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

April 2017

In This Issue

CoMSEF Executive Committee Elections

Congratulations to Jim Pfaendtner (Vice-Chair, Washington), Joe Golab (Secretary/ Treasurer, Environmental Standards), Christina Payne (Liaison Director, Kentucky), and Andrew Ferguson (Liaison Director, Illinois) who were elected to the CoMSEF Executive Committee in the fall of 2016! Thanks to David Sholl (Past-Chair, Georgia Tech) and Erik Santiso (Liaison Director, NC State) who have completed their terms! Also, thanks to Michael Shirts (Liaison Director, Colorado) who is staying on an extra year to fill a Liaison Director vacancy.

The Vice-Chair and Secretary/Treasurer are elected every two years. A key responsibility of the Vice-Chair is to organize the programming activities of the Forum. The Vice-Chair also transitions to the Chair role after two years. Two CoMSEF Liaison Directors are elected each year and serve two-year terms. Their responsibilities include facilitating programming with other organizations by identifying opportunities for co-sponsorship, communicating and advocating CoMSEF activities with other organizations, and aiding the other officers in developing and carrying out CoMSEF activities and preparing the CoMSEF newsletter.

Call for Nominations

****Graduate Student Awards in Computational Molecular Science and Engineering****

AIChE's Computational Molecular Science and Engineering Forum (CoMSEF) graduate student awards recognize excellence in research by graduate students. The intent of the awards is to reward significant contributions to research in computational molecular science and engineering by students. The award consists of a certificate and an honorarium. Two awards are to be given annually.

Nominations should consist of a **nominating letter** from the student's research advisor and the **curriculum vitae** of the nominee. These should be sent by the advisor via e-mail in pdf format to the CoMSEF co-Chair (co-chair@comsef.org) by **October 1.** In addition, nominees must **present a poster** at the CoMSEF Poster session at the AIChE annual meeting. The nominee must be a **graduate student** at the time of the poster presentation, and **the faculty nominator must be a member of CoMSEF**. The winners will be selected by a committee composed of CoMSEF officers based on the student's CV, the nomination letter from the advisor (who must be a **member of CoMSEF**), and the quality of the poster presentation.

2016 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering were awarded at the annual AIChE Meeting in San Francisco. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. Two awardees were selected based on the nomination letters received from each student's advisor, their CV, and a poster presented at the CoMSEF poster session. The winners were announced at the CoMSEF/ Area 1a annual General Meeting.

- Gül Zerze (Lehigh University, advisor: Jeetain Mittal)
- Kayla Sprenger (University of Washington, advisor: Jim Pfaendtner)

From left: Prof. Jeff Errington (CoMSEF Chair), Gül Zerze (Lehigh), Kayla Sprenger (Washington), and Prof. Coray Colina (CoMSEF Past-Chair)

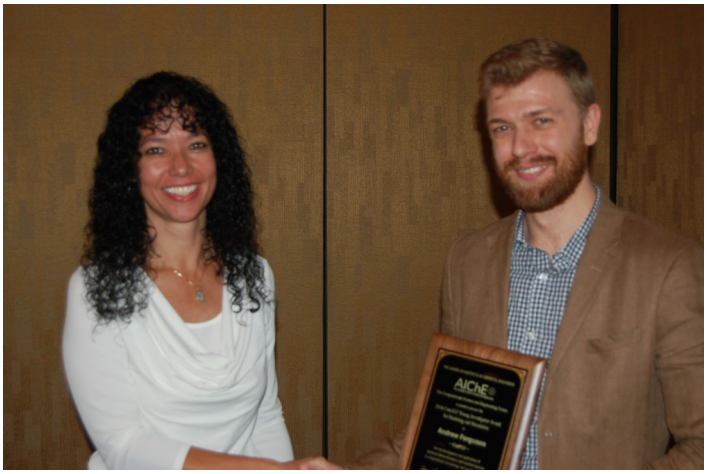
Truskett Winner of 2016 CoMSEF Impact Award

Professor Thomas Truskett from the University of Texas at Austin is the winner of the 2016 CoMSEF Impact Award which cites his "***creative and pioneering work elucidating how nanoscale interfaces impact structure, dynamics, and self-assembly of complex fluids and biomolecular systems***." Thomas has been on the faculty at Texas-Austin since 2002 following an NIH NRSA postdoc at California-San Francisco, PhD at Princeton, and his Bachelor at Texas.

