Computational Molecular Science and Engineering Forum
for the combined community of engineers and scientists developing and applying molecularly based theories, modeling, and simulation
http://comsef.org/

CoMSEF Newsletter

AIChE

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In This Issue

Abrams Winner of 2015 CoMSEF Impact Award

Professor Cameron F. Abrams from Drexel University is the winner of the 2015 CoMSEF Impact Award, which cites his work "***For the development and application of enhanced sampling and free-energy methods for elucidating thermodynamics and kinetics of protein conformational changes and ligand interactions***," Cameron has been on the faculty at Drexel University since 2002 after completing a postdoctoral appointment at Max-Planck-Institute for Polymer Research, Mainz, Germany, PhD at University of California, Berkeley and his Bachelor at North Carolina State University.

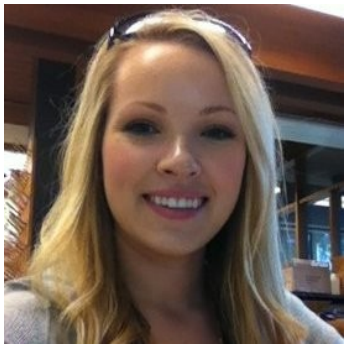
Cameron will receive his award during the CoMSEF Plenary Session at the 2015 AIChE Annual Meeting, where he will also give a talk describing his research. The CoMSEF Impact Award is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

Anderson Winner of the 2015 CoMSEF Young Investigator Award

Joshua A. Anderson from the Department of Chemical Engineering at the University of Michigan is the 2015 winner of the CoMSEF Young Investigator Award. Joshua joined the Dept. of Chemical Engineering, University of Michigan, as a Senior Research Area Specialist in 2009, after obtaining his Ph.D. from the Department of Physics and Astronomy, Iowa State University and Ames Laboratory. With this award, Joshua is cited "***For contributions to the development and dissemination of open source, GPU-enabled molecular simulation software, HOOMD-blue, which enables scientific computations with unprecedented speed***." Joshua will receive his award during the CoMSEF Plenary Session at the 2015 AIChE Annual Meeting, where he will also give a talk describing his research.

The CoMSEF Young Investigator Award for Modeling and Simulation is awarded annually to a member of CoMSEF who is within 7 years of completion of their highest degree in the year of the award.

Kayla Springer Wins CoMSEF Conference Presentation Award



Congratulations to Kayla Sprenger of the University of Washington (Advisor: Jim Pfaendtner) who won the 2015 CoMSEF Conference Presentation Award for her poster presentation "Obtaining Thermodynamic and Structural Information of Surface-Bound Biomolecules from Biased Simulations" at FOMMS 2015 (http://fomms.org).

The CoMSEF Conference Presentation Award recognizes excellence in research by undergraduate students, graduate students and/or postdoctoral researchers. The intent of the award is to reward significant contributions to research in computational molecular science and engineering by young researchers. The award consisted of an announcement for the presentation and a waived conference registration fee for the awardee.

2015 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded for the 10th consecutive year at the annual AIChE Meeting in Salt Lake City. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. Up to three awardees will be selected based on the nomination letters received from each student's advisor, their CV, and a poster presented at the CoMSEF poster session (session #247) to be held Monday evening from 6 - 8 pm in the Salt Palace CC: Exhibit Hall 1. The winners will be announced at the CoMSEF/ Area 1a annual General Meeting (Wednesday, from 6:15-7:15 pm).

Upcoming Conferences of Interest to CoMSEF Members

ARC 2015 – Advancing Research through Computing
October 29, 2015
Pittsburgh, PA
http://www.sam.pitt.edu/arc2015/

AIChE Annual Meeting
November 8-13, 2015
Salt Lake City, UT
http://www.aiche.org/conferences/aiche-annual-meeting/2015

Quantum dynamics in molecular systems: theory, modelling, simulation
November 9-13, 2015
Orsay, France
http://www.cecam.org/workshop-1177.html

Understanding function of proteins in membrane by atomistic and multiscale simulations
November 10-12, 2015
Switzerland
http://www.cecam.org/workshop-1112.html

