Schedule for Monday, June 14

All times CT; invited speakers/events in green; long breaks in blue; short breaks in gray.

Time	Name	Title
8:45	Reid Van Lehn	Introduction and Conference Overview

Session 1: Nonequilibrium Systems and Active Matter 1 **Moderator:** Reid Van Lehn		
9:00	Vikram Jadhao	Probing Rheological Properties of Liquids at High Shear Rates using Nonequilibrium Simulations and Machine Learning
9:18	Antonio Tavera-Vazquez	Activity of 2D Platelets at the Light – Induced Nematic – Isotropic Interface of a Thermotropic Liquid Crystal
9:36	Kathleen Krist	Equilibrium Theory for Binding-Driven Molecular Chemotaxis
9:54	Break	
10:00	Vivek Sharma	Surface Forces and Stratification in Micellar Foam Films & Soap Bubbles
10:40	Break	

Session 2: Biological Systems **Moderator:** Reid Van Lehn		
11:10	Shashank Pant	Mechanistic Picture for Chemo-Mechanical Coupling in Human Glutamate Transporter
11:28	Ramin Mehrani	Understanding Protein Dimerization and Identifying Small Molecule Inhibitors using Molecular Simulations.
11:46	Oghosa Akenuwa	Organization and Dynamics of Crosslinked Actin Filaments in Confined Environments
12:04	Break	

Session 3: Polymer Coarse-Graining **Moderator:** Michael Webb		
1:00	Aditi Khot	Top-Down Coarse-Grained Framework for Characterizing Mixed Conducting Polymers
1:18	Ashley Knoerdel	Transfer Matrix Model of pH Effects in Polymeric Complex Coacervation
1:36	Nobahar Shahidi	Developing Polymer Coarse-Grain Models with Local Density Potentials
1:54	Break	

Session 4: Nonequilibrium Systems and Active Matter 2 **Moderator:** Randall Snurr		
2:00	Abhinendra Singh	Towards Designing the Constraints in Dense Particle Suspensions
2:18	Caleb Wagner	Dynamical Systems Approach to Active Nematic Flows
2:36	Break	

Keynote Presentation and Poster Session		
3:00	Robin Selinger	Modeling Programmable Shape-Morphing Dynamics in Liquid Crystal Elastomers
3:55	Break	
4:00	Poster Session A	

Schedule for Tuesday, June 15

All times CT; invited speakers/events in green; long breaks in blue; short breaks in gray.

Time	Name	Title
8:55	Reid Van Lehn	Introduction

Session 5: Machine Learning and Reaction Predictions **Moderator:** Nick Jackson		
9:00	Nick Iovanac	Synthesizable by Design: The Importance of Thermodynamics in Generative Chemical Models
9:18	Vinita Boolchandani	Molecular Dynamics Simulations in TensorFlow
9:36	Sina Chiniforoush	Theoretical Insights into the Polymerization of rac-Lactide by Aluminum Indolide Catalysts
9:54	Break	
10:00	Brett Savoie	How Things Fall Apart: Discovering New Chemistry with Automated Reaction Prediction
10:40	Break	

Session 6: Assembly, Adsorption, and Partitioning **Moderator:** Kevin Hinkle		
11:10	Richard Elliott	On The Fly Second Virial Coefficients
11:28	Vy (Jasmine) Tran	Predicting Octanol/Water Partition Coefficients from Molecular Structure
11:46	Himanshu Singh	Finding the Equilibrium Adsorption Morphologies of Surfactant Molecules at Metal-Water Interfaces via Advanced Molecular Dynamics Simulations
12:04	Break	
1:00	Julia Dshemuchadse	Self-Assembly Simulations for Crystal Structure Discovery
1:40	Break	

Session 7: Porous Materials **Moderator:** Yamil Colón		
1:45	Bandar Bashmmakh	Krypton, Xenon Separation Performance via DD3R Zeolitic Membrane
2:03	Cory Simon	A Toy Statistical Mechanical Model of Gas Adsorption in a Metal-Organic Framework Containing a Rotaxane Molecular Shuttle
2:21	Break	

Faculty Q&A Panel and Poster Session	
2:30	Faculty Q&A Panel (Viviana Monje-Galvan, Neeraj Rai, Brett Savoie, Robin Selinger)
3:30	Break
4:00	Poster Session B

Schedule for Wednesday, June 16

All times CT; invited speakers/events in green; long breaks in blue; short breaks in gray.

