degrees of confinement, these material systems exhibit self-assembly of their mesogens into interesting mesostructures under relatively mild conditions.

These subunits then subsequently pack together into cubic arrangements with periodicity on the order of hundreds of nanometers. This behavior has been extensively investigated for its optical response; however, little is understood about the mechanical properties of the resultant disclination architectures. This work utilizes a combinatorial approach to generate a catalogue of disclination textures formed under varying conditions to explore their various elasto-mechanical properties for materials design across multiple length scales. First, Landau-De Gennes guided simulations are utilized to predict thermodynamically stable architectures formed by disclination lines in confined liquid crystal systems. The resultant disclination lattices are then scaled to macroscopic (millimeter) dimensions, fabricated via Stereolithography additive manufacturing techniques, and evaluated under uniaxial compression. Of the unique geometries which arise from these liquid crystal systems, the bicontinuous, interpenetrating double diamond lattice that forms from the bulk behavior shows promise for structural applications. Study of the mechanical response of these geometries indicate potential toughening mechanisms induced by contact between the two interpenetrating lattices, consistent with results from adjacent studies. In addition to its variable strut diameter and reinforced nodal regions, the simulated lattice void fraction, or relative density, can be adjusted rapidly using a threshold value for the mean orientational order of the mesogens adjacent to disclination cores. These features, unique to liquid crystal systems, offer an additional set of adjustable parameters which can add to the architected materials design space.

Illuminating the mechanism of DNA origami folding with a new mesoscopic model

Mr. Daniel Duke, Marcello Deluca^{Duke}, Tao Ye, Michael Poirier, Yonggang Ke, Carlos Castro, **Dr. Gaurav Arya**

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Scaffolded DNA origami exploits the highly specific canonical base pairing rules of DNA to fabricate intricate and dynamic nanostructures. In this method, single-stranded oligonucleotides (staples) are designed to collectively hybridize with a single long strand (scaffold), causing it to fold into the target shape. Despite the centrality of folding to DNA origami, the details of this process are unclear because current models cannot access the long timescales necessary to simulate the folding of full-sized origamis in standard conditions. Here, we present a new mesoscopic model that captures the entire folding process, from freely floating strands to the eventual product. To accomplish this, the model coarse grains DNA at levels up to 8 base pairs per bead, integrates motion with Brownian dynamics, and uses switchable force fields to depict the change in mechanical properties of DNA after hybridization and dehybridization. Simulations of a 4-helix-bundle (4HB) with a straight scaffold routing show hierarchical folding with first-order kinetics in two regimes. The folding starts with fast initial constraint of the scaffold associated with a transitional zipping action, leading to gradual incorporation of the remaining staples. Conversely, simulations of a 32-helix bundle (32HB) reveal heterogeneous staple incorporation, frequent trapping in metastable states, and lower yield compared to the more accessible 4HB structure. In addition to these analyses, we investigate the role of hybridization strength, scaffold routing, and staple design on the folding process. This model opens an avenue for predicting and understanding how origami design impacts the speed and quality of the folding.

[1] DeLuca, M. et al. Mechanism of DNA origami folding elucidated by mesoscopic simulations. Nat Commun 15, 3015 (2024).

Inducing hydrophobicity in biobased foams by the addition of lignin

Dr. Tero Mäkinen, Kourosh Mobredi, Juha Lejon, Xiang Hu, Isaac Miranda Valdez, Mohamed Elamir, Dr. Leevi Viitanen, Luisa Jannuzzi, Dr. Juha Koivisto, Prof. Mikko Alava

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Replacing plastics with biobased materials is of utmost importance, especially in packaging solutions and hydrophobic coatings. In our research group, we have previously demonstrated how to use forest-industry sidestreams (namely methylcellulose and cellulose fibers) to produce fully biobased foam materials suitable for packaging solutions [1], by mimicking the structure of wood.

The main problem in the widespread utilization of these biobased foams as plastic substitutes is their lack of water resistance. Continuing on this road of biomimicry, we again looked into the structure of wood and saw promise in the the addition of lignin to the foam manufacturing process [2], mimicking the function lignin has in the structure of wood. Although not completely hydrophobic---the lignin molecules comprise a combination of hydrophobic and hydrophilic end-groups---lignin essentially acts as a water-resistant barrier. We achieve great improvements in the hydrophobicity of these methylcellulose foams both by incorporating lignin into the manufacture of bulk foams [3] or using a lignin-methylcellulose combination as a hydrophobic coating [4].

