



# Foundations of Molecular Modeling and Simulation

July 28 – August 1

Snowbird Resort ♦ Snowbird, Utah

## FINAL PROGRAM

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All FOMMS 2024 events will take place at the Cliff Lodge. [Map available here.](#)

### Sunday July 28

1:00 p.m. – 7:00 p.m.	<b>Conference Registration – <u>Atrium Overlook</u></b>
2:00 p.m. – 5:00 p.m.	<b>Free Time and Outdoor Activities at Snowbird</b>
6:00 p.m. – 7:20 p.m.	<b>Welcome Reception – <u>Golden Cliff/Eagles Nest</u></b>
7:30 p.m. – 8:40 p.m.	<b>Opening Session – <u>Primrose Ballroom</u></b> <i>Session Chair: Shikha Nangia, Syracuse University</i>
7:30 p.m. – 7:40 p.m.	<b>Welcome Address – Jim Pfaendtner</b>
7:40 p.m. – 8:40 p.m.	<b>Keynote Address</b> 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.	<b>Hospitality – <u>Golden Cliff/Eagles Nest</u></b>

## 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**  
[Sign up via this link: Accelerated DFT Workshop](#)
- 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/Al<sub>2</sub>O<sub>3</sub> 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- $\beta$ : 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**