Tom received his award during the CoMSEF Plenary Session at the 2016 AIChE Annual Meeting, where he also gave 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.

Ferguson Winner of the 2016 CoMSEF Young Investigator Award

Andrew Ferguson from the Materials Science and Engineering Department at the University of Illinois at Urbana-Champaign is the 2016 winner of the CoMSEF Young Investigator Award. Andy joined the faculty at Illinois in 2012 after a postdoc at MIT, Ph.D. from Princeton, and MEng from Imperial College London. With this award, Andy is cited "***For the development and application of statistical thermodynamics and machine learning to computational immunology and vaccine design***." Andy received his award during the CoMSEF Plenary Session at the 2016 AIChE Annual Meeting, where he also gave 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.

Nominations Solicited for CoMSEF Awards

The CoMSEF Impact and Young Investigator awards recognize outstanding research in computational molecular science and engineering, encompassing both methods and applications.

Impact Award in Computational Molecular Science and Engineering
Recipients must be within 15 years of completion of their highest degree.

Young Investigator Award for Modeling and Simulation
Recipients must be within 7 years of completion of their highest degree.

Nominees may hold positions in academia, industry, or a government lab and must be current members of CoMSEF. The CoMSEF Chair and Vice-Chair are ineligible for nomination while they hold these offices. Other CoMSEF officers are eligible for nomination. A single nomination package consisting of the nominee's CV, a nomination letter (typically from the nominee's department chair or supervisor) and two supporting letters of recommendation should be submitted as a single pdf file to the CoMSEF chair (chair@comsef.org). The nomination should provide a clear statement as to the impact of the nominees work on the field and an award citation of 25 words or less, beginning with the word 'For'. Self-nominations are discouraged. Call for nominations will coincide with the announcement of the AIChE Annual Meeting's call for papers. Deadline for receipt of nominations will be May 1st annually. Renomination of candidates is encouraged. It is recommended but not required that the contents of the nomination package be updated each year; while supporting letters may be re-used, the nomination form must have current dates.

More info about these awards (including lists of past-winners) is available at http://comsef.org/awards

Annual Meeting Sessions

CoMSEF has an exciting range of programming at the upcoming 2017 AIChE Annual Meeting in Minneapolis. Of special note are the Computational Molecular Science and Engineering Plenary Session, the CoMSEF Poster Session, a new session featuring Faculty Candidates in CoMSEF/Area 1a, and a Hands-on with Molecular Simulation workshop.

The call for abstracts is open through Monday, April 17, 2017

- Applications of Molecular Modeling to Study Interfacial Phenomena
- Data Mining and Machine Learning in Molecular Sciences
- Industrial Applications of Computational Chemistry and Molecular Simulation
- Molecular Simulation of Protein Adsorption and Molecular Recognition Processes
- Plenary Session: Computational Molecular Science and Engineering Forum
- Recent Advances in Molecular Simulation Methods I
- Software Engineering in and for the Molecular Sciences
- The Industrial Fluid Properties Simulation Challenge
- Honoring Keith Gubbins [Invited Talks]
- Faculty Candidates in CoMSEF / 1a [co sponsor]
- Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)
- CoMSEF Workshop: Hands-on with Molecular Simulation

Research Highlight: G.C. Sosso et al., "Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations", Chem. Rev. 116, 7078-7116 (2016)

Erik Santiso, Chemical & Biomolecular Engineering, N.C. State
Link to article: http://pubs.acs.org/doi/abs/10.1021/acs.chemrev.5b00744

