CONFERENCE PROGRAM

Midwest Thermodynamics and Statistical Mechanics (MTSM) Conference

June 7–8, 2023
Smith Ballroom, The Morris Inn
University of Notre Dame

MTSM is a regional meeting for interdisciplinary researchers in all aspects of thermodynamics and statistical mechanics, especially those in the early stages of their academic careers. It brings together faculty and students from diverse fields to exchange new ideas and research results.

The conference provides an ideal forum for researchers to present their work and engage in intense discussions about topics of similar interest, enabling camaraderie within other groups and fostering sustainable research programs. Each session features an invited speaker and presentations representing a diverse range of research topics and populations. The keynote address will be given at the conference banquet.

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Thank you for attending the 32nd annual MTSM Conference. We look forward to your participation!
If you have questions, please contact Prof. Yamil Colón at ycolon@nd.edu or 574-631-8246.

Conference Site
University of Notre Dame Morris Inn, 1399 N. Notre Dame Avenue, South Bend, IN 46617, Phone: 574-631-2000

Event Locations
Morris Inn Smith Ballroom – Technical Sessions
Morris Inn Private Dining Rooms – Breakfasts, Lunches, and Breaks
Corbett Family Hall Downes Club – Poster Session, Reception and Dinner, and Keynote Lecture

Parking and Directions
Between the hours of 6:00 a.m. and 4:00 p.m., visitors must purchase a permit at the Walsh Architecture Visitor lot. Please use code **NDENFX1851** to park free and place the printed receipt on your dashboard to serve as your parking permit. The Walsh lot and other parking lots are located on the south side of campus.

- View this link for a complete list of visitor parking lots.
- View this link for parking and directions to Morris Inn.
- View this link for directions to Notre Dame.

Explore Campus
Get to know your surroundings before you arrive!

- View this link for a map of Notre Dame's campus highlighting the building locations of the Morris Inn, Corbett Family Hall, Knott Hall, and visitor parking lots.
- View this link for a campus tour via Live Webcams and learn about famous landmarks on campus.

Conference Check-in
Conference attendees arriving before 6:30 p.m. on **Tuesday, June 6**, should check in at the Morris Inn Smith Ballroom. If arriving after 6:30 p.m., please go directly to your dorm or hotel. Early arrivers may also attend the evening welcome reception to meet and mingle with other conference attendees.

- **2:00 – 6:30 p.m. Check-in, Morris Inn Smith Ballroom**
  Pick up your name badge, conference book, and get directions to Knott Hall, the on-campus residence hall for conference attendees, and to Embassy Suites hotel.
- **6:30 – 8:00 p.m. Welcome Reception, Morris Inn Private Dining Rooms**
  Early-arrivers will have a chance to mingle with other conference attendees while enjoying light refreshments. We hope you will stop in!

Housing Contact Information

- Knott Hall, 574-634-2125 (Sunday–Thursday, 7 p.m.–8 a.m.; Friday 7 p.m.–Sunday 6 p.m.)
  Area Summer Coordinator: Gina Alderson, galderso@nd.edu or 574-634-2138
  (Monday–Friday, 10 a.m.–7 p.m.)
  Additional Support: Office of Residential Life, residentiallife@nd.edu or 574-631-5878
  (Monday–Friday, 8-10 a.m.)
- Embassy Suites by Hilton South Bend at Notre Dame
  1140 E. Angela Blvd, South Bend, IN 46617
  Phone: 574-400-2600

Wi-Fi Access
Visitors can access the ND-Guest Wi-Fi network by following the instructions below. If you have credentials from your home institution for the Eduroam network, you can connect through the Notre Dame network.

- **Notre Dame-Guest Wi-Fi Network:** ND-Guest is an unencrypted wireless network accessed by browsing through available wireless networks on any wireless device.
- **Eduroam Wireless Network:** Eduroam allows visitors from participating institutions to have internet connectivity with only a one-time initial configuration**.** Follow these instructions to connect your devices to eduroam: (1) Connect to any wireless network such as ND-guest. (2) Using a browser on the device, go to eduroam.nd.edu and follow the instructions to configure your device. (3) If you do not immediately connect to eduroam, reboot your device.

