Foundations of Molecular Modeling and Simulation

July 28 – August 1

Snowbird Resort ◆ Snowbird, Utah

~ PRELIMINARY PROGRAM ~

Sunday July 28

1:00 p.m. – 7:00 p.m.	**Conference Registration**
2:00 p.m. – 5:00 p.m.	**Educational Workshop**
	Workshops open to all Participants, no registration is required
6:15 p.m. – 7:30 p.m.	**Welcome Reception**
7:30 p.m. – 8:40 p.m.	**Opening Session** *Session Chair: Shikha Nangia, Syracuse University*
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**

Monday July 29

7:00 a.m. – 8:30 a.m.	**Continental Breakfast**
8:30 a.m. – 10:45 a.m.	**ML/AI in MMS 1** *Session Chairs: TBD1* *TBD2*
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 (SN/PiV)
10:45 a.m. – 11:15 a.m.	**Refreshment Break**
11:15 a.m. – 12:15 p.m.	**Panel 1: Topic TBD** *Moderator: TBD*
12:15 p.m. – 2:00 p.m.	**Lunch** (on your own)
2:00 p.m. – 4:00 p.m.	**Poster Session I**
4:00 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 Chair: TBD*
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**

Tuesday July 30

7:00 a.m. – 8:30 a.m.	**Continental Breakfast**
8:30 a.m. – 10:45 a.m.	**Advances in Materials Simulations** *Session Chairs: TBD* *TBD*
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**
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** (information coming soon)
7:15 p.m. – 9:30 p.m.	**ML/AI in MMS 2** *Session Chairs: TBD* *TBD*
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 Melon 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**

Wednesday July 31

7:00 a.m. – 8:30 a.m.	**Continental Breakfast**
8:30 a.m. – 12:15 p.m.	**Advances in MMS** *Session Chairs: TBD* *TBD*
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 II (SN/PiV)
10:45 a.m. – 11:15 a.m.	**Refreshment Break**
11:15 a.m. – 12:15 p.m.	**Panel 2: Topic TBD** *Moderator: TBD*
12:15 p.m. – 2:00 p.m.	**Lunch** (on your own)
2:00 p.m. – 4:00 p.m.	**Poster Session II**
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: TBD*
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**

Thursday August 1

7:00 a.m. – 8:30 a.m.	**Continental Breakfast**
8:30 a.m. – 10:45 a.m.	**Crystallization** *Session Chairs: TBD* *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**
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.	**Educational Workshops**
1:30 p.m. – 4:00 p.m.	Introduction to Azure Quantum Elements Microsoft Azure Team
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 "TBD"
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**
7:00 p.m. – 9:30 p.m.	**Conference Banquet**