The key physics influencing the hydrophobicity of the foams relates to the interface phenomena in the bubble films. By varying the type of lignin used in the manufacturing process, and characterizing the created surfaces using microscopy methods, we see that the best performance is achieved when the lignin particles self-assemble uniformly on the bubble film surface. When the lignin concentration is increased above a certain level, the lignin particles start to cluster and the surface coating starts to detach from the substrate. There is thus an optimal lignin concentration for hydrophobicity.

In this work we have shown that by adding lignin to the manufacture process of cellulose foams we can achieve lightweight, biodegradable, and hydrophobic foams, which can be produced in a scalable manner and used as future plastic substitutes. We have also made functional, full-scale prototypes of the products envisioned to be made from the foam material with water resistance, most notably a coffee cup, made using fully bio-based---even edible---constituents.

[1] Reichler et. al "Scalable method for bio-based solid foams that mimic wood", Scientific Reports 2021.
[2] Miranda-Valdez et. al "Foam-formed biocomposites based on cellulose products and lignin", Cellulose 2023.
[3] Miranda-Valdez et. al "Bio-based foams to function as future plastic substitutes by biomimicry: inducing hydrophobicity with lignin", Advanced Engineering Materials (in review).

[4] Mobredi et. al "On hydrophobicity of biobased coatings based on organosolv lignin", Soft Matter (in review).

Magnetoelastic microscopic multistate machines

Dr. Melody Lim, Dr. Zexi Liang, Prof. Paul McEuen, Prof. Itai Cohen

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The creation of microscopic machines that extract energy from their environment to perform multiple targeted functions is an outstanding challenge in soft matter. Current strategies for achieving multiple functionalities in a single device require reprogramming of interactions between the device subunits. Here, we demonstrate a design and experimental platform for a microscopic structure which achieves multifunctionality without reprogramming. Our structures consist of rigid particles connected by an elastic backbone. Each panel is patterned with single-domain nano-magnetic patches, enabling precise control over the magnetic dipole moment, orientation, and spatial distribution of the magnetization of each panel. Applying an external magnetic field to these devices actuates designed patterns of folding. Additionally, when panels are sufficiently close, the magnetic interaction between their magnetic patches causes them to attach and move as a rigid body. We leverage this hierarchical folding to create reconfigurable, multistate, magneto-elastic microscopic machines.

Materials characterization of a self-assembling elastin-like polypeptide fusion protein as a platform for immunotherapies

Ms. Kat Lazar, Dr. Yulia Shmidov, Rachel L. Strader, Shamitha Shetty, Dr. Joel H. Collier, Dr. Ashutosh Chilkoti

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Self-assembling polypeptides a class of materials that undergo spontaneous organization into nano- or microstructures whose morphology is dictated by precise interactions such as hydrogen bonds, ionic and electrostatic interactions, π-stacking, and hydrophobic effects. Some of these self-assembling materials are also stimuli-responsive and undergo morphological changes based on external cues such as temperature, pH, or enzymatic activity. These stimuli-responsive self-assembling materials have grown increasingly popular in the realm of immune engineering as they can improve vaccine delivery and immunogenicity by increasing plasma residence time, improving uptake by antigen-presenting cells, or targeting specific locations within lymphoid tissues.

We have identified a novel self-assembling fusion protein, termed K2(E36)115, which forms a diverse array of nano and microstructures in a concentration and temperature dependent manner. The protein is comprised of a short, zwitterionic peptide (K2) derived from an immunomodulatory class of drugs called Glatiramoids, as well as (E36)115, a long and hydrophobic elastin-like polypeptide (ELP). ELPs are a family of repetitive proteins that undergo lower critical solution temperature (LCST) phase behavior, wherein they transition from a soluble to coacervate state upon heating above a characteristic transition temperature (Tt). This thermosensitive assembly makes them attractive for a wide variety of applications in drug delivery, including injectable depots for the controlled release of protein or peptide therapeutics and nanomaterial-mediated delivery of covalently conjugated cargo. Using UV-Vis spectrophotometry, we observed that K2(E36)115 exhibits two sharp increases (a primary and secondary Tt) in absorbance upon heating, suggesting molecular self-assembly is occurring before polypeptide coacervation. Using Cryo-TEM, we determined that the fusion protein forms distinct nano- and micro- structures before, after, and in between both transition temperatures. These structures include bilayer sheets at low temperatures, polymeric vesicles at intermediate temperatures, and heterogeneous rod and coil coacervates at high temperatures.