32nd Annual Midwest Thermodynamics and Statistical Mechanics (MTSM) Conference

June 7-8, 2023 • Morris Inn • University of Notre Dame

Tuesday, June 6	
2:00-6:30 pm	Registration • Morris Inn Smith Ballroom
6:30-8:00 pm	Welcome Reception • Morris Inn Private Dining Room

Wednesday, June 7 ***Morris Inn Smith Ballroom***		
7:30-8:00 am	Registration and Breakfast	
8:00 am	**Welcome from Professor Yamil Colón, University of Notre Dame**	
	Session I	
	Presenter	*Presentation Title*
8:15-8:45 am **Invited Speaker**	**Rebecca Lindsey** **University of Michigan**	**Machine Learning: A Route to High Accuracy Simulation of Complex Systems**
8:45-9:00 am	Montana Carlozo University of Notre Dame	Bayesian Optimization for Force Field Calibration
9:00-9:15 am	Hilal Daglar Northwestern University	Machine Learning Assisted Molecular Simulation of MOF Membranes and MOF/Polymer Mixed Matrix Membranes for Gas Separations
9:15-9:30 am	Gregory Cooper University of Notre Dame	Metal–Organic Framework Clustering Through the Lens of Transfer Learning
9:30-9:45 am	Meiirbek Islamov University of Pittsburgh	Accelerating MOF Discovery: Predicting Thermal Conductivity Using Graph Convolutional Neural Networks
9:45-10:00 am	**Morning Break**	
10:00-10:15 am	Chun-I Wang University of Illinois, Urbana-Champaign	Identifying Coarse-Grained Representations for Electronic Predictions
10:15-10:30 am	Zheng Yu University of Illinois, Urbana-Champaign	Machine Learning Quantum-Chemical Bond Scission Accelerates Thermoset Large Deformation Simulations
10:30-10:45 am	Kevin Adams University of Illinois, Urbana-Champaign	Microkinetic Models in Catalysis: Chic Designs from Wallpaper and Tile
10:45-11:00 am	Safa Alzaim University of Michigan	Toward Accurate Prediction of Hydrogen and Oxygen Properties Under Extreme Conditions
11:00-11:15 am	Robert Wexler Washington University, St. Louis	Path of Least Resistance: Predictive Thermochemical Cycles for Bulk and Surface Catalysis
11:15-11:30 am	Denver Haycock University of Notre Dame	Application of the Maximization of Entropy Production Theory for Nonthermal Ethane Plasmas
11:30-11:45 am	Veerupaksh Singla Purdue University	Learning Material Stability Scores from Computationally Generated Kinetic Data
11:45 am-1:00 pm	**Lunch Break**	

	Session II	
	Presenter	*Presentation Title*
1:00-1:30 pm Invited Speaker	**Sumit Sharma Ohio University**	**Probing the Adsorption Behavior of Surfactants at Metal-Water Interfaces Using Molecular Simulations**
1:30-1:45 pm	Nikhil Nambiar University of Tennessee	Particle Deformability Enables Control of Interactions Between Membrane-Anchored Nanoparticles
1:45-2:00 pm	Thomas Gaetjens University of Tennessee	Applied Force Modulates the Organization of Pathogen-Macrophage Interfaces
2:00-2:15 pm	Hossam Farag University of Illinois, Urbana-Champaign	Modeling Thermal Hysteresis of Anti-Freeze Proteins on Ice: Effects of Supercooling, Footprint Size, Surface Coverage, and Engulfment Avalanches
2:15-2:30 pm	Hemant Nagar Ohio University	Microcystin Adsorption Studied Using Molecular Simulations
2:30-2:45 pm	Greg Cantrall University of Tennessee	Effects of Macromolecular Crowding on the Collapse and Adsorption of Biopolymers with Nonuniform Bending Stiffness
2:45-3:00 pm	**Afternoon Break**	
3:00-3:15 pm	Ravi Kumar Reddy Addula University of Illinois, Urbana-Champaign	Extracting Homogeneous and Heterogeneous Rate Parameters from Ice Nucleation Survival Assays
3:15-3:30 pm	Howard Weatherspoon University of Illinois, Urbana-Champaign	Broken Bond Models, Magic-Sized Clusters, and Nucleation Theory in Nanoparticle Synthesis
3:30-3:45 pm	Camila Faccini de Lima Indiana University	Multilayered Ordered Arrays Self-Assembled from a Mixed Population of Nanoparticles
Poster Session, Conference Banquet, and Keynote Lecture: Corbett Family Hall Downes Club (east side of stadium)		
4:00-4:30 pm	Poster Session Setup for Poster Presenters and Break	
4:45-6:00 pm	Poster Session and Reception	
6:00-6:15 pm	Group Photo	
6:15-7:30 pm	Conference Banquet (bar closes at 7:30 pm)	
7:30-8:30 pm Keynote Lecture	**Linda Broadbelt, Northwestern University "Polymer Redesign through Reaction Pathway Analysis"**	

