

**5th International Conference on
Foundations of Molecular Modeling and Simulation
FOMMS 2012**

Foundations for Discovery and Data

Edward Maginn, Chair (University of Notre Dame)
Kristen Fichthorn, co-Chair (Pennsylvania State University)
J. Ilja Siepmann, co-Chair (University of Minnesota)

The 5th triennial FOMMS conference was held July 22-26, 2012 at the Resort at the Mountain, near Mount Hood, Oregon. A total of 129 participants and 11 guests took part in the meeting, which focused on showcasing the latest developments in the use of molecular modeling and simulation in both fundamental and applied application areas. After the opening evening reception on July 22, **Prof. Matthias Scheffler** of the Fritz-Haber Institute in Germany gave the opening keynote lecture entitled “Role of van der Waals Interactions in Physics, Chemistry and Biology”.

On Monday, **Prof. Mike Greenfield** (University of Rhode Island), **Dr. Bruce Murch** (Procter and Gamble) and **Dr. Edward Seidel** (National Science Foundation) gave presentations in a session focused on “Cyberinfrastructure and Future Trends”. A second session called “Multi-Resolution Modeling” featured talks by **Prof. Sharon Hammes-Schiffer** (Penn State) and **Jih Wei Chu** (University of California, Berkeley). The first contributed poster session also occurred on Monday, with over 50 posters being presented.



Matthias Scheffler giving the opening keynote address.

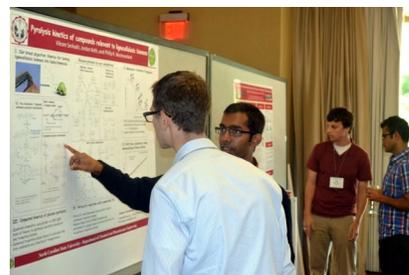
On Tuesday, **Prof. Phil Westmoreland** (North Carolina State), **Dr. Krzysztof Moorthi** (Mitsui Chemicals) and **Prof. Claire Adjiman** (Imperial College London) spoke in the “Products and Process Design” session. Participants took Tuesday afternoon off to enjoy group outings, including a waterfall tour, whitewater rafting, hiking, wine tasting and fly fishing. We went back to work Tuesday evening, with a workshop on “Software Suites and Application Interfaces”. There were short presentations made by **Dr. Wibe De Jong** (NWChem), **Prof. Matthias Scheffler** (FHI-aims software), **Dr. George Fitzgerald** (Accelrys), **Dr. Hannes Schweiger** (Materials Design), **Dr. Lalitha Subramanian** (Scienomics), **Dr. Paul Crozier** (LAMMPS) and **Dr. Shyamal Nath** (Culgi). Following this, participants engaged in a lively and spirited exchange on the merits of different packages, the future of modeling software, and best practices.



FOMMS 2012 participants in the main lecture room.

Wednesday began with talks on “Energy and Environment” by **Prof. David Sholl** (Georgia Institute of Technology), **Prof. Fumio Hirata** (Institute for Molecular Science, Japan) and **Dr. Bruce Garrett** (Pacific Northwest Laboratory). The second poster session (again with about 50 poster presentations) took place Wednesday afternoon and the day ended with evening presentations in the “Life Sciences” session by **Prof. Sarah Price** (University College – London) and **Prof. Joan Emma Shea** (University of California, Santa Barbara).

The final day of FOMMS 2012 began with a session on “Complex Fluids” in which **Prof. Mark Asta** (University of California, Berkeley), **Prof. Juan de Pablo** (University of Wisconsin) and **Prof. Pablo Debenedetti** (Princeton University) all gave outstanding talks. The afternoon was dedicated to the second conference workshop, with the theme being “Validation of Simulations”. **Prof. Ellad Tadmor** (University of Minnesota) and **Prof. Michael Shirts** (University of Virginia) challenged the participants to think of ways in which simulation methods and results can be better validated,



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



Conference chair Ed Maginn presenting Keith Gubbins the FOMMS Medal.

archived, and trusted. The conference ended with the presentation of the FOMMS Medal to **Prof. Keith Gubbins** of North Carolina State University, who gave a talk entitled “Molecular Modeling and Simulation of Confined Nano-Phases”. Following this, the traditional FOMMS movie was screened (<http://www.youtube.com/watch?v=6sWSBttSf4c>) and the conference ended with a wonderful outdoor banquet on the grounds of the resort.

Overall, FOMMS 2012 was a great success. We are especially grateful to the National Science Foundation, whose grant enabled us to award 30 graduate student / postdoc fellowships that enabled many people to attend the meeting who otherwise would not have been able to do so. Other sponsors include Accelrys, Procter and Gamble, Scienomics, Materials Design, and Culgi.

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. They also loved the venue! At the end of the meeting, Prof. Randy Snurr of Northwestern University agreed that, pending approval by CACHE, he would take on the role of Chair for FOMMS 2015.

Thank you to all who attended and supported FOMMS 2012. A special thanks goes out to Robin Craven, who helped provide organizational and logistic support for the meeting. We look forward to seeing you at FOMMS 2015!

Edward Maginn
University of Notre Dame

Kristen Fichthorn
Pennsylvania State University

J. Ilja Siepmann
University of Minnesota

1.

