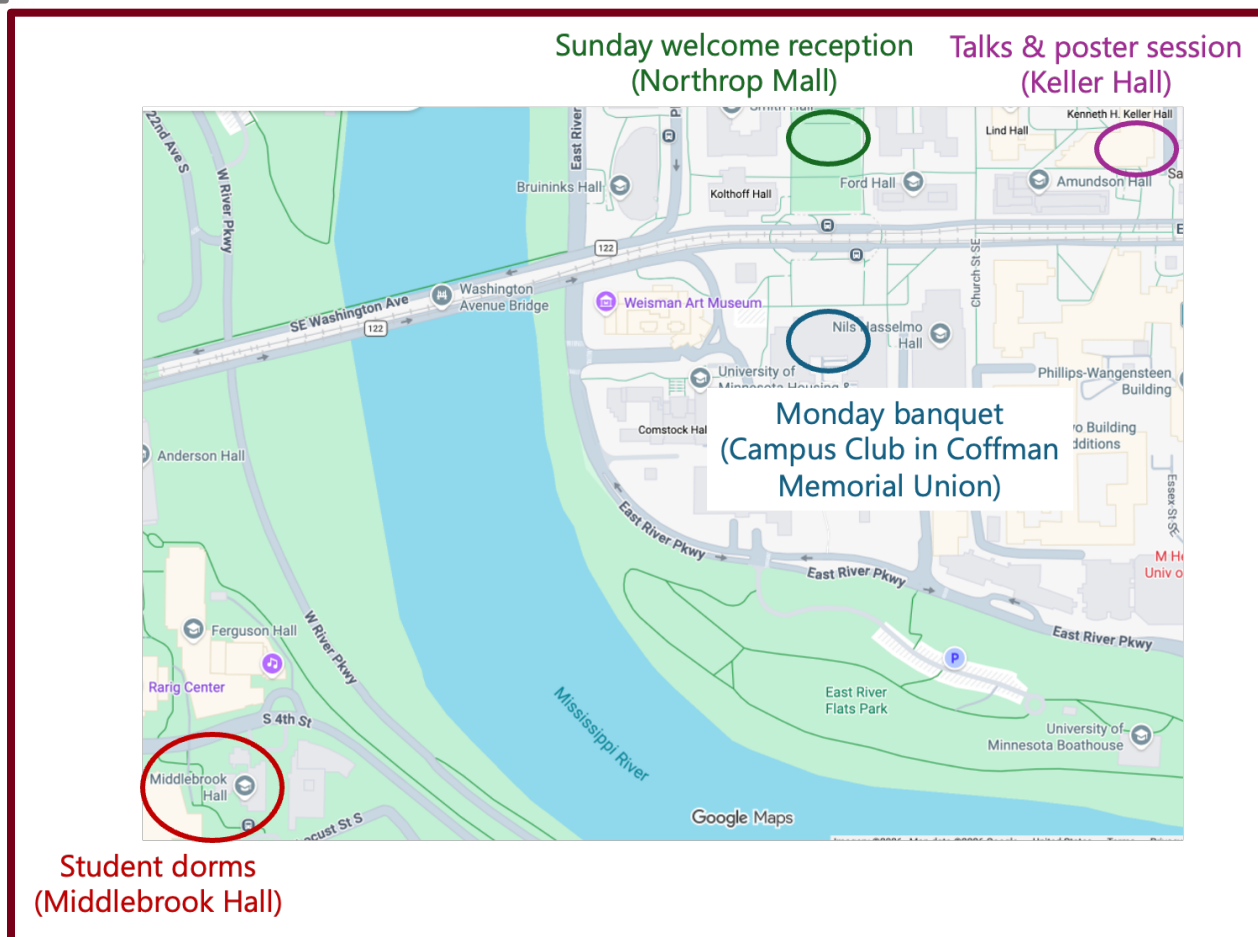




35th Midwest Thermodynamics and Statistical Mechanics (MTSM) Conference

Sunday June 14th to Tuesday June 16th | Minneapolis, MN



The conference will take place on the **University of Minnesota Twin Cities East Bank campus** in Minneapolis, with technical and poster sessions in **Keller Hall**.

For those arriving early, there will be an informal welcome reception **Sunday 6/14 from 5-7 pm on Northrop Mall**. This will be an opportunity to pick up your badge, meet fellow attendees, and spend some time outside (weather permitting) before the conference starts in earnest. Pizza will be provided. You are also welcome to **pick up your badge Monday morning in Keller Hall from 8:00-8:45 am**.

Those that **signed up for dorms will be staying at Middlebrook Hall**. Those that also signed up for parking should receive a parking pass when you check in at Middlebrook.

If you are driving to campus, but not staying in the dorms, we recommend **parking in the Washington Ave Ramp** next door to Keller Hall for \$15 per day. Public transit is also available and can be accessed via the **Metro Transit App**.



