
# Foundations of Molecular Modeling and Simulation

July 17 – 21, 2022

Lake Lawn Resort ◆ Delavan, Wisconsin

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*All General Sessions will be located in the Geneva Ballroom*

## Sunday July 17

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| 1:00 p.m. – 7:00 p.m. | **Conference Registration** *(Upper Pre-Function)* |
| 2:00 p.m. – 5:00 p.m. | **Educational Workshop** *(Geneva Ballroom)*<br>Joshua Anderson and Brandon Butler, University of Michigan<br>"Workshop: HOOMD-blue"<br>*Workshops open to all Participants, no registration is required* |
| 6:15 p.m. – 7:30 p.m. | **Welcome Reception** *(Great Room)* |
| 7:30 p.m. – 8:40 p.m. | **Opening Session**<br>*Session Chair: Jim Pfaendtner, University of Washington* |
| 7:30 p.m. – 7:40 p.m. | **Welcome Address – Jeff Errington** *(Geneva Ballroom)* |
| 7:40 p.m. – 8:40 p.m. | **Keynote Address**<br>Claire Adjiman, Imperial College London<br>"Engineering molecules: a view from process design" |
| 8:40 p.m. – 10:00 p.m. | **Hospitality** *(Great Room)* |

# Monday July 18

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| 7:00 a.m. – 8:30 a.m. | **Continental Breakfast** *(Geneva Ballroom Foyer)* |
| 8:30 a.m. – 10:45 a.m. | **Energy and Environment**<br>*Session Chairs: Laura de Sousa Oliveira, University of Wyoming*<br>*Wei Shi, National Energy Technology Laboratory* |
| 8:30 a.m. – 9:30 a.m. | Scott Shell, University of California Santa Barbara<br>"Computational Inverse Design of Surfaces and Water-Mediated Interactions" |
| 9:30 a.m. – 10:30 a.m. | Sapna Sarupria, University of Minnesota<br>"Pushing the Frontiers of Simulations to Study Crystallization in Complex Systems" |
| 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: Careers in computational molecular science**<br>*Moderator: Jim Pfaendtner, University of Washington* |
| 12:15 p.m. – 2:00 p.m. | **Lunch** (on your own) |
| 2:00 p.m. – 4:00 p.m. | **Poster Session I** *(Lake Lawn / Queen's Table)*<br>Molecular Modeling Fundamentals, Product Design |
| 4:00 p.m. – 7:15 p.m. | **Free time and dinner** (on your own) |
| 7:15 p.m. – 9:30 p.m. | **New Approaches in Computational Catalysis**<br>*Session Chair: David Cantu, University of Nevada* |
| 7:15 p.m. – 8:15 p.m. | Heather Kulik, Massachusetts Institute of Technology<br>"New Strategies for Catalyst Discovery from Machine Learning Exploration" |
| 8:15 p.m. – 9:15 p.m. | Randall Snurr, Northwestern University<br>"How Molecular-Level Modeling and Machine Learning Can Accelerate the Discovery of Nanoporous Materials" |
| 9:15 p.m. – 9:30 p.m. | Open Discussion |
| 9:30 p.m. – 11:00 p.m. | **Hospitality** *(Great Room)* |

# Tuesday July 19

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| 7:00 a.m. – 8:30 a.m. | **Continental Breakfast** *(Geneva Ballroom Foyer)* |
| 8:30 a.m. – 10:45 a.m. | **Product Design**<br>*Session Chairs: Qing Shao, University of Kentucky*<br>*Sabry Moustafa, Trinity University* |
| 8:30 a.m. – 9:30 a.m. | Edward Maginn, University of Notre Dame<br>"Molecular Simulation of Molten Salts" |
| 9:30 a.m. – 10:30 a.m. | Jose Tabora, Bristol-Myers Squibb<br>"On the evolution of mathematical modeling in pharmaceutical research and development" |
| 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: Supporting inclusive excellence in computational molecular science**<br>*Moderator: Sharon Glotzer, University of Michigan* |
| 12:15 p.m. – 7:00 p.m. | **Conference Outings & Free Time** (pre-registration required) |
| 7:15 p.m. – 9:30 p.m. | **Biological Systems**<br>*Session Chairs: Kayla Sprenger, University of Colorado Boulder*<br>*Eric Jankowski, Boise State University* |
| 7:15 p.m. – 8:15 p.m. | Andrew Ferguson, University of Chicago<br>"Data-Driven Protein Design and Ultra-Fast Molecular Simulators" |
| 8:15 p.m. – 9:15 p.m. | Shikha Nangia, Syracuse University<br>"Molecular Challenges to Treating Alzheimer's Disease" |
| 9:15 p.m. – 9:30 p.m. | Open Discussion |
| 9:30 p.m. – 11:00 p.m. | **Hospitality** *(Great Room)* |