Given this discovery, we sought to determine which features of the zwitterionic peptide K2 contributed to this self-assembly and to identify lead formulations for further application as immunotherapies. We used dynamic light scattering, UV-Vis spectrophotometry, and cryo-electron microscopy to characterize the temperature and concentration dependence of nanoparticle self-assembly. To investigate the contributions of specific amino acids to ionic and π-stacking interactions, we designed a library of fusion proteins with single amino acid alterations in the parent peptide K2 and evaluated them for disruption in nanoparticle formation. In our ongoing work, we aim to characterize a second library of fusion proteins with varied length and hydrophobicity in the ELP domain to investigate how the features of the hydrophobic block influence morphology. Together, this information provides insight into the molecular characteristics governing the self-assembly of (K2)E36115 and guides further investigation into the development of a tunable, stimuli-responsive platform for immunotherapies.

Multifunctional MXene-PAA microgel hybrids for high-performance conductive 3D printing inks and aerogels

Dr. Farivash Gholamirad, Dr. Monirosadat Sadati, **Dr. Nader Taheri-Qazvini**

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

This work presents a novel approach for designing a multifunctional MXene-based ink with record-low solid content for 3D printing applications. By leveraging the unique properties of Ti3C2Tx MXene nanosheets and polyacrylic acid-based microgels, we engineer a hybrid ink that exhibits a combination of high elasticity, high electrical conductivity, and low solid content. The ink formulation process involves a thermodynamically guided assembly approach, where MXene nanosheets are spatially confined within the jammed microgel network. This confinement prevents uncontrolled aggregation of MXene while simultaneously imparting favorable rheological properties for extrusion-based 3D printing.

The resulting MXene-microgel hybrid ink demonstrates remarkable printability, enabling the fabrication of high-fidelity 3D structures with excellent shape retention. Printed structures can be transformed into free-standing hydrogels and subsequently freeze-dried to yield highly porous, electrically conductive aerogels. This enhanced performance stems from the percolated conductive network formed by aligned MXene nanosheets, even at low concentrations. The aerogels exhibit an excellent electrical conductivity of 360 S/m and electromagnetic interference shielding (EMI) effectiveness of 57 dB.

The engineered MXene-microgel system exhibits excellent mechanical properties, with the aerogels demonstrating resilience to over 5000 times their own weight without structural collapse.

This approach opens up new avenues for the development of 3D printable, multifunctional soft materials with potential applications spanning EMI shielding, energy storage, and wearable electronics.

Optimal face-to-face coupling for fast self-folding kirigami

Mr. Maks Pecnik Bambic, Prof. Nuno Araujo, Dr. Benjamin Walker, Prof. Duncan Hewitt, Dr. Pei Qing Xiang, Prof. Ran Ni, Prof. Giorgio Volpe

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Kirigami is a design method through which two-dimensional templates are transformed into complex three-dimensional structures by a series of cuts and folds. In practice, templates consist of flat and rigid panels connected through flexible hinges. Kirigami designs are easily scalable, providing a straightforward route to intricate structures at small scales. Unfortunately, at the meso-scale, folding around hinges is difficult to control directly. A possibility is to rely on indirect forces to drive actuation, such as collision with solvent molecules when suspending the template in a fluid. However, the lack of control over the folding process results in low yields and rates of folding, a problem made worse when target structures consist of several hierarchical levels. Here, I will discuss how Brownian motion is used to simulate the temperature driven folding of two-leveled kirigami structures consisting of coupled panels tethered on one side to a substate. The motion of panel pairs is coupled due to constraints of force and torque in an inertia-less system, which we parameterize using a hydrodynamic drag law. This coupling is tuned through simple modification of the panels and can significantly enhance the rate and yield of folding of our structures. The coupling resulting in the highest yield and rate can be predicted solely by the folding of the upper level, whose initial state depends on the folding time of the lower level. Exploiting hydrodynamic coupling in this way can improve the design of hierarchical multi-leveled meso-scale structures for many applications from soft robotics to drug encapsulation.