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Sunday, June 14th

Pizza and badge pickup (Northrop Mall)

5:00–7:00 pm

Monday, June 15th

Light breakfast and badge pickup (Keller Atrium)

8:00–8:45 am

Technical Session I (Keller 3-180)

8:45 am – 12:00 pm

8:45 am	Prof. Chris Bartel , University of Minnesota Opening remarks
9:00	<u>Invited</u> : Prof. Alex Albaugh , Wayne State University Catalysts, Motors, and Vapor Deposition: Nonequilibrium Applications of Grand Canonical Monte Carlo
9:30	Tim Tan , University of Minnesota Toward Molecular Simulations of Low-solubility Salt Nucleation with Constant Chemical Potential Molecular Dynamics
9:45	Jordan Loeffler , University of Wisconsin Developing Low-Dimensional Order Parameters for Automated Detection of Crystallization in Complex Molecules
10:00	Paul Amagada , University of Notre Dame Kirkwood–Buff Integral-Based Framework for Constructing Solid–Liquid Equilibria in Non-Ideal Mixtures
10:15	Fadeshola Shodipe-Dosunmu , University of Notre Dame Evaluating The Impact of Pressure Tensor Averaging Conventions on Green-Kubo Viscosity Precision
10:30	Coffee Break (Keller Atrium)
11:00	Hwigwang Lim , University of Wisconsin Impact of electrostatic interaction models in colloidal morphology and phase behavior in highly concentrated electrolytes



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11:15	Benjamin Schwartz , University of Michigan Phase separation and collective motion of self-propelled cell-like "flexicle" mixtures
11:30	George Yeh , University of Texas at Austin Bidisperse Colloidal Monolayers with Competing Interactions
11:45	Christian Jorgensen , University of Wisconsin scikit-matter: A Suite of Generalizable Machine Learning Methods Born out of Chemistry and Materials Science

Lunch (Keller Atrium)
12:00-1:30 pm

Technical Session II (Keller 3-180) 1:30-4:00 pm

1:30	<u>Invited</u> : Prof. Sara Kadkhodaei , University of Illinois Chicago Finite temperature diffusion transition states in strongly anharmonic solids
2:00	Jane Schlesinger , University of Minnesota A thermodynamic assessment of machine learning models for synthesis prediction
2:15	Orlando Mendible-Barreto , University of Notre Dame DynaMate2: Democratization of Agentic AI for Expert-Designed Custom Workflows
2:30	Coffee Break (Keller Atrium)
3:00	Fathya Salih , University of Notre Dame Predicting the environmental and safety properties of refrigerants and refrigerant mixtures using sigma profiles
3:15	Prof. Sumit Sharma , Ohio University Hydration Free Energies of Linear Alkanes and Surfactants
3:30	John Michael Lane , Mississippi State University Theoretical Insights on B-site Cation Diffusion into Core-shell Perovskites
3:45	Amir Orvati Movaffagh , University of Illinois Chicago Defect Energy Formalism for CALPHAD Thermodynamics of Dilute Point Defects



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Poster Session (Keller Atrium) 4:00-5:30 pm	
1	Christopher Akiki , University of Minnesota Strain-enhanced miscibility in (Sn,Ti)O ₂ rutile alloys grown by molecular beam epitaxy
2	Charles Carroll , University of Wisconsin Identifying the Origins of Stability in an Organic Vapor Deposited Glass Former
3	Max Depperschmidt , University of Wisconsin An active machine learning framework for designing nanoprobe targeting chronic pain signaling
4	Chiara Corsini , University of Illinois Urbana-Champaign Glassy Dynamics in Polyelectrolyte Complexes
5	Jung Min Lee , University of Wisconsin Molecular Dynamic Investigation of Calcium-Sugar Interactions under Alkaline Conditions
6	Changsu Kim , University of Wisconsin Effect of Protonation Equilibrium on the Hydrophobicity of Charged, Chemically Heterogeneous Surfaces
7	Armand Lannerd , University of Minnesota Proton insertion across the perovskite-brownmillerite transition in La _{0.5} Sr _{0.5} CoO _{3-δ}
8	Haisu Kang , University of Illinois Urbana-Champaign Shape-driven assembly of bottlebrush homopolymers in melts
9	Ethan Deutsch , University of Wisconsin Persistent Homology Identifies Dynamics-Property Correlations in Simulated Glass Formers
10	Avery Greene , University of Wisconsin Predicting Sodium-Ion Battery Electrolyte Performance with Molecular Dynamics
11	Yuhui Huang , University of Wisconsin Understanding Nanoparticle-Protein Interactions through Molecular Dynamics and Surface-Based Machine Learning
12	Precious Okolo , University of Notre Dame Computational Screening of Refrigerant Solubility in Deep Eutectic Solvents via Pre-sampled Solvent Trajectories and Configurational-Bias Monte Carlo
13	Letian Wang , University of Wisconsin Enhanced Sampling-Guided Machine Learning for the Rational Design of Orthogonal Polymer Sensor Arrays in Serum
14	Anushna Bhattacharyya , University of Illinois Urbana-Champaign Simulations of Bond Network Dynamics in Vitrimers