## Wednesday July 20

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|---|---|
| 7:00 a.m. – 8:30 a.m. | **Continental Breakfast** *(Geneva Ballroom Foyer)* |
| 8:30 a.m. – 12:15 p.m. | **Sustainability**<br>*Session Chairs: Janani Sampath, University of Florida*<br>*Maximilian Kohns, TU Kaiserslautern* |
| 8:30 a.m. – 9:30 a.m. | Thomas Truskett, University of Texas Austin<br>"Linked Assembly of Plasmonic Colloidal Nanocrystals" |
| 9:30 a.m. – 10:30 a.m. | Styliani Consta, Western Ontario University<br>"Chemistry in Small Volumes: Bridging Electrostatic Properties Between Nanoscopic and Microscopic Droplets" |
| 10:30 a.m. – 11:00 a.m. | **Refreshment Break** |
| 11:00 a.m. – 12:00 p.m. | Erich Muller, Imperial College London<br>"Machine-Learned Equations of State for the Prediction of Thermodynamic and Transport Properties of Fluids" |
| 12:00 p.m. – 12:15 p.m. | Open Discussion |
| 12:15 p.m. – 2:00 p.m. | **Lunch** (on your own) |
| 2:00 p.m. – 4:00 p.m. | **Poster Session II** *(Lake Lawn / Queen's Table)*<br>Applications of Machine Learning, Biological Systems, Energy and Environment, New Approaches in Computational Catalysis, Sustainability |
| 4:00 p.m. – 7:15 p.m. | **Free time and dinner** (on your own) |
| 7:15 p.m. – 9:30 p.m. | **Molecular Modeling Fundamentals**<br>*Session Chair: Yamil Colon, University of Notre Dame* |
| 7:15 p.m. – 8:15 p.m. | Fernando Escobedo, Cornell University<br>"Choreographing Lattice-Symmetry Transitions in Particle Assemblies and Monolayers Through Entropic and Energetic Rhythms" |
| 8:15 p.m. – 9:15 p.m. | Michael Shirts, University of Colorado Boulder<br>"The Statistical Mechanics of Being Stingy: Using Reweighting Techniques for Fun and Profit" |
| 9:15 p.m. – 9:30 p.m. | Open Discussion |
| 9:30 p.m. – 11:00 p.m. | **Hospitality** *(Great Room)* |

## Thursday July 21

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|---|---|
| 7:00 a.m. – 8:30 a.m. | **Continental Breakfast** *(Geneva Ballroom Foyer)* |
| 8:30 a.m. – 10:45 a.m. | **Applications of Machine Learning**<br>*Session Chairs: Niki Vergadou, NCSR "Demokritos"*<br>*Amber Mace, Uppsala University* |
| 8:30 a.m. – 9:30 a.m. | Rebecca Lindsey, Lawrence Livermore<br>"Enabling an Atomistically-Resolved View into Chemistry Under Extreme Conditions" |
| 9:30 a.m. – 10:30 a.m. | Bingqing Cheng, IST Austria<br>"Predicting Materials Properties with the Help of Machine Learning" |
| 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: Best practices for publishing in computational molecular science**<br>*Moderators: Edward Maginn, University of Notre Dame*<br>*Michael Shirts, University of Colorado Boulder* |
| 12:15 p.m. – 1:00 p.m. | **Lunch** (on your own) |
| 1:00 p.m. – 4:00 p.m. | **Educational Workshops**<br>*(Geneva Ballroom, Geneva Club & Chicago)* |
| 1:00 p.m. – 2:30 p.m. | Peter Cummings, Vanderbilt University<br>"Workshop: MoSDeF" |
| 2:30 p.m. – 4:00 p.m. | Corwin Kerr and Sharon Glotzer, University of Michigan<br>"Workshop: signac" |
| 4:00 p.m. – 4:30 p.m. | **Break** |
| 4:30 p.m. – 6:15 p.m. | **FOMMS Medal Lecture, Poster Awards & FOMMS Movie**<br>*Session Chair: Jeff Errington, University at Buffalo* |
| 4:30 p.m. – 5:45 p.m. | Doros Theodorou, National Technical University of Athens<br>"Meeting the Challenge of Long Times in Entangled Macromolecules: From Atomistic to Mesoscopic Modeling and Simulations" |
| 5:45 p.m. – 6:00 p.m. | **Screening of "FOMMS 2022: The Movie"**<br>*FOMMS Movie Director: Chris Wilmer, University of Pittsburgh* |
| 6:00 p.m. – 6:15 p.m. | Presentation of Poster Awards, *Jeff Errington*<br>Presentation of Movie Awards, *Chris Wilmer* |
| 6:15 p.m. – 7:00 p.m. | **Reception** *(Queen's Table)* |
| 7:00 p.m. – 9:30 p.m. | **Conference Banquet** *(Lake Lawn)* |