ICMMN 2015 : XIII International Conference on Molecular Materials and Nanosystems
November 12-13, 2015
Kyoto, Japan
https://www.waset.org/conference/2015/11/kyoto/ICMMN/

SC15 Workshop: Producing High Performance and Sustainable Software for Molecular Simulation
November 20, 2015
Austin, TX
http://www.apes-soft.org/sc15

2nd Workshop on High-Throughput Molecular Dynamics 2015
November 26-27, 2015
Barcelona, Spain
http://workshop.htmd.org/

MRS Fall Meeting
November 29-December 4, 2015
Boston, MA
http://www.mrs.org/fall2015/

Big Data of Materials Science -- Critical Next Steps
November 30-December 4, 2015
Lausanne, Switzerland
http://www.cecam.org/workshop-1147.html

MolSim-2016
January 4-15, 2016
Netherlands
http://www.cecam.org/workshop-1329.html

Gordon Conference: Protein Folding Dynamics
January 10-15, 2016
Galveston, TX
https://www.grc.org/programs.aspx?id=13060

High Throughput materials discovery: Perspectives and Challenges in theory and experiment
February 3-5, 2016
University of Tel Aviv, Israel
http://www.cecam.org/workshop-1204.html

Models for Protein Dynamics
February 15-19, 2016
Lausanne, Switzerland
http://www.cecam.org/workshop-1116.html

Structure Based Drug Design Conference 2016
February 21-24, 2016
San Diego, CA
http://www.zingconferences.com/conferences/structure-based-drug-design-conference-2016/

251st ACS National Meeting: Computers in Chemistry
March 13-17, 2016
San Diego, CA
http://www.acs.org/content/acs/en/meetings/spring-2016.html

ICMCC 2016 : 18th International Conference on Mathematical and Computational Chemistry
March 14-15, 2016
Paris, France
https://www.waset.org/conference/2016/03/paris/ICMCC/

American Physical Society
March 14-18, 2016
Baltimore, MD
http://www.aps.org/meetings/march/index.cfm

12th International Conference of Computational Methods in Science and Engineering
March 17-20, 2016
Athens, Greece
http://www.iccmse.org/

MRS Spring Meeting
March 28-April 1, 2016
Phoenix, AZ
http://www.mrs.org/spring2016/

30th Molecular Modelling Workshop 2016
April 4-6, 2016
Erlangen, Germany
http://mmws2016.mgms-ds.de/

5th International Conference on Mathematical Modeling in Physical Sciences
May 23-27, 2016
Chania, Crete, Greece
http://www.icmsquare.net/

Properties and Phase Equilibria for Product and Process Design (PPEPPD)
May 22-26, 2016
Porto, Portugal
http://paginas.fe.up.pt/~ppeppd2016/PPEPPD/Home.html

Modeling and Design of Molecular Materials 2016
June 26-30, 2016
Wrocław, Poland
http://mdmm.pl/2016/

STATPHYS26
July 18-22, 2016
Lyon, France
http://statphys26.sciencesconf.org/

Gordon Conference: Polymer Physics
July 24-29, 2016
South Hadley, MA
http://www.grc.org/programs.aspx?id=11989

Hermes Summer School on Materials Modelling and Science Communication
July 27-31, 2016
Windsor Great Park, UK
http://hermessummerschool.org/

Gordon Conference: Quantum Science
July 31 - August 5, 2016
Easton, MA
http://www.grc.org/programs.aspx?id=14962

11th Asian Thermophysical Properties Conference
October 2- 6, 2016
Yokohama, Japan
http://atpc2016.org/

11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2017)
August 27-September 1, 2017
Munich, Germany
http://www.watoc2017.com/home.html

21st European Conference on Thermophysical Properties
September 3-8, 2017
Graz, Austria
http://ectp2017.tugraz.at/

Research Highlight: Energy is Hot

Michael Shirts, Department of Chemical and Biological Engineering, University of Colorado Boulder

Energy is hot (pun intended)! We are becoming more aware of issues surrounding climate change, energy scarcity, and pollutants. As computational power increases and more and more problems become amenable to molecular simulation, we can start to think more about finding new ways to apply our molecular modeling expertise to solve energy related problems.