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15	Poornima Moremada , University of Michigan Machine Learning Interatomic Potential Model for H/O system under Extreme Conditions using ChIMES
16	Brian Wood , University of Illinois Urbana-Champaign Evaluating Image Recognition as a Tool for Classifying Sequence-Defined Polymer Self-Assembly
17	Caleb Youngwerth , University of Wisconsin Using MD Simulation with Energetic and Structural Analysis to Examine DLVO Theory in Highly-Ionic Colloidal Gel Systems
18	Zach Hart , University of Michigan A cautionary tale: Hyperparameter selection for machine-learned interatomic potentials to maintain quantum accuracy & macroscopic consistency
19	Liang-Ching Chen , University of Illinois Urbana-Champaign Impact of Structural Regularity on the Crystallization of Crosslinked Networks
20	Bridget Ferris , Washington University in St. Louis Developing a Predictive Model for Anion Vacancy Formation Energies in Binary Metal Chalcogenides
21	Eyob Tewelde , Washington University in St. Louis Surface Characterization of CaTiO ₃ as a Model for Perovskite-Based Solar Thermochemical Water Splitting
22	Benjamin Chiu , University of Illinois Urbana-Champaign Using Molecular Models and Recovery Rheology to Predict the Stress Response of Polymer Networks
23	Grady Clopton , University of Illinois Urbana-Champaign Multiscale Modeling of Swift Heavy-Ion Track Formation in Redox-Active Ceria
24	Luis Felipe Gabriel Zanardo , University of Campinas Building Bridges

Banquet (Coffman Memorial Union, Campus Club, 4 th floor, West Wing) 6:00-9:00 pm	
6:00	Bar opens
6:30	Buffet dinner served
7:30	<u>Keynote:</u> Prof. Elif Ertekin , University of Illinois Urbana-Champaign Machines, Molecules, and Many-Body Physics: Statistical Mechanics in the Age of Generative AI



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Tuesday, June 16th

Light breakfast (Keller Atrium)

8:00-9:00 am

Technical Session III (Keller 3-180)

9:00-11:30 am

9:00	<u>Invited</u> : Prof. Daphne Wui Yarn Chan , Carnegie Mellon University Self-assembled protein nanofibrils for renewable materials
9:30	Gopal Parthasarathy , University of Minnesota Entropic segregation of bottlebrush ring polymers
9:45	James Tallman , University of Illinois Urbana-Champaign Morphologies of Lipid--Block Co-polymer Bilayers: Phase Separation and Mixing Behavior
10:00	Coffee break (Keller Atrium)
10:30	Arthur Lin , University of Wisconsin Anisotropic Coarse-Graining with Machine Learning Representations
10:45	Tyla Holoman , University of Texas at Austin Coarse-grained modeling of dynamic star polymer networks
11:00	Lakshmi Ananthabhotla , University of Pittsburgh Probing Polyurethane Pyrolysis Chemistry with Reaction-Aware Machine Learning Interatomic Potentials
11:15	Min-Hsien Lin , University of Illinois Urbana-Champaign Molecular Simulation Study of Penetrant Diffusion in Vitrimer Networks

Lunch (Keller Atrium)

11:30 am – 1:00 pm



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Technical Session IV (Keller 3-180) 1:00-2:45 pm	
1:00	<u>Invited:</u> Prof. Tyler Josephson , UMBC Formally-verified thermodynamics and molecular simulations
1:30	Pragya Parihar , University of Minnesota Assessing force fields for adsorption in Zeolitic Imidazolate Framework (ZIF-8)
1:45	Abdullah Al Mahmud , Ohio State University Unraveling Adsorption Hydrophilic FAU Zeolites: Coupling DFT-Derived Charge Distributions with Statistical Mechanical Simulations
2:00	Yufeng Qian , University of Pittsburgh Synergistic Adsorption of Lead and PFOA in MOFs: A Combined Computational and Experimental Study
2:15	Wilson Raney , University of Notre Dame Halogenated Metal–Organic Frameworks for Entangled Photon Pair Generation
2:30	Prof. Chris Bartel , University of Minnesota Closing remarks

If you find yourself with free time, a few suggested things to do near campus are [East River Flats Park](#) (nice view of the river), [Weisman Art Museum](#) (free museum on campus), and [Stone Arch Bridge](#) (landmark ~30 min walk from campus). For food near campus, there's [Afro Deli](#), [Kinzo Udon](#), [Lu's Sandwiches](#), and [Kimchi Tofu House](#). For a drink, there's [Stub and Herbs](#) and [Sally's Saloon](#), among many other options.



If you have questions, please reach out to Chris Bartel (cbartel@umn.edu).