Thursday, June 8 ***Morris Inn Smith Ballroom***		
7:30-8:00 am	Registration and Breakfast	
8:00 am	**Welcome from Professor Yamil Colón, University of Notre Dame**	
	Session III	
	Presenter	*Presentation Title*
8:15-8:45 am **Invited Speaker**	**Vikram Jadhao** **Indiana University**	**Computational Studies of Soft Materials at the Nanoscale**
8:45-9:00 am	Seonghwan Kim University of Illinois, Urbana-Champaign	Open Macromolecular Genome: Generative Design of Synthetically Accessible Polymers
9:00-9:15 am	Neha Tyagi University of Illinois, Urbana-Champaign	Transport of Tracer Particle in Flowing Semidilute Polymer Solutions
9:15-9:30 am	Wenhui Li Indiana University	Linking Rheological Properties with Molecular-Scale Features via Molecular Dynamics Simulations and Machine Learning
9:30-9:45 am	Alex Albaugh Wayne State University	Understanding and Designing Artificial Molecular Motors with Nonequilibrium Simulation
9:45-10:00 am	**Morning Break**	
10:00-10:30 am **Invited Speaker**	**Svetlana Morozova** **Case Western University**	**Polymer Dynamics Near Surfaces**
10:30-10:45 am	Yamara Matos Oliveira University of Notre Dame	Potential of Mean Force between Polyethylene Nanoplastic and Bisphenol A
10:45-11:00 am	Hyeonmin Jeong University of Illinois, Urbana-Champaign	Developing a Phase-Field Model to Study Polymerization-Induced Self-Stratification
11:00-11:15 am	Dervis Vural University of Notre Dame	A Closer Look at Maxwell's Demon: Counterfactual Measurements and Finite Size Effects
11:15-11:30 am	George Curtis Purdue University	Self-Adjoint Formulation and Approximations for the Construction of Stochastic Bridges
11:30-11:45 am	Grant Mathews University of Notre Dame	Simulations of Multi-Component Relativistic Thermalization in Big Bang Cosmology
11:45 am-1:00 pm	**Lunch Break**	
	Session IV	
1:00-1:15 pm	Brendan Mahoney University of Notre Dame	Entanglement Spread and Quantum Phase Transitions
1:15-1:30 pm	Atefeh Ahmadbeigi Ohio University	Thermodynamic Modeling of Water Solubility in Supercritical CO_2
1:30-1:45 pm	Qing Shao University of Kentucky	Deciphering Hydrogen Bond Features to Develop Machine Learning Models for Predicting Non-ionic Deep Eutectic Solvents
1:45-2:00 pm	Ryan Smith University of Notre Dame	An Efficient Implementation of the Test Particle Insertion Method for High-Throughput Screening of Gas Absorption in Liquids
2:00-2:15 pm	Mingrui Yang Washington University, St. Louis	Surface Phase Diagrams from Nested Sampling
2:15-2:30 pm	**Closing Remarks from Professor Yamil Colón, University of Notre Dame**	

