

**7th International Conference on
Foundations of Molecular Modeling and Simulation
FOMMS 2018**

Innovations for Complex Systems

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Claire Adjiman, co-Chair (Imperial College London)
Jeffrey Errington, co-Chair (University at Buffalo)

The 7th triennial FOMMS conference was held July 15-20, 2018 at Lake Lawn Resort, located in Delavan, Wisconsin. Over 150 participants took part in the meeting, with approximately 10% of these from industry, 10% from national labs, and 22% from countries outside the U.S. After the opening reception on Sunday evening, one of the leading figures in the field, Dr. Sharon Glotzer of the University of Michigan, gave the opening keynote lecture on “The Entropic Bond, and Colloidal Crystallization Pathways.”

On Monday, Prof. Tina Düren (University of Bath), Dr. Peter Ravikovitch (ExxonMobil), and Prof. Yaroslava Yingling (North Carolina State University) gave presentations in a session focused on “Materials Design.” The first contributed poster session took place Monday afternoon, with 53 posters presented and lively discussion over beverages and light refreshments. The evening session was devoted to “Nano-composite and Bio-Inspired Materials,” with talks by Prof. Arthi Jayaraman (University of Delaware) and Prof. Igal Szleifer (Northwestern University). An entertaining hospitality session capped the evening.



Participants at FOMMS 2018

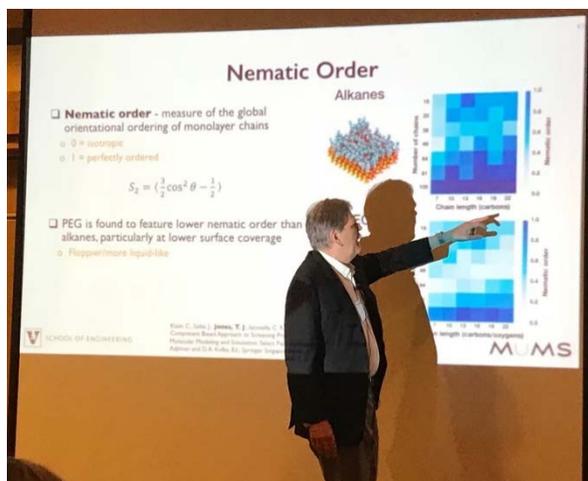
The Tuesday morning session featured talks by Prof. Alenkar Luzar (Virginia Commonwealth University), Dr. Chris Mundy (Pacific Northwest National Laboratory), and Prof. Kenji Yasuoka (Keio University) on the topic of “Water: Substrates and Ions.” Participants took Tuesday afternoon off to enjoy group 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 “Theory for Complex Systems,” with talks by Prof. Peter Monson (University of Massachusetts – Amherst) and Prof. Lourdes Vega (Khalifa University of Science and Technology). The evening again came to a close with a hospitality session.

Wednesday began with talks on “Enhanced Sampling” by Prof. Nandini Ananth (Cornell University), Prof. Heather Mayes (University of Michigan), and Prof. Jim Pfendtner (University of Washington). The second contributed poster session was held in the afternoon, with 52 posters, refreshments, and robust discussions. The evening session featured presentations related to the subject “Quantum Chemistry for Challenging Systems,” with talks by Prof. Maytal Caspary-Toroker (Technion-Israel Institute of Technology) and Prof. Angela Wilson (Michigan State University). 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 “Coarse Graining and the Mesoscale,” featuring talks by Prof. Amparo Galindo (Imperial College London), Dr. Peter in ‘t Veld (BASF), and Prof. Huai Sun (Shanghai Jiao Tong University). Three concurrent workshops were held during the afternoon period. One focused on “Software Development Best Practices in Molecular Science,” and was led by Drs. Eliseo Marin Rimoldi (MoISSI), Jessica Nash (MoISSI), and Paul Saxe (MoISSI). A second addressed “Reproducibility of Molecular Modeling and Simulation,” and was led by Drs. David Kofke (University at Buffalo), Michael Shirts (UC Boulder), Christopher Iacovella (Vanderbilt University), Peter Cummings (Vanderbilt University), Clare McCabe (Vanderbilt University), and Ilja Siepmann (University of Minnesota). The third workshop covered “Enhanced Sampling in Biomolecular Simulations,” and was delivered by Prof. Harish Vashisth (University of New Hampshire).

After a short break, the afternoon continued with the awarding of poster prizes. We extend our thanks to Swati Meherishi (Springer) and Rhea Williams (American Chemical Society) for participating in the recognition ceremony.

The conference ended with the presentation of the FOMMS Medal to Prof. Peter Cummings of Vanderbilt University, who gave a talk entitled “Computational Screening of Soft Materials Systems with Application to Nano-Lubrication Systems.” Following this, the traditional FOMMS movie, produced by Prof. Christopher Wilmer (University of Pittsburgh) and Dr. Christopher Iacovella (Vanderbilt University), was screened (watch for it soon on youtube). The conference ended with a lively banquet.



Peter Cummings delivers the FOMMS Medal lecture

Overall, FOMMS 2018 was a great success. We are especially grateful to the Department of Energy, the National Science Foundation, and our other sponsors, whose generosity enabled us to award 26 graduate student fellowships that enabled people to attend the meeting who otherwise might not have been able to do so. Other sponsors were ExxonMobil, Solvay, the AIChE Computational Molecular Science and Engineering Forum, the American Chemical Society, Springer, The Dow Chemical Company Foundation, and the University of Minnesota.



Recipients of Department of Energy (left) and National Science Foundation (right) fellowships



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. Jeff Errington (University at Buffalo) agreed that, pending approval by CACHE, he would take on the role of Chair for FOMMS 2021 with co-Chairs Sabrina Prici (University of Trieste) and Jim Pfaendtner (University of Washington).

Thank you to all who attended and supported FOMMS 2018. 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 2021!

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