Session 8: Polymer Theory **Moderator:** Charles Sing		
9:00	Yuecheng Peter Zhou	Probing Viscoelastic Hysteresis in Single Polymer Dynamics using Crooks Fluctuation Theorem
9:18	Liliana Bello Fernández	Mechanisms of Diffusive Charge Transport in Redox-Active Polymer Solutions
9:36	Miron Kaufman	The Volume Transition in Polymer Gels is Driven by the Crosslinking Entropy
9:54	Break	
10:00	Qian Chen	Nanoscale Cinematography of Nanoscale Crystallization and Protein Fluctuation
10:40	Break	

Session 9: Applications of Machine Learning **Moderator:** Antonia Statt		
11:10	Geemi Wellawatte	Applications of Machine Learning in Coarse-Grained (CG) Molecular Dynamics (MD)
11:28	Jiale Shi	Machine Learning Predicting Adhesive Free Energy of Polymer-Surface Interaction
11:46	Carlos Borca	Smiles4Psi: Automated Conformational Search with a Genetic Algorithm for Quantum-Mechanical Featurization of Synthetic Polymers
12:04	Break	
Session 10: MOFs and Optical Materials **Moderator:** Andrew Paluch		
1:00	Yamil Colón	Engineering Entangled Photon Pairs with MOFs
1:18	Kaihang Shi	Two-Dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Metal-Organic Frameworks
1:36	Tadej Emersic	Directed Self-Assembly of Blue-Phase Liquid Crystals into Thermally Stable Monocrystals
1:54	Break	

Session 11: Charged Systems **Moderator:** Vikram Jadhao		
2:00	Ning Wang	Elucidating the Effect of Ionic Liquid Structure on the Separation of Hydrofluorocarbon Mixtures: A Molecular Modeling Study
2:18	Jason Madinya	Field Theory Description of Polyelectrolyte-Surfactant Coacervate Phase Behavior
2:36	Break	

Session 12: Coarse-Grained Modeling of Soft Materials **Moderator:** Reid Van Lehn		
3:00	Xueying Ko	Adsorption Behavior of Corrosion Inhibitors on Partial Metal Surfaces Studied using Molecular Simulations
3:18	Tianyuan Pan	Interaction Potential for Coarse-Grained Models of Bottlebrush Polymers

Poster Presentations

Poster Session A: Monday, June 14, 4-5 PM

Name	Title
Rusen Argun	Simulations of the Internal Structure of Microgel Particles
Salman Bin Kashif	Towards a Standard Tool for Generating Atomistic Cross-Linked Polymers
Whitney Blocher McTigue	Simulating the Depolymerization of Cyclic and Linear Polymers
Gaurav Chauhan	Crowding-Induced Interactions of Biopolymers
Brian Day	Computational Design of a MOF-Based Electronic Nose for Exhaled Breath Analysis
Hyeonmin Jeong	Modeling of Polymerization-Induced Self-Stratifying Coatings
Jaehyeok Jin	Many-Body Projection Theory in CG Modeling: Bottom-Up Many-Body Projected Water (BUMPer)
Carl Lira	Thermodynamic Modeling of Mixtures with Associating Species
Spencer Sabatino	Predicting Octanol/Water Partition Coefficients Using Molecular Simulation for the SAMPL7 Challenge: Comparing the Use of Neat and Water Saturated 1-Octanol
Sydney Shavalier	Investigation of Thermal Transport in Solvated Gold Nanoparticle Systems using Reverse Non-Equilibrium Molecular Dynamics Methods
Ryan Szukalo	Understanding the Energetic and Entropic Contributions to Effective Coarse-Grained Potentials

Poster Session B: Tuesday, June 15, 4-5 PM

Name	Title
Aseel Bala	Development of a COSMO-Based Activity Coefficient Model for Associating Systems
William Killian	Spectroscopy-Assisted Thermodynamic Modeling of Cooperative Hydrogen-Bonding
Nitesh Kumar	Interfacial Competitive Interactions and Transport Mechanism of Uranyl Across the Liquid/Liquid Phase Boundary
Zhao Li	Molecular Simulation of Adsorption Hysteresis and Spinodal of n-Alkanes in Nanoporous Materials
Tsai-Wei Lin	Coarse-Grained Modeling of Molecular Transport in Permanent Polymer Network
Varun Mandalaparthy	Impact of Solvent Interactions upon Interfacial Phenomena
Kathleen Mitcheltree	Mixed-Surfactant Adsorption on Single-Walled Carbon Nanotubes: Insights from Molecular Simulations
Gustavo Andres Vasquez Montoya	Acoustic Optofluidics on Nematic Liquid Crystals
Alexander Smith	Topological Data Analysis: Applications in Molecular Simulation
Hang Zhang	Molecular-Level Characterization of Water in Contact Charging Phenomena