2019 Midwest Thermodynamics & Statistical

Sunday, June 2, 2019 (Welcome and Evening Reception, 6pm-8pm):

- Registration opens on Sunday at 6:00pm at the Beckman Institute (the same building where the talks and posters will take place).
- The reception will be on the first floor of the Beckman Institute in the Center Atrium.
- Drinks and appetizers will be provided.
- Address of the Beckman Institute: 405 North Mathews Avenue, Urbana, IL 61801
- There is limited parking at the Beckman Institute.
    - If you are driving, you should be able to park at a designated space at your hotel or Hendrick House student housing location.
    - It is a short walk across the street to the Beckman Institute from the Hampton Inn. It is a several-block walk from Hendrick House to Beckman.
    - If you are driving, but are not staying in town overnight, please contact Laura Thurlwell at thurlwel@illinois.edu or (217) 300-1166 for assistance with parking.

2019 Midwest Thermodynamics & Statistical

Monday, June 3, 2019 - (Talks), Location: Beckman Institute Auditorium, Room 1025

7:30 AM	**Breakfast**	**Breakfast will be served in the Center Atrium**
8:00 AM	**Jeffrey Moore and Charles Sing**	**Opening remarks**
8:15 AM	**Cari Dutcher**	**Lattice-based adsorption isotherms for solute activities and surface tensions of complex aqueous electrolyte solutions**
9:00 AM	Nabil Ramlawi	Medium-amplitude oscillatory shear (MAOS) predictions for the Johnson-Segalman non-affine deformation model
9:15 AM	Vikram Jadhao	Shear-thinning in viscous fluids at high shear rates and pressures
9:30 AM	Michael Quevillion	Effects of a Polarizable Model on the Phase Behavior of Ionic Liquid Crystals
9:45 AM	Simon Rogers	Elastic to Liquid Transitions in Soft Solids
10:00 AM	Shiyan Wang	Biased sampling of 3D polymer conformations in an external field using Brownian bridges
10:15 AM	**Coffee break**	**Coffee and refreshments will be served in the Center Atrium**
10:45 AM	Nicholas Brunk	Soft Nanoparticle Shape Control: Competing Electrostatic, Elastic, and Hydrophobic Forces
11:00 AM	Jiale Shi	Novel Elastic Response in Twist-Bend Nematic Models
11:15 AM	Kartik Kamat	A free-energy diabat approach to polymorph stability
11:30 AM	Ashesh Ghosh	Theory of interchain packing, ideal kinetic arrest and emergent elasticity in associating copolymer liquids
11:45 AM	**Lunch and Poster Session**	**Lunch will be served in the Center Atrium, Poster session will be in East Atrium**
1:00 PM	**Reid van Lehn**	**Computational Design of Nanoparticles with Tunable Water-Mediated Interactions**
1:45 PM	Christian Leitold	Solid–solid phase transitions in the NaCl–KCl system
2:00 PM	Alex Chew	Understanding the Influence of Polar Aprotic Solvents on Reaction Selectivities in Biomass Conversion Processes using Classical Molecular Dynamics Simulations
2:15 PM	Sumit Sharma	Quantitatively Accurate Theory to Predict Adsorbed Configurations of Surfactants on Metal Surfaces
2:30 PM	Haimeng Wang	Computing the Structural and Transport Properties of Molten Alkali Halide Salts
2:45 PM	**Coffee break**	**Coffee and refreshments will be served in the Center Atrium**
3:15 PM	Steven Strong	Tennis with Water Molecules: IR spectroscopy of supercritical water
3:30 PM	Himanshu Singh	Adsorption and Disintegration of Surfactant Micelles at Metal-Water Interfaces: A Computational Investigation
3:45 PM	William Killian	Improved Methods for Obtaining Thermodynamic Model Parameters from Spectroscopy
4:00 PM	Maghesree Chakraborty	Importance of Symmetry Preservation in Coarse-Grained Alkanes
4:15 PM	Garrett Tow	Aging of Solid Propellant
4:30 PM	Xueying Ko	Self-Assembly of Adsorbed Surfactant Molecules at Metal-Water Interfaces
5:00 PM	**Monica Olvera de la Cruz**	**Puzzles in Molecular Electrolytes**
6:00 PM	**Banquet Dinner**	**Banquet buffet dinner to be held in the Center Atrium**