Usually when we think about energy applications, we think in terms of quantum mechanics; electron transfer mechanisms, catalysis, redox reactions, and so forth. Indeed, when large amounts of energy are involved, bonds must be broken and electrons must be moved, which necessitates a level of theory that can model such behavior. But there are a surprising number of scientific questions that require classical simulation as well. Most energy-producing processes require some level of molecular motion, and these motions require classical modeling. Problems of carbon capture and gas separations are well-known examples, but a number of new problems are becoming more amenable to simulation approaches to understand molecular details in other energy-related problems.

One large class of problems where classical molecular simulations is required is in understanding mechanisms of biological systems involved in energy production. A series of papers from Beckham and a large number of collaborators at NREL have elucidated many of the mechanistic details of cellulase complexes, from binding, procession along the chain, catalysis, to release (1). Molecular simulations can also be useful in understanding the properties of crystalline cellulose, making it possible to more easily better break the crystals apart for enzymatic digestion. Work in the Smith lab at ORNL combined simulation with neutron scattering to examine how hydration affects cellulose properties (2), and work from Bu et al. at NREL unraveled the molecular origins of the twist in cellulose fibers (3). Ionic liquids can dissolve cellulose to make them more accessible to enzymatic degradation, but requiring a better understanding of how the ionic liquids affect enzymes themselves (4).

Another important area where classical simulation is required is understanding the transport and thermodynamics of ions in batteries. For example, in lithium-ion batteries, energy is stored in the electrostatic interactions of intercalated ions, and the ions must move back and forth during the charging and discharging. Webb and coworkers (5) used long time scale molecular dynamics to study the diffusion of lithium in PEO and newer polyester polymers. They were able to explain the ion conductivity in terms of polymer segment mobility, as current theories typically emphasize, but also in terms of comparative differences in intrachain and interchain hopping, details which are not accessible to theory alone. Molecular details can also be revealed in the differences in the intercalation rates of lithium ions on free surfaces and at grain boundaries (6).

There are certainly many more applications than those listed here; I would encourage readers to think broadly about their techniques, tools, and expertise, and think about how to apply them to solve new and different problems in energy engineering at the molecular level.

(1) G. T. Beckham, J. Ståhlberg, B. C. Knott, M. E. Himmel, M. F. Crowley, M. Sandgren, M. Sørlie, and C. M. Payne, Current Opinion in Biotechnology, 2014, 27, 96-106, http://dx.doi.org/10.1016/j.copbio.2013.12.002
(2) L. Petridis, H. M. O'Neill, M. Johnsen, B. Fan, R. Schulz, E. Mamontov, J. Maranas, P. Langan, and J. C. Smith, Biomacromolecules, 2014, 15 (11), 4152-4159, http://dx.doi.org/10.1021/bm5011849
(3) L. Bu, M. E. Himmel, and M. F. Crowley, The molecular origins of twist in cellulose I-beta, Carbohydrate Polymers, 2015, 125, 146-152, http://dx.doi.org/10.1016/j.carbpol.2015.02.023
(4) P. R. Burney, E. M. Nordwald, K. Hickman, J. L. Kaa, and Pfaendtner, J. Proteins 2015 83: 670-680. http://dx.doi.org/10.1002/prot.24757
(5) M. A. Webb, Y. Jung, D. M. Pesko, B. M. Savoie, U. Yamamoto, G. W. Coates, N. P. Balsara, Z.-G. Wang, and T. F. Miller, III, ACS Central Science 2015 1 (4), 198-205 http://dx.doi.org/10.1021/acscentsci.5b00195
(6) Christopher M. Shumeyko, Edmund B. Webb, Scripta Materialia, 2015, 102 43-46 http://dx.doi.org/10.1016/j.scriptamat.2015.02.010