1. Pecnik Bambic, M., Araújo, N. A. M., Walker, B. J., Hewitt, D. R., Pei, Q. X., Ni, R., & Volpe, G. (2024). Optimal face-to-face coupling for fast self-folding kirigami. Soft Matter, 2(5), 1114–1119. https://doi.org/10.1039/d3sm01474f

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Overcoming Kinetic Traps in Self-Assembly using Magnetic Decoupling

Dr. Zexi Liang, Dr. Melody Lim, Dr. Chrisy (Xiyu) Du, Dr. Conrad Smart, Dr. Tanner Pearson, Qianze Zhu, Dr. Michael Brenner, Dr. Paul McEuen, Dr. Itai Cohen

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Recent advances in self-assembly offer the potential for creating complex, functional materials. Yet, a persistent challenge lies in the formation of off-target structures, hindering the yield of the desired product. Here, we introduce a novel strategy to escape these kinetic traps by decoupling the target structure from the driving force. Using lithographically patterned magnetic microparticles driven by rotating magnetic fields, we demonstrate how magnetic decoupling selectively stabilizes the target structure while destabilizing incomplete by-products. By tailoring the magnetic field amplitude and frequency, we achieve selective disassembly of the by-products, effectively recycling their components. Our approach employs tailored magnetic driving patterns that fully convert these by-products into the desired target structure, significantly enhancing assembly yields.

Peptide Nanomaterial Active Immunotherapy to counteract IL-22 Binding Protein for Intestinal Regeneration in Inflammatory Bowel Disease

Deleah Pettie, Dr. Joel Collier

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Current treatments for Inflammatory Bowel Disease (IBD) consist of anti-inflammatory drugs, immunosuppressants, and biologics against inflammatory cytokines. These treatments lead to increased risk of infection due to immune suppression, focus only on treating inflammation, and do not promote adequate intestinal epithelial regeneration. As an alternative, active immunotherapies are receiving increased interest and aim at reducing inflammation and promoting intestinal healing within broad populations. An active immunotherapy made from engineered immunogens can generate antibodies that help anti-inflammatory responses and promote intestinal regeneration. Supramolecular assemblies of proteins and peptides combined with B- and T-cell epitopes can form nanomaterials that raise therapeutic antibody responses. Coil29 is an alpha helical peptide platform that oligomerizes into supramolecular nanofiber immunogens. This work describes the design of an immunotherapy using Coil29 against Interleukin-22 binding protein (IL-22BP), a critical mediator in inflammatory bowel disease (IBD). IL-22BP is a regulator of IL-22 which promotes cellular proliferation and inhibition of apoptosis. The central hypothesis is that antibody responses against IL-22BP can promote IL-22-mediated regeneration of the intestinal epithelial layer in a chronic colitis mouse model. Kolaskar Tongaonkar antigenicity testing and Bepipred 2.0 were used to predict B-cell epitopes within mouse IL-22 binding protein, and these 9 epitopes were synthesized in tandem with Coil29 self-assembling peptides to make supramolecular peptide nanofiber immunogens. Nanofiber formulations were assessed for fibrilization using Atomic Force Microscopy and Transmission Electron Microscopy. To test immunogenicity of the engineered Coil29-IL-22BP candidates, female C57BL/6 mice (n=5 per group) were subcutaneously immunized and boosted. To measure IgG responses, sera was collected at multiple time points and probed against IL-22BP epitopes and whole mouse IL-22 binding protein via indirect ELISA. Results showed IL-22BP Coil29 immunized mice exhibited significant increase in antibody responses against the IL-22BP epitopes (titer and AUC). Multiple predicted epitopes raised antibodies that also bound whole IL-22BP. These studies showed that predicted IL-22BP epitopes can be synthesized onto supramolecular peptide platform Coil29 and form nanofiber structures that raise IgG antibodies against the predicted epitopes and against IL-22 binding protein in mice. Future studies will be performed to assess the intestinal regenerative properties of the active immunotherapy in a colitis mouse model. If successful, this work will be a proof-of-concept for an active immunotherapy that both reduces inflammation and promotes tissue regeneration in IBD.

