



Foundations of Molecular Modeling and Simulation

July 28 – August 1

Snowbird Resort ♦ Snowbird, Utah

FINAL PROGRAM

All FOMMS 2022 events will take place at the Cliff Lodge. [Map available here.](#)

Sunday July 28

1:00 p.m. – 7:00 p.m.	Conference Registration – <u>Atrium Overlook</u>
2:00 p.m. – 5:00 p.m.	Free Time and Outdoor Activities at Snowbird
6:00 p.m. – 7:20 p.m.	Welcome Reception – <u>Golden Cliff/Eagles Nest</u>
7:30 p.m. – 8:40 p.m.	Opening Session – <u>Primrose Ballroom</u> <i>Session Chair: Shikha Nangia, Syracuse University</i>
7:30 p.m. – 7:40 p.m.	Welcome Address – Jim Pfaendtner
7:40 p.m. – 8:40 p.m.	Keynote Address Mark Tuckerman, New York University “Crystal Math: A new topological and data-driven approach to the crystal structure prediction problem”
8:40 p.m. – 10:00 p.m.	Hospitality – <u>Golden Cliff/Eagles Nest</u>

Monday July 29

All Oral Presentations and Workshops are in Primrose Ballroom

- 7:00 a.m. – 8:30 a.m. **Continental Breakfast – Golden Cliff/Eagles Nest**
- 8:30 a.m. – 10:45 a.m. **ML/AI in MMS 1**
Session Chairs: Yamil Colón, Notre Dame
Rebecca Lindsey, University of Michigan
- 8:30 a.m. – 9:30 a.m. Nathan Baker, Microsoft
“Accelerating Scientific Discovery with HPC and AI”
- 9:30 a.m. – 10:30 a.m. Paulette Clancy, Johns Hopkins University
“A Chemistry-Informed Machine Learning Framework for Closed-Loop Material Discovery”
- 10:30 a.m. – 10:45 a.m. Poster Lightning Talks (*Nangia & in ‘t Veld*)
- 10:45 a.m. – 11:15 a.m. **Refreshment Break – Golden Cliff/Eagles Nest**
- 11:15 a.m. – 12:15 p.m. **Panel 1: Best Practices for Publishing in MMS**
Moderator(s): Janani Sampath
- 12:15 p.m. – 1:45 p.m. **Lunch** (on your own)
- 1:45 p.m. – 3:45 p.m. **Poster Session I – Primrose Foyer**
- 3:45 p.m. – 4:00 p.m. **Break**
- 4:00 p.m. – 5:30 p.m. **Educational Workshop: Accelerating Scientific Discoveries with Microsoft Azure Quantum Elements**
- 5:30 p.m. – 7:15 p.m. **Free time and dinner** (on your own)
- 7:15 p.m. – 9:30 p.m. **Catalysis and Reaction Engineering**
Session Chairs: Tyler Josephson, UMBC
Xin Qi, Dartmouth
- 7:15 p.m. – 8:15 p.m. Shaama Sharada, University of Southern California
“Beyond Conventional Transition State Theory in Catalysis: Applications of Matrix Completion”
- 8:15 p.m. – 9:15 p.m. Rachel Getman, The Ohio State University
“Influence of Liquid Water on the Thermodynamics, Kinetics, Mechanism, and Rate of Hydrogen Production from Methanol over Pt/Al₂O₃ Catalysts”
- 9:15 p.m. – 9:30 p.m. Open Discussion
- 9:30 p.m. – 11:00 p.m. **Hospitality – Golden Cliff/Eagles Nest**

Tuesday July 30

All Oral Presentations and Workshops are in Primrose Ballroom

- 7:00 a.m. – 8:30 a.m. **Continental Breakfast – Golden Cliff/Eagles Nest**
- 8:30 a.m. – 10:45 a.m. **Advances in Materials Simulations**
Session Chairs: Ashley Guo, Rutgers
Janani Sampath, University of Florida
- 8:30 a.m. – 9:30 a.m. Tiffany Walsh, Deakin University
“Advanced Sampling of Resilin-Like Peptides on 2D-Material Surfaces to Control Elastomer Cross-Linking”
- 9:30 a.m. – 10:30 a.m. Jianwen Jiang, National University of Singapore
“Computational Chemical Separations”
- 10:30 a.m. – 10:45 a.m. Open Discussion
- 10:45 a.m. – 11:15 a.m. **Refreshment Break – Golden Cliff/Eagles Nest**
- 11:15 a.m. – 12:15 p.m. Sukrit Mukhopadhyay, Dow
“Machine Learning Approaches for Polyurethane Foam Discovery”
- 12:15 p.m. – 7:00 p.m. **Conference Outings & Free Time** (see FOMMS.org for info)
- 7:15 p.m. – 9:30 p.m. **ML/AI in MMS 2**
Session Chairs: Sumit Sharma, Ohio University
Michael Webb, Princeton
- 7:15 p.m. – 8:15 p.m. Pratyush Tiwary, University of Maryland
“From chemical identity to Boltzmann ensembles for proteins, RNA and crystals with generative AI and statistical mechanics”
- 8:15 p.m. – 9:15 p.m. Oleksandr Isayev, Carnegie Mellon University
“AIMNet2: A Neural Network Potential to Meet Your Neutral, Charged, Organic, and Elemental-Organic Needs”
- 9:15 p.m. – 9:30 p.m. Open Discussion
- 9:30 p.m. – 11:00 p.m. **Hospitality – Golden Cliff/Eagles Nest**