Annual Meeting Sessions

CoMSEF has an exciting range of programming at the upcoming 2015 AIChE Annual Meeting in Salt Lake City. Of special note are the Computational Molecular Science and Engineering Plenary Session at 12:30 on Wednesday and the CoMSEF Poster Session on Monday from 6:00-8:00 pm. Full details on all of the CoMSEF sessions are available on the web at:

https://aiche.confex.com/aiche/2015/webprogram/21.html

Day	Time	Session
Sunday	3:30 PM	The Industrial Fluid Properties Simulation Challenge
Sunday	3:30 PM	Multiscale Modeling (co-sponsor)
Monday	8:30 AM	Industrial Applications of Computational Chemistry and Molecular Simulation I
Monday	8:30 AM	In Honor of Stanley Sandler I (co-sponsor)
Monday	12:30 PM	Industrial Applications of Computational Chemistry and Molecular Simulation II
Monday	12:30 PM	In Honor of Stanley Sandler II
Monday	12:30 PM	Tools for Product Design (co-sponsor)
Monday	3:15 PM	Software engineering in and for the molecular sciences
Monday	6:00 PM	CoMSEF Poster Session
Tuesday	8:30 AM	Recent Advances in Molecular Simulation Methods I
Tuesday	12:30 PM	Recent Advances in Molecular Simulation Methods II
Tuesday	3:15 PM	Recent Advances in Molecular Simulation Methods III
Wednesday	8:30 AM	Molecular Simulation of Protein Adsorption and Molecular Recognition Processes
Wednesday	8:30 AM	Data Mining and Machine Learning in Molecular Sciences I
Wednesday	12:30 PM	Plenary Session: Computational Molecular Science and Engineering Forum
Wednesday	3:15 PM	Data Mining and Machine Learning in Molecular Sciences II
Thursday	8:30 AM	Applications of Molecular Modeling to Study Interfacial Phenomena I
Thursday	12:30 PM	Applications of Molecular Modeling to Study Interfacial Phenomena II
Thursday	3:15 PM	Applications of Molecular Modeling to Study Interfacial Phenomena III
Friday	8:30 AM	Molecular Modeling in Solid Form Design (co-sponsor)

CoMSEF General Meeting in Salt Lake City

CoMSEF will hold its annual General Meeting on Wednesday November 11 from 6:15-7:15 pm in room 255B (Salt Palace Convention Center) during the Fall 2015 AIChE Annual Meeting. As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend. The winners of the CoMSEF Graduate Student Awards and Liaison Directors elections will be announced and programming for future AIChE meetings will be discussed.

Member Spotlights

Patricia Taboada-Serrano (Rochester Institute of Technology)

Dr. Patricia Taboada-Serrano is an Assistant Professor in the Chemical Engineering Department at the Rochester Institute of Technology. She obtained her B.Sc. degree in Chemical Engineering from University Mayor de San Andrés in La Paz, Bolivia, and a Ph.D. degree in Environmental Engineering from the Georgia Institute of Technology, in Atlanta Georgia. Patricia's research interests are in the area of colloids and surface science, specifically on the challenges encountered in the water-energy nexus. Her current research projects include the rational design of nanostructured materials and novel processes for energy storage and ion-separation applications. Research efforts involve combining molecular and phenomenological modeling with electrochemistry experiments in order to study basic electrochemical phenomena that can be manipulated in order to design ion-specific processes and electrodes. Patricia's research group develops its own algorithms and codes for the molecular simulation of electrolyte systems and electrostatic interfacial phenomena. The focus of the molecular modeling work has been on equilibrium thus far and, therefore, on Monte Carlo-based methods.

Member Spotlights

Dirk Reith (University of Mainz)

Dirk Reith studied physics and mathematics at Mainz University, Germany and at Uppsala University, Sweden. Concentrating on computational physics, he received his diploma in 1998. After that, he was a short-term guest researcher at the Australian National University, Canberra. In 1999, he went back to Mainz to join the Max-Planck Institute for Polymer Research, where he completed his Ph.D. in 2001. During this time he developed new techniques for the simulation of mesoscopic molecular simulations and applied them to various polymer systems.

From 2002-2006, Dirk Reith worked as business analyst, working in the “Global Ordering Center of Competence” at the headquarters of DaimlerChrysler AG in Stuttgart. Thereafter, he joined the Fraunhofer Institute SCAI, where he led the Computational Chemical Engineering Group until 2012. Since then, he holds a professorship for modelling and simulation at the Bonn-Rhein-Sieg University of Applied Sciences
. Scientifically, Reith’s emphasis lies on simulations techniques for soft matter and materials including their visualization.

