

**8th International Conference on
Foundations of Molecular Modeling and Simulation
FOMMS 2022**

Molecular Modeling and the Data Revolution

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The 8th triennial FOMMS conference was held July 17-21, 2022 at Lake Lawn Resort, located in Delavan, Wisconsin. Over 130 participants took part in the meeting, with approximately 6% of these from industry, 7% from national labs, and 15% from countries outside the U.S. The conference began with a Sunday afternoon workshop focused on “HOOMD-blue,” which was led by Dr. Joshua Anderson and doctoral student Brandon Butler (University of Michigan). After the opening reception on Sunday evening, one of the leading figures in process design, Dr. Claire Adjiman of Imperial College London, gave the opening keynote lecture on “Engineering molecules: a view from process design.”



Lake Lawn Resort, Delavan, WI

On Monday, Prof. Scott Shell (University of California Santa Barbara) and Prof. Sapna Sarupria (University of Minnesota) gave presentations in a session focused on “Energy and Environment.” The first contributed poster session took place Monday afternoon, featuring 44 posters presented with lively discussion over beverages and light refreshments. The evening session was devoted to “New Approaches in Computational Catalysis,” with talks by Prof. Heather Kulik (Massachusetts Institute of Technology) and Prof. Randall Snurr (Northwestern University). An entertaining hospitality session capped the evening.

The Tuesday morning session featured talks by Prof. Edward Maginn (University of Notre Dame) and Dr. Jose Tabora (Bristol-Myers Squibb) on the topic of “Product Design.” Participants took Tuesday afternoon off to enjoy group outings, including a thrilling trip to Zip Line Canopy Adventure, a visit to Yerkes Observatory, and a boat tour of Lake Geneva. Attendees returned for an evening session focused on “Biological Systems,” with talks by Prof. Andrew Ferguson (University of Chicago) and Prof. Shikha Nangia (Syracuse University). The evening again came to a close with a hospitality session.

Wednesday began with talks on “Sustainability” by Prof. Thomas Truskett (University of Texas at Austin), Prof. Styliani Consta (University of Western Ontario), and Prof. Erich Muller (Imperial College London). The second contributed poster session was held in the afternoon, with 45 posters, refreshments, and robust discussions. We thank *Molecular Systems Design & Engineering* (MSDE) for graciously supporting the second poster session. The evening session featured presentations related to the subject “Molecular Modeling Fundamentals,” with talks by Prof. Fernando Escobedo (Cornell University) and Prof. Michael Shirts (University of Colorado Boulder). Following the evening session, hospitality again brought participants together for spirited discussions.

The final day was a busy one. The morning began with a session on “Applications of Machine Learning,” featuring talks by Dr. Rebecca Lindsey (Lawrence Livermore National Laboratory) and Prof. Bingqing Cheng (IST Austria). Two workshops were held during the afternoon period. One addressed “The Molecular Simulation Design Framework (MoSDeF),” and was led by Prof. Peter Cummings (Vanderbilt University). A second focused on “signac,” a framework that aids in the management of large and heterogeneous data spaces, which was led by Corwin Kerr (University of Michigan).

The final session featured a presentation from the FOMMS Medal recipient, Prof. Doros Theodorou of the National Technical University of Athens, who gave a talk entitled “Meeting the Challenge of Long Times in Entangled Macromolecules: From Atomistic to Mesoscopic Modeling and Simulations.” Following this presentation, the traditional FOMMS movie, produced by Prof. Christopher Wilmer (University of Pittsburgh), was screened to a vibrant applause ([watch it on YouTube](#)).



(left) Prof. Doros Theodorou delivering the FOMMS Medal lecture and (right) a screenshot from the FOMMS movie

The afternoon continued with the awarding of seven poster awards and three movie prizes. We extend our thanks to *The Journal of Physical Chemistry* and *Journal of Chemical & Engineering Data* for supporting the poster awards as well as *Physical Chemistry Chemical Physics* and *Digital Discovery* for sponsoring the movie prizes. The conference ended with a lively banquet.



Recipients of poster (left) and movie (right) awards

FOMMS 2022 introduced a new component to the traditional format. Specifically, professional development panels focused on “Careers in computational molecular science”, “Supporting inclusive excellence in computational molecular science”, and “Best practices for publishing in computational molecular science” were held during the Monday, Tuesday, and Thursday morning sessions, respectively. We are grateful to Jim Pfaendtner (University of Washington), Sharon Glotzer (University of Michigan), Edward Maginn (University of Notre Dame), and Michael Shirts (University of Colorado Boulder) for serving as moderators. The panels spurred lively discussion and afforded early career researchers an

opportunity to obtain valuable advice regarding areas important to the computational science community. Feedback related to the new component was very positive.

Overall, FOMMS 2022 was a great success. We are especially grateful to the National Science Foundation for supporting 25 Early Career Researcher Awards and the Department of Energy for supporting an additional 14 of these awards targeted at graduate students and post-doctoral scholars. The awards enabled people to attend the meeting who otherwise might not have been able to do so. Other sponsors were The Dow Chemical Company and the AIChE Computational Molecular Science and Engineering Forum (CoMSEF).



Recipients of National Science Foundation (left) and Department of Energy (right) Early Career Researcher Awards

Participants commented favorably on the location, the speakers, and the format. Participants seemed appreciative of the ample time scheduled into the program for informal meetings and interactions, the quality of the speakers and the poster sessions. Jim Pfaendtner (University of Washington) agreed that, pending approval by CACHE, he would take on the role of Chair for FOMMS 2024 with co-Chairs Shikha Nangia (Syracuse University) and Pieter in't Veld (BASF).

Thank you to all who attended and supported FOMMS 2022. A special thanks goes to Robin Craven, who helped provide organizational and logistic support for the meeting. We look forward to seeing you at FOMMS 2024!

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