Programming Bio-inspired Nanoscale Chiral Self-Assembly in 3D Printed Composites

Dr. Monirosadat (Sanaz) Sadati, Dr. Mohsen Esmaeili, Mr. Kyle George, Dr. Nader Taheri Qazvini

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

The emergence of three-dimensional (3D) printing has advanced the fabrication of on-demand architectures for various applications, from functional devices to organs. However, 3D printing is limited to feature size and lacks the nanoscale design of the constituents vital for functional devices. Herein, we combine the "bottom-up" approach with a "top-down" fabrication strategy to program the nano/microscale 3D chiral self-assembly of colloidal nanoparticles in the printed objects. The chiral or helical arrangement, in which layers of nanoparticles/fibers are slightly twisted by a fixed angle relative to the neighboring layers, is known as the origin of the superior fracture resistance of the mineralized chitin in the "smasher-type" mantis shrimp's dactyl club, and compressive and torsional strength of collagen in mammalian cortical bones. Here, we design chiral inks derived from cellulose nanocrystals (CNC) to induce nano/microscale chiral self-assembly, achieving precise control over helical pitch length. We leverage the interplay between ink’s inherent chiral twist energy, the flow dynamics of the 3D printing process and the spatial constraints of the printed filament to orchestrate hierarchical chiral self-assembly within the fabricated constructs. Our mechanical evaluations revealed a marked improvement in toughness attributed to these chiral configurations within the 3D printed structure. Additionally, the process of mineralization of these 3D chiral nanostructures substantially enhanced mechanical toughness under axial tension, surpassing the performance of structures featuring randomly arranged CNC nanoparticles. This phenomenon can be attributed to the chiral-induced order of inorganic mineralized particles embedded in the printed constructs. Our biomimetic concept offers a novel way to developing materials with enhanced mechanical properties, naturally emerging from the synergy of nano/microscale chiral assemblies and biominerals, and is transferred into the larger scale printed architectures, expanding 3D printing material technologies well beyond what has been conceived and attempted so far, into a new generation of nanocomposite and process design.

Reconfigurable self-assembly of peptide-peptoid hybrids

Yuan Gao

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Molecular control of self-assembly and mechanical stiffness in artificial peptide amphiphile matrices offers a chemical strategy to control biological phenomena such as stem cell differentiation and cell morphology. We synthesize a series of peptide-peptoid (an emerging peptide-mimetic) amphiphiles (PAs) with systematically modified amino acid sequences to corresponding peptoid counterparts to investigate the effect and structural properties in their self-assembly. By rationally manipulating the different domains of amino acids in the amphiphiles, we designed and built up our library in the lab to study their self-assembly behavior. We found that variable interesting structures were formed based on peptide/peptoid substitutes and showed different properties such as sizes and mechanics by our control. We also demonstrate that the self-assembly of our peptide-peptoid hybrids was reconfigurable and reversible, which is rare among traditional bio-materials. This type of self-assembled materials and structures showed precise shape designs and kinetic paths like other well-developed classes such as carbon nanotube (CNT) and DNA origami and opened a gate for more bio-applications from soft matter.