Wednesday July 31

All Oral Presentations and Workshops are in Primrose Ballroom

- 7:00 a.m. – 8:30 a.m. **Continental Breakfast – Golden Cliff/Eagles Nest**
- 8:30 a.m. – 12:15 p.m. **Advances in MMS**
Session Chairs: Shuwen Yue, Cornell.
Alex Pak, Colorado School of Mines
- 8:30 a.m. – 9:30 a.m. Thijs Vlugt, TU Delft
“Accurate Free Energies of Aqueous Electrolyte Solutions from Molecular Simulations with Non-Polarizable Force Fields”
- 9:30 a.m. – 10:30 a.m. Tamar Schlick, NYU
“Biomolecular Modeling and Simulation Today: Examples From Deciphering Mechanisms of Gene and Chromosomal Folding to Viral Frameshifting”
- 10:30 a.m. – 10:45 a.m. Poster Lightning Talks (*Nangia & in 't Veld*)
- 10:45 a.m. – 11:15 a.m. **Refreshment Break – Golden Cliff/Eagles Nest**
- 11:15 a.m. – 12:15 p.m. **Panel 2: Careers in MMS**
Moderators: Sumit Sharma and Rebecca Lindsey
- 12:15 p.m. – 2:00 p.m. **Lunch** (on your own)
- 2:00 p.m. – 4:00 p.m. **Poster Session II – Primrose Foyer**
- 4:00 p.m. – 7:15 p.m. **Free time and dinner** (on your own)
- 7:15 p.m. – 9:30 p.m. **Biomolecular Simulations**
Session Chair: Kayla Sprenger, CU Boulder
Qing Shao, University of Kentucky
- 7:15 p.m. – 8:15 p.m. Birgit Strodel, University Düsseldorf
“Structural Odyssey of Amyloid- β : Navigating the Conformational Landscape in Alzheimer's Pathogenesis”
- 8:15 p.m. – 9:15 p.m. Jeetain Mittal, Texas A&M University
“Multiscale Computational Models for Uncovering the Molecular Language of Biomolecular Condensates”
- 9:15 p.m. – 9:30 p.m. Open Discussion
- 9:30 p.m. – 11:00 p.m. **Hospitality – Golden Cliff/Eagles Nest**

Thursday August 1

All Oral Presentations and Workshop 1 are in Primrose Ballroom; **Workshop 2 is in Superior A/B**

- 7:00 a.m. – 8:30 a.m. **Continental Breakfast – Golden Cliff/Eagles Nest**
- 8:30 a.m. – 10:45 a.m. **Crystallization**
Session Chairs: Rose Cersonsky, Wisconsin
TBD
- 8:30 a.m. – 9:30 a.m. Erik Santiso, NC State University
“Molecular Modeling of Nucleation of Molecular Crystals”
- 9:30 a.m. – 10:30 a.m. Julia Dshemuchadse, Cornell University
“Self-Assembly Models for Crystal Growth and Phase Transitions”
- 10:30 a.m. – 10:45 a.m. Open Discussion
- 10:45 a.m. – 11:15 a.m. **Refreshment Break – Golden Cliff/Eagles Nest**
- 11:15 a.m. – 12:15 p.m. **Panel: TBD Panel 3**
Moderators: TBD
TBD
- 12:15 p.m. – 1:30 p.m. **Lunch** (on your own)
- 1:30 p.m. – 4:00 p.m. **Concurrent Educational Workshops (see FOMMS.org for info)**
- 1:30 p.m. – 4:00 p.m. **Workshop 1 Title:** Introduction to MoSDEF
Offered by: Clare McCabe, Eric Jankowski, and Peter Cummings
- 1:30 p.m. – 4:00 p.m. **Workshop 2 Title:** Simulation Setup and Management with EMC
Offered by: Pieter J. in ’t Veld
Workshop 2 Location: Superior A&B
- 4:00 p.m. – 4:30 p.m. **Break**
- 4:30 p.m. – 6:15 p.m. **FOMMS Medal Lecture, Poster Awards & FOMMS Movie**
Session Chair: Jim Pfaendtner, NC State University
- 4:30 p.m. – 5:45 p.m. Sharon Glotzer, University of Michigan
- 5:45 p.m. – 6:00 p.m. **Screening of “FOMMS 2024: The Movie”**
FOMMS Movie Director: Chris Wilmer, University of Pittsburgh
- 6:00 p.m. – 6:15 p.m. Presentation of Poster Awards, *Jim Pfaendtner*
Presentation of Movie Awards, *Chris Wilmer*
- 6:15 p.m. – 7:00 p.m. **Reception – Golden Cliff/Eagles Nest**
- 7:00 p.m. – 9:30 p.m. **Conference Banquet – Golden Cliff/Eagles Nest**