

**6<sup>th</sup> International Conference on  
Foundations of Molecular Modeling and Simulation  
FOMMS 2015**

*Conference Theme: Molecular Modeling and the Materials Genome*

Randy Snurr, Chair (Northwestern University)  
Claire Adjiman, co-Chair (Imperial College London)  
David Kofke, co-Chair (University at Buffalo, SUNY)

The 6<sup>th</sup> triennial FOMMS conference was held July 12 – 16, 2015 at The Resort at the Mountain, near Mount Hood, Oregon. A record 172 participants took part in the meeting, which had a general theme related to the White House's Materials Genome Initiative: *Molecular Modeling and the Materials Genome*. Approximately 10% of the participants were from industry, 10% from national labs, and 20% from countries outside the U.S. After the opening reception on Sunday evening, one of the pioneers in the field, **Dr. Frank Stillinger** of Princeton University, gave the opening keynote lecture on “Chiral Symmetry Breaking via Computer Simulation.”



FOMMS 2015 participants in the main lecture room.

On Monday, **Dr. Andrea Browning** (Boeing), **Prof. Alan Aspuru-Guzik** (Harvard University), and **Prof. Jinghai Li** (Chinese Academy of Sciences) gave presentations in a session focused on “Future Trends in Modeling, Simulation, and Data Mining.” An afternoon workshop focused on “Data Mining, Machine Learning, and Materials Informatics” was led by **Prof. Johannes Hachmann** (University at Buffalo) and **Dr. Jonathan Moore** (Dow Chemical Company). The evening session was devoted to “Biomaterials and Biological Systems.,” with talks by **Prof. Sabrina Priel** (University of Trieste) and **Prof. Yiannis Kaznessis** (University of Minnesota).

The Tuesday morning session featured talks by **Prof. Chris Wolverton** (Northwestern University), **Prof. Kristen Fichtorn** (Penn State University), and **Dr. Jonathan Moore** (Dow Chemical Company) on the topic of “Energy and Environmental Applications.” Participants took Tuesday afternoon off to enjoy group outings, including whitewater rafting, hiking, and a microbrew tour. The first contributed poster session took place Tuesday evening, with ~58 posters presented and lively discussion over beverages and light refreshments.

Wednesday began with talks on “Complex Fluids and Materials” by **Prof. Edward Maginn** (University of Notre Dame), **Prof. Coray Colina** (Penn State University), and **Prof. Marjolein Dijkstra** (Utrecht University). The afternoon was devoted to two hands-on workshops. The first was on “Using GPUs for Bigger and Faster Simulations,” led by **Dr. Joshua Anderson** (University of Michigan), and the second was on “Solving Common Software Problems in



Poster sessions were well attended and gave participants the opportunity to present their latest work.

University) spoke in an afternoon session on “Reactive Force Fields.” After a short break, the afternoon continued with the awarding of poster prizes to **Brian Barnes** (US Army Research Laboratory), **Rebecca Lindsey** (University of Minnesota), and **Kayla Sprenger** (University of Washington).

The conference ended with the presentation of the FOMMS Medal to **Prof. Carol Hall** of North Carolina State University, who gave a talk entitled “Confessions of a Slow Learner: Lessons Learned over a Decade of Protein Aggregation Simulations.” Following this, the traditional FOMMS movie was screened (watch for it soon on youtube), and the conference ended with an outdoor banquet.

Overall, FOMMS 2015 was a great success. We are especially grateful to the **National Science Foundation** and our other sponsors, whose generosity enabled us to award 23 graduate student or postdoc fellowships that enabled people to attend the meeting who otherwise might not have been able to do so. Other sponsors were **UOP, Materials Design, Procter and Gamble, the Nanoporous Materials Genome Center, Northwestern University, the National Institute of Standards and Technology, ExxonMobil, the AIChE Computational Molecular Science and Engineering Forum, the Journal of Physical Chemistry, Scienomics, Imperial College London, the Royal Society of Chemistry, and Springer.**

At the end of the meeting, participants were given surveys to fill out so they could provide feedback on the meeting. People had many favorable comments on the location, the speakers, and the format. Participants seemed most appreciative of the ample time scheduled into the program for informal meetings and interactions, the quality of the speakers and the poster sessions. **Ilja Siepmann** (University of Minnesota) agreed that, pending approval by CACHE, he would take on the role of Chair for FOMMS 2018 with co-chairs **Claire Adjiman** (Imperial College London) and **Jeff Errington** (University at Buffalo).

Computational Labs,” led by **Patrick Fuller** (NuMat Technologies) and **Prof. Chris Wilmer** (University of Pittsburgh). The day ended with the second poster session, again with ~58 posters, refreshments, and discussions that were still going strong at 10:00 p.m.

The final day was a busy one. The morning began with a session on “Catalysis and Interfaces,” featuring talks by **Prof. Joachim Sauer** (Humboldt University, Berlin), **Prof. Daniela Kohen** (Carleton College), and **Prof. Jeffrey Errington** (University at Buffalo). After lunch, **Prof. Susan Sinnott** (University of Florida) and **Prof. Adri van Duin** (Penn State



Conference co-chairs Dave Kofke and Claire Adjiman presenting Carol Hall the FOMMS Medal.

Thank you to all who attended and supported FOMMS 2015. 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 2018!

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