Self-assembly of bidisperse colloidal gels

Mr. Rony Waheibi, Dr. Lilian Hsiao

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Self-assembled colloidal depletion gels are important model systems for many industrial processes and applications, such as inks and pharmaceuticals. These nonequilibrium gels persist due to a dynamical arrest resulting in dense, percolated structures with cluster-level architectures. The self-assembly process is well studied with monodisperse colloids; however, the introduction of size polydispersity changes the network microstructure in ways that are not well understood. Here, we investigate the microstructure of three sets of fluorescent poly(methyl methacrylate) colloidal gels comprising sterically stabilized poly(methyl methacrylate) (PMMA) particles of size ratios $\alpha = 1$, 0.7, and 0.62 (average diameter $2a = 1.20$ μm) mixed with polystyrene ($M_w = 900{,}000$ g/mol) as a depleting agent. Colloidal gels are synthesized at a range of volume fractions ($0.1 < \phi < 0.4$) by suspending mixtures of bidisperse PMMA particles in a refractive index and density matched solvent. Confocal light scanning microscopy is used to obtain 3D image volumes from which particle centroids are detected. As the size disparity and volume fraction increases, gels exhibit increased signatures of reduced short-range and local order. We further investigate the origin of this reduced order through particle contact distributions, finding that increasing the size disparity leads to a decrease in the average contact number. Separating distributions into small-small, small-large, and large-large particle contact pairings show that small particle contacts are much less frequent compared to small-large and large-large particle contacts, due to differences in the available surface area and attractive potential. This disparity grows with increasing volume fraction, where the occurrence of large particle contacts increases linearly with ϕ. We hypothesize that differences in the behavior of different sized colloids across volume fractions may influence the mechanical integrity of the network structure underlying these gels.

Synthetic modular building blocks for self-limited assembly

Mr. Rupam Saha, Mr. Daichi Hayakawa, Dr. Thomas Videbaek, Dr. Wei-Shao Wei, Dr. W. Benjamin Rogers, Dr. Seth Fraden

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Among biological systems, entities such as microtubules and viral capsids exhibit a remarkable ability for self-limited growth, achieving precise sizes and shapes through inherent biological processes. Recent material science advancements enable the creation of synthetic building blocks capable of emulating this self-assembly. However, with increasing size and complexity the number of unique blocks with distinct interactions increases, resulting in substantial costs. Here we tackle this challenge by introducing a pluripotent DNA origami subunit whose interaction specificity and angle of binding can be independently programmed, conserving 100% of the core design.

Our approach utilizes equilateral triangle building blocks that interact through DNA hybridization via linker strands. Linkers, arranged in top, middle, and bottom rows, activate positive or negative binding angles. These linkers feature a short flexible single-stranded DNA region and a longer rigid double-stranded DNA domain, with the length of the double-stranded DNA domain determining the binding angle.

Demonstrating our method's effectiveness in programming the binding angles we have constructed platonic capsids by varying the length of the double-stranded DNA domain. We have further characterized the angles of binding with vertex and ring assemblies, validated by cryo-electron microscopy. Notably, we find the bevel angle of bonds changes linearly with the length of the double-stranded DNA domain. Encouraged by these findings, we leverage the combined programmability of bevel angle and interaction specificity of DNA sequences to build various low-symmetrical capsids with high yields.

Looking forward, our strategy holds promise for fabricating synthetic biomaterials, offering new avenues to mimic nature's sophisticated assembly processes.

Theory and Simulations of Light-Induced Self-Assembly in Colloids with Quantum Chemistry Derived Empirical Potentials

Dr. Remya Ann Mathews Kalapurakal, Dr. Prateek K. Jha, Dr. Harish Vashisth

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

Light-induced self-assembly (LISA), a nanoscale phenomenon, leverages photo-responsive ligands to precisely control particle interactions, enabling dynamic, reversible assembly with applications in materials, optics, and biomedicine. Photo-responsive ligands like azobenzene dithiol (ADT) aid in the control of the light-induced self-assembly of gold nanoparticles coated with ADT (ADT-AuNPs).
The exposure to the ultraviolet (UV) light drives the trans-to-cis transition of ADT. The higher dipole-moment in the cis-ADT than trans-ADT results in the reversible transition from a disordered to an aggregated phase, induced by the dipole-dipole attraction. Singh et al., (Comput. Theor. Chem., vol. 1206, pp. 113492, 2021) reported the interaction energy of a pair of ADT ligands in the cis and trans conformations, as a function of distance between the center of mass of the azo-groups. The calculations were performed for different solvent compositions using quantum chemistry calculations. The data was fit onto a generalized potential energy equation similar to the Lennard-Jones (LJ) form, but having different attractive and repulsive contributions for each isomer. Using this generalized equation for the ligand-pair interaction, we calculated the effective interaction energy between a pair of ADT-AuNPs in the cis and trans conformations. The effective energy calculated was compared using discrete and continuous descriptions. In order to identify the optimum length of the ligand which incorporated experimental effects like bending and steric repulsion, we also studied the effect of the ligand length on the effective energy. Further, we fit the effective energy to a generalized potential energy equation, and investigated the detailed phase-behaviour of ADT-AuNPs using Langevin Dynamics simulations.