"I really like computational molecular science and engineering because it is a very stimulating challenge to work interdisciplinary and to deal efficiently with many different length- and time-scales. To transform the insight from small scales into innovation on the large scales is a great reward whenever it succeeds."

The Ninth Industrial Fluid Properties Simulation Challenge

The Industrial Fluid Properties Simulation Challenge is an open competition organized by employees of the Army Research Lab, the National Institute of Standards and Technology (NIST), The Dow Chemical Company, 3M, and United Technologies Research Center with support from CoMSEF and the ACS. The goals of the competition are to drive improvements in the practice of molecular modeling, formalize methods for the evaluation and validation of simulation results with experimental data, and ensure relevance of simulation activities to industrial requirements. The Simulation Challenge was initiated by the workshop on "Predicting the Thermophysical Properties of Fluids by Molecular Simulation" held at NIST in 2001.

The topic of the ninth challenge will be announced at a CoMSEF-sponsored session at the AIChE annual meeting in Salt Lake City at 3:30 PM on Sunday November 8. The challenge problem will be related to the topic of predicting water/oil interfacial tension at high temperatures and pressures.

In addition to announcing the challenge topic, the 2015 IFPSC session will feature invited talks by experts in the field of molecular modeling of interfacial systems who will comment on the topic of the ninth challenge in addition to presenting some of their recent research. The confirmed speakers include: Alberto Striolo (University College London), Jeffrey Errington (University at Buffalo), Walter Chapman (Rice University), Ilja Siepmann (University of Minnesota), Ahmed Ismail (West Virginia University), and Vishnu Sresht (from the Blankschtein group at MIT).

A detailed agenda for the session will be posted at the following link prior to the conference:
https://aiche.confex.com/aiche/2015/webprogram/Session29975.html

Note that there are also three CoMSEF-sponsored sessions on “Applications of Molecular Modeling to Study Interfacial Phenomena” scheduled for Thursday at the annual meeting.

The IFPSC is always eager to receive feedback regarding the types of physical properties challenges that would be of special interest and to recruit industrial researchers to get involved in organizing the challenges. Please contact the IFPSC at admin@fluidproperties.org with any comments or questions or to let us know that you’d like to get involved!

More information about previous challenges can be found at http://fluidproperties.org/simulation-challenge

Why CoMSEF?

CoMSEF has over 230 dues-paying members, and occasionally it is worthwhile to remind everyone what CoMSEF does for our community and why your membership support is important. CoMSEF was founded in 2000, and since that time it has worked to advance molecular science and engineering in diverse ways:

* We provide a forum for communication and networking within the community. The document you're reading now is a prime example, but there is more. The annual membership meeting provides a venue for communication and interaction among members. The CoMSEF web site http://comsef.org is another useful resource for this purpose. It often hosts notices about upcoming workshops, available post-doc positions, etc.

* We provide a vehicle for communication and advocacy for molecular science and engineering in relation to other research communities. For example, our four Liaison Directors identify opportunities for co-sponsorship of sessions at the AIChE Annual Meeting, facilitate programming with other organizations, and communicate and advocate CoMSEF activities with other organizations.

* We help to recognize and promote outstanding researchers and promising graduate students by funding and administering several awards. Most recently we initiated the Young Investigator Award for Modeling and Simulation. This and our other awards help the contributions of some of our best researchers to be recognized by a broad audience, extending into the larger chemical engineering community. Your dues make these awards possible.

* We provide technical programming support, ensuring we have sessions of interest to you at the AIChE meeting. These include the many sessions we sponsor or co-sponsor, as well as the CoMSEF plenary, CoMSEF poster, and Industrial Fluid Properties Simulation Challenge sessions. We also work externally to AIChE, providing technical sponsorship to conferences in our discipline (e.g., FOMMS), where we help to ensure that these events have molecular science and engineering content of the highest quality.

Your support of CoMSEF through your membership is very important in enabling us to fulfill our mission. The financial element is valuable of course, but we also gain strength in demonstrating the size of the community we represent. So please make sure to check the box to include renewal of your CoMSEF membership whenever you pay your annual dues to AIChE. When the opportunity arises, encourage your non-member colleagues in the molecular science and engineering community to join too!