2019 Midwest Thermodynamics & Statistical

Tuesday, June 4, 2019 - (Talks), Location: Beckman Auditorium, Room 1025

7:30 AM	**Breakfast**	Breakfast will be served in the Center Atrium
8:00 AM	**Clare McCabe**	**Molecular Dynamics Simulations of Stratum Corneum Lipid Mixtures: A Multiscale Perspective**
8:45 AM	Shashank Pant	Microscopic characterization of proton binding and lipid-protein interactions in glutamate transporters using advanced simulation techniques
9:00 AM	Anne Leonhard	Utilizing Advanced Sampling to Understand Host-Guest Binding Dynamics
9:15 AM	Mohammadreza Aghaaminiha	Spatial Distribution of Cholesterol in Symmetric and Asymmetric Lipid Bilayers studied using Coarse Grained MD Simulations
9:30 AM	Lauren Nilsson	Probing Heterogeneous Virus Capsid Self-Assembly using Molecular Dynamics Simulations of Elastic Capsomeres
9:45 AM	Shuting Yan	Base Stacking in the Loop of an RNA Aptamer: Investigation of the Geometry and Energetics with Molecular Dynamics Simulation
10:00 AM	Jonathan Sheavly	Curvature-driven adsorption and alignment of cationic nanoparticles to phase boundaries in multicomponent lipid bilayers
10:15 AM	**Coffee break**	**Coffee and refreshments will be served in the Center Atrium**
10:45 AM	Heta Gandhi	A GPU-Accelerated Machine Learning Framework for Molecular Simulation: Hoomd-blue with TensorFlow
11:00 AM	Tyler Josephson	Partial molar properties from molecular simulation using multiple linear regression
11:15 AM	Zahra Shamsi	Transfer learning in Potts models
11:30 AM	Michael Webb	Graph-Based Coarse-Graining
11:45 AM	**Lunch and Poster Session**	**Lunch will be served in the Center Atrium, Poster session will be in East Atrium**
1:00 PM	**Steven Abel**	**Antigen Recognition at Immune-Cell Surfaces: Probing the Role of Mechanical Forces**
1:45 PM	Brett Savoie	Improved Chemical Prediction from Scarce Data Sets Using Transfer Learning
2:00 PM	Matthew Chan	Substrate-induced conformational transitions of the human serotonin transporter
2:15 PM	Alex Pak	Systematically Derived Coarse-Grained Lipid Models with Semi-Explicit Solvation
2:30 PM	Shanghui Huang	Surveying the Free Energy Landscape of Clusters of Attractive Colloidal Spheres
2:45 PM	**Coffee break**	**Coffee and refreshments will be served in the Center Atrium**
3:15 PM	Bing Li	Shaping membrane vesicles by adsorption of a semiflexible polymer
3:30 PM	Artem Rumyantsev	Complex Coacervates of Semiflexible Polyanions and Flexible Polycations: Isotropic and Liquid Crystalline States
3:45 PM	Daniel Sinkovits	Many-Body Effects in Assemblies of Polarizable Rigid Polyelectrolytes
4:00 PM	Natalia Markiewicz	The Effect of Short-range Attractions on Sequence-Defined Polyelectrolyte Coacervation
4:15 PM	Daniel Davies	Understanding the Polymorphic Transition Mechanisms of n-Type Organic Semiconductors
4:30 PM	Ernesto Carlos Cortes Morales	Theory of equilibration and aging in colloidal fluids of non-spherical interacting particles.
4:45 PM	Yuxing Zhou	Local structure and phase behavior of dense polymer-particle mixtures: improved theory and comparison with simulation

2019 Midwest Thermodynamics & Statistical

Monday and Tuesday, June 3 and June 4, 2019 - (Posters), Location: Beckman East Atrium

Note: Posters will be up throughout the duration of the conference, but you will only be asked to stand by your poster during your designated poster session time.

1. Derrick Poe	A Study of Solvation Structure and Dynamic Properties of Ethaline and Glyceline via Molecular Dynamics
2. Bradley Dallin	Perturbations to Hydrophobicity by Physical Properties Create Chemically Heterogeneities in Self-assembled Monolayers
3. Tianyuan Pan	Rheology behaviors of bottlebrush semi-dilute solution
4. Samarthaben Patel	Predicting the Morphologies of Self-Assembled Quorum Sensing Signal Molecules
5. Jiming Chen	Simulations reveal divergent substrate binding pathways in Striga hermonthica and Arabidopsis thaliana strigolactone receptors
6. Bridgette Befort	Discovery of New Ionic Liquids via Molecular Simulations for the Separation of Azeotropic Mixtures of High Global Warming Potential Hydrofluorocarbon Refrigerants
7. Atharva Kelkar	Combining Molecular Dynamics Simulations and Deep Learning to Predict Interfacial Properties
8. Rand Dickson	Three-Body Interaction in Parallel
9. Scotty Bobbitt	Computational Screening of Nanoporous Materials for Hydrogen Storage
10. Gary Min Chiang Ong	Self-assembly of diblock copolyelectrolytes
11. Randy Ewoldt	Weakly-nonlinear viscoelasticity is a stat mech playground
12. Zhizhang Shen	Atomistic Simulations of Carbon Nanotube Deposition on Functionalized Silicon Substrates
13. Craig Vandervelden	Catalysts on amorphous supports II: importance learning estimate of the site-averaged kinetics
14. Bijal Patel	Nonequilibrium Assembly of Bottlebrush Block Copolymers for Tunable Nanoscale Morphology
15. Zack Jarin	How Shape, Flexibility, and Crowding Affect Curvature Sensing and Generation by Generic Scaffolding Proteins
16. Andres Arango	Molecular Docking to Estimate Binding Affinities of Anthracyclines to Cytochrome P450s

17. Arun Gopalan	Fast and Accurate Prediction of Hydrogen Adsorption in Nanoporous Materials
18. Mayank Boob	Critical phenomena in the temperature-pressure-crowding phase diagram of a protein
19. Jason Madinya	Self-Coacervation of Sequence-defined Polyampholytes
20. Stephen Shiring	Surface Cation Substitution-Effects on 2-D Perovskite Stability and Optoelectronic Properties
21. Nicolae Iovanac	Improved Chemical Prediction from Scarce Data Sets via Latent Space Enrichment
22. Aditi Khot	Effects of the Mapping Operator in Bottom-Up Coarse-Graining
23. Qiyan Zhao	Enthalpy of Formation Prediction via TAFFI Group Increment Theory
24. Jack Yungbluth	An Excess Internal Energy Model Describing Super-Arrhenian Relaxation Dynamics of Super-Cooled Liquids
25. Lili Bello	Structure and Dynamics of Redoxmers in Dilute Solution
26. Ying Tan	Charge Transport in TEMPO-Based Radicals
27. Charles Young	Conformational distributions in flowing semidilute polymer solutions
28. Sarit Dutta	Coarse-Grained Modeling of Bottlebrush Polymers in Dilute Solution
29. Richard Elliott	Combined Temperature and Density Series for Fluid-Phase Properties. 2. Lennard-Jones Spheres