Tunable alignment of highly-oriented silver nanowires through polymer-assisted evaporation processing for anisotropic electrical and optical coatings

Mr. Liyimin Tao, Mr. Zechao Jiang, Prof. Xingkun Man, **Dr. Ye Xu**

Poster Session 1, Exhibit Hall A, July 30, 2024, 6:00 PM - 8:00 PM

The self-assembly of one-dimensional (1D) nanomaterials into specific configurations is one of the approaches in achieving novel functionalities, including enhanced anisotropy in electrical and optical properties. However, the controlled alignment of nanomaterials, such as silver nanowires, presents considerable challenges due to the intricate interplay of forces at the nanoscale. In this talk, I will introduce our novel methods for aligning Ag NWs in drying suspensions by manipulating the evaporation-induced fluid flow with the addition of polymeric components. This approach allows us to achieve highly-oriented deposition near the drying edge. Through combined in situ microscopic observations and theoretical modeling, we reveal that this alignment mechanism is predominantly due to the increased concentration of the polymeric component near the drying edge, which induces a compressive flow near the contact line. Furthermore, by integrating this alignment method with the shear-alignment effect of the dip-coating process, we demonstrate the ability to pattern Ag NW coatings with alternating alignment directions. Our findings propose a scalable, cost-effective strategy for the alignment of 1D nanomaterials, offering new fabrication methods for the development of materials with tailored anisotropic functionalities for next-generation electronic, photonic, and energy devices.

Uncovering Supramolecular Chirality Codes for the Design of Tunable Biomaterials

Mr. Stephen Klawa, Michelle Lee, Kyle Riker, Tengyue Jian, Qunzhao Wang, Yuan Gao, Margaret Daly, Shreeya Bhonge, W. Seth Childers, Tolulope Omosun, Anil Mehta, David Lynn, Ronit Freeman

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

Supramolecular assembly and polymorphism of β-sheet amyloids play a major role in neurodegenerative diseases and can adopt either a left- or right-handed supramolecular chirality. However, the underlying relationship between sequence and supramolecular chirality remains largely unknown. Here, we characterize the sequence specificity of the central core of amyloid-β 42 and design peptide derivatives which enable chirality inversion at biologically relevant temperatures. We further find that C-terminal modifications can tune the energy barrier of a left-to-right chiral inversion. Leveraging this design principle, we demonstrate how temperature-triggered chiral inversion of peptides hosting therapeutic payloads modulates the dosed release of an anticancer drug. These results suggest a generalizable approach for fine-tuning supramolecular chirality in actuated biomaterials and could be applied in developing treatments to regulate amyloid morphology in neurodegeneration.

Unraveling the conformational dynamics of ‘clasping’ polymer-grafted nanoparticles and their networks

Kireeti Akkunuri

Poster Session 2, Exhibit Hall A, August 1, 2024, 6:00 PM - 8:00 PM

In recent years, increased focus has been placed on creating open network morphologies using polymer-functionalized nanoparticles (NPs). Such structures are of interest due to their immediate applications across a range of sectors including membranes, optics, and stimuli-responsive materials. However, a priori design of such “soft” NPs exhibiting the requisite directional interactions needed to target open lattices remains an ongoing challenge. In this work, we use experiment-theory-simulation integrated to study patch-patch interactions between polymer-functionalized triangular NPs. We first show that the observed patchy interactions give rise to robust yet rotationally flexible “bonds” between NPs. We then extend polymer scaling laws to elucidate the fundamental driving forces governing chain rearrangement, NP relative orientation, and structural relaxation of the “bonded” NPs. Our results show that directionality in NP interaction, branching, and patchy flexibility can be computationally designed and mapped to experimentally relevant parameters, providing powerful handles to aid in targeting non-close-packed NP assemblies.