Poster Session Roster
Wednesday, June 7 • 4:45 – 6:00 pm

Poster #	Poster Title & Authors
1	"Evaluating Suitability of the ChIMES Machine-Learned Interatomic Model for Zeolite Materials" Sayed Ahmad Almohri (University of Michigan) and Rebecca K. Lindsey
2	"An Attempt to Accelerate Rigid-Body Molecular Dynamics Simulations" B. Ruşen Argun (University of Illinois, Urbana-Champaign) and Antonia Statt
3	"Use MOSCED for Azeotrope Prediction and Efficient Entrainer Selection" Md Abdus Samad Azad (Miami University), Alim Dewan, and Andrew S. Paluch
4	"Directed Self-Assembly of Complex Liquid Crystalline Phases" Kushal Bagchi (University of Chicago), Tadej Emeršič, Juan J. de Pablo, and Paul Nealey
5	"Effect of Water on Local Solvation Structure of Carbon Dioxide Towards Understanding the Microscopic Level Environment of Deep Eutectic Solvent" Sanchari Bhattacharjee* (Clemson University) and Rachel B. Getman
6	"Structure Property Relationships for the Effect of External Electric Fields on Thermophysical Properties of Ionic Liquids" Fernando Carmona-Esteva (University of Notre Dame), Yong Zhang, Yamil J. Colón, and Edward Maginn
7	"Atomistic Simulations of Soft Porous Coordination Polymers" James Carpenter (University of Notre Dame) and Yamil J. Colón
8	"Exploring Phase Behavior in Dynamic Covalent and Permanent Diblock Copolymer Melts: A Self-Consistent Field Theory Approach" Yun-Ju Chen (University of Illinois, Urbana-Champaign) and Charles E. Sing
9	"Predicting the Solubility of Pharmaceuticals Using MOSCED" Anisha Parsub Chhoan (Miami University) and Andrew S. Paluch
10	"Structure and Charge Transport in Ionic Liquid Crystals" Marvin Diaz-Segura (University of Notre Dame), Jiacheng Liu, Jennifer L. Schaefer, and Jonathan K. Whitmer
11	"Practical Approaches to Bottom-Up Coarse-Graining for Liquid Crystalline Conducting Materials" Dylan Fortney (Purdue University) and Brett Savoie
12	"Morphological Dependence of Electronic Transport in Conjugated Polyelectrolytes" David Friday (University of Illinois, Urbana-Champaign) and Nicholas Jackson
13	"Estimation of Solvation Free Energy of Lanthanides Capture with Lanmodulin Peptide for Selective Rare Earth Element Recovery" Ricardo Garcia (Clemson University), Sayani Biswas, and Rachel Getman
14	"Thermodynamics of Li+—Crown Ether Interactions in Aqueous Solvent" Ramón González-Pérez (University of Notre Dame), Stephen Adams, Alexander W. Dowling, William A. Phillip, and Jonathan K. Whitmer
15	"Mechanistic Study of the Effects of Ligand Structure on Nanoparticle Adsorption to Lipid Bilayers" Carlos A. Huang-Zhu (University of Wisconsin-Madison) and Reid C. Van Lehn
16	"Exploring the Impact of Structural Characteristics on Thermal Transport Properties of Metal-Organic Frameworks: A High-Throughput Screening Study" Meiirbek Islamov (University of Pittsburgh), Hasan Babaei, Ryther Anderson, Kutay B. Sezginel, Jeffrey R. Long, Alan J.H. McGaughey, Diego A. Gomez-Gualdron, and Christopher E. Wilmer

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Poster #	Poster Title & Authors
17	"Molecular Dynamics Simulations and Graph-Based Analyses of Nanostructure Formation in Ionic Liquids" Lisa Je (University of Wisconsin-Madison), Victor M. Zavala, and Reid C. Van Lehn
18	"Construct the Aimed Electrolyte Materials with a Fundamental Understanding Between Molecular Structures and Electrolyte Properties" Yinke Jiang (University of Notre Dame)
19	"Coarse-Grained Model for Evaporation-Induced Self-Assembly of Bottlebrush Block Copolymers" Haisu Kang (University of Illinois, Urbana-Champaign) and Charles Sing
20	"A Molecular Dynamics Study Using Weighted Ensemble Advanced Sampling of Distamycin Binding to d(GTATATAC)2 DNA in 1:1 and 2:1 Configurations" Nell Karpinski (University of Notre Dame) and Steven A. Corcelli
21	"MD Simulation Study of Choline Chloride-Alkanediol Deep Eutectic Solvents" Daniel Kim (University of Notre Dame), Yong Zhang, Edward Maginn, Rathiesh Pandian, and Clemens Burda
22	"Temperature, Flow and Chain Length Distribution Effects in Flow Induced Crystallization" Tzortzis Koulaxizis (University of Illinois, Urbana-Champaign) and Antonia Statt
23	"Cooperative Hydrogen Bonding Quantified by Infrared Spectroscopy and Applied to Phase Equilibria Modeling" Carl T. Lira (Michigan State University), William G. Killian, Andrew T. Norfleet, and Lars Peereboom
24	"Modeling the Effect of Molecular Walkers on Microtubule Substrates" Jutta Luettmer-Strathmann (University of Akron) and Matthew Murrow
25	"Enabling Quantum-Accurate Carbon Melt Line Prediction with a Machine Learned Interatomic Model" Yanjun Lyu (University of Michigan) and Rebecca K. Lindsey
26	"Distilling Graph Neural Networks to Generate Target-Optimized Coarse-Grained Representations" J. Charlie Maier (University of Illinois, Urbana-Champaign) and Nicholas E. Jackson
27	"Neural Network Force Fields for Free Energy Landscape Determination of MOF Self-Assembly" Orlando Mendible Barreto (University of Notre Dame)
28	"Active Learning for Efficient Navigation of Multi-Component Gas Adsorption Landscapes in a MOF" Krishnendu Mukherjee (University of Notre Dame), Etinosa Osaro, and Yamil J. Colón
29	"Non-Mean Field Approaches for Surface Catalysis: Analytical Description of Adsorbate-Adsorbate Interactions" Purva Paranjape (Purdue University) and Jeffrey Greeley
30	"Mechanistic and Thermodynamic Characterization of the Dynamic Membrane Topology in an Unassembled Membrane Protein" ByungUk Park (University of Wisconsin-Madison) and Reid C. Van Lehn
31	"Classical Molecular Dynamics Simulations to Design Anchoring Species to Fine-Tune Threshold for Sensing in Liquid Crystal Mixtures" Juriti Rajbangshi (University of Wisconsin-Madison), Jonathan K. Sheavly, and Reid C. Van Lehn
32	"Utilizing Molecular Dynamics Simulations and Machine Learning Methods to Predict α/β-Peptide Experimental Labels for Antifungal Drug Development" Joshua Richardson (University of Wisconsin-Madison)

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Poster #	Poster Title & Authors
33	"High-Throughput Screening of MOFs for Entangled Photons Using Type-I SPDC" Sanoj (University of Notre Dame), Simon Paiva, Rubén A. Fritz, Felipe Herrera, and Yamil J. Colón
34	"Using Genetic Algorithms to Discover Stable Fluoride Electrolytes" Vignesh Sathyaseelan (Purdue University) and Brett M. Savoie
35	"First-Principles Investigation of N_2O Formation over H-SSZ-13 Zeolite Catalyst" Raghav Saxena (University of Notre Dame), Matthew Tyler Caudle, Subramanian Prasad, Ahmad Moini, Rajamani Gounder, and William F. Schneider
36	"Thermal Transport in Functionalized Gold Interfaces using a Polarizable Force Field" Sydney A. Shavalier (University of Notre Dame) and J. Daniel Gezelter
37	"Bridging Field Theory and Ion Pairing in the Theory of Polymer Complex Coacervation" Charles E. Sing (University of Illinois, Urbana-Champaign)
38	"A Tactile Statistical Mechanics Activity for College Physics I" Daniel W. Sinkovits (University of Wisconsin-Stout)
39	"Predicting Noble Gas Solubility in Alkali Halide Molten Salts" Cole Strickling (University of Notre Dame) and Edward Maginn
40	"Polymers in Confinement: Free Energy Scaling and Finite-Size Corrections" Mark P. Taylor (Hiram College)
41	"Revisiting the Clausius-Clapeyron Equation and the Cause of Linearity" Jason E. Thompson (Miami University) and Andrew S. Paluch
42	"Towards Chemically General Activation Energy Prediction Models" Sai Mahit Vaddadi (Purdue University) and Brett M. Savoie
43	"Ion Clustering and Transport in $MgCl^{2-}$ Based Electrolytes for Rechargeable Magnesium Batteries" Vallabh Vasudevan (University of Michigan), Mingchao Wang, Nick Birbilis, and Nikhil Medhekar
44	"Monte Carlo Framework for Molecularly Doped Organic Semiconductors" Archana Verma (University of Illinois, Urbana-Champaign) and Nicholas Jackson
45	"Evaluating Suitability of ChIMES for Coarse-Grained Nanoparticle Systems" Melody Zhang (University of Michigan), Sharon C. Glotzer, and Rebecca K. Lindsey
46	"Computational Modeling of Dissolution-based Plastic Recycling: Solubility Prediction, Solvent Screening, and Process Design" Panzheng Zhou (University of Wisconsin-Madison), Jiuling Yu, Aurora del Carmen Munguía-López, Kevin L. Sánchez-Rivera, George W. Huber, Victor M. Zavala, and Reid C. Van Lehn