Despite its apparent simplicity and technological relevance, the study of crystal nucleation in liquids remains one of the most challenging problems to study both experimentally and using molecular simulation tools. The stochastic nature of nucleation, and its uncanny ability to amplify the effect of minute molecular-level details, make it very difficult to achieve consistent experimental results even for simple systems [L. Ickes *et al.*, *Phys. Chem. Chem. Phys.* **17**, 5514 (2015)]. On the other hand, simulation studies are challenging for several reasons: (1) nucleation is a rare event with a substantial entropic contribution to the free energy barrier, requiring sophisticated enhanced sampling methods to model it; (2) available force fields have usually been parameterized to reproduce liquid-state or solution properties, and usually need to be re-fitted to model the solid state correctly; (3) methods based on equilibrium thermodynamics fail to account for transport limitations, which become crucial at high supersaturations; (4) some of the common assumptions in molecular dynamics simulations, such as periodic boundary conditions and constant number of molecules, can greatly bias the results, and (5) the most technologically relevant form of nucleation, heterogeneous nucleation, requires placing a surface in the simulation, which implies molecular-level knowledge of the relevant surfaces and, specially, their high-energy sites. In recent years, however, the development of novel experimental methods such as cryo-transmission electron microscopy, the possibility of running increasingly long molecular dynamics (MD) simulations, and the application of modern rare event methods to the study of nucleation, have given us a more detailed view of the molecular-level complexity of crystal nucleation. In a recent review, G.C. Sosso *et al.* have compiled a summary of the theoretical background of crystal nucleation, the experimental methods employed for its study, and a survey of MD-based simulation methods that have been recently used to learn about the molecular-level details of nucleation [G.C. Sosso *et al.*, *Chem. Rev.* **116**, 7078-7116 (2016)]. The paper outlines the basic ideas of classical nucleation theory (CNT), two-step nucleation theory, and modifications of CNT to account for transport effects and heterogeneous nucleation, and discusses the application of MD-based methods to the study of nucleation in several systems, including colloids, Lennard-Jonesium, water, organic crystals, metals, alloys, sodium chloride, and clathrate hydrates. The paper is a great introduction to the field for new researchers, and outlines some of the many remaining challenges left to achieve a true molecular-level understanding of nucleation.

Research Highlight: Computational Design of Robust Superhydrophobic Surfaces

Andrew L. Ferguson, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign

The wettability of a surface is characterized by its contact angle with water. Surfaces admitting contact angles below 90° are classified as hydrophilic, above 90° as hydrophobic, and above 150° as "superhydrophobic" [1]. Superhydrophobic materials have garnered interest in many sectors due to their water and ice repellency, high slip, and self-cleaning properties, and offer technological applications as coatings against fouling, corrosion, and icing, and for drag reduction and enhanced heat transfer [1,2,3]. Superhydrophobicity can be promoted by introducing surface roughness to stabilize a Cassie-Baxter (Cassie) state in which water perches upon surface asperities to ride on a layer of air trapped within the nanotextured surface [1,3]. Exposure to shocks, high pressures, surface defects, or external fields can destabilize the Cassie state and induce a transition to the fully wetting Wenzel state in which water penetrates the textured surface and destroys its superhydrophobicity [1,3]. Although the Cassie state remains thermodynamically favored after removal of the perturbation, the system can become trapped in the metastable Wenzel state due to large free energy barriers associated with the unfavorable nucleation of a vapor-liquid interface within the texture [3]. Engineering surface textures to promote the Wenzel-Cassie transition is of great interest in designing resilient superhydrophobic surfaces that can robustly recover the Cassie state and its attendant superhydrophobicity after a temporary excursion to the Wenzel state.

A recent study led by Amish Patel (CBE, U Penn) reports a pioneering simulation study that sheds light on the important role of microscopic water density fluctuations in opening up non-classical dewetting pathways and informing the rational design of resilient superhydrophobic surface textures [3]. Employing the elegant indirect umbrella sampling (INDUS) approach to drive sampling between the wet and dry states [4], the free energy barriers for the Wenzel-Cassie transition computed from simulation are ~120 k_BT compared to ~270 k_BT predicted by macroscopic classical thermodynamics [3]. Analysis of the simulations reveals this large discrepancy to arise from the opening of non-classical dewetting pathways that are not captured by the theory. These pathways are initiated by the nucleation of nanoscopic vapor bubbles at the base of the surface asperities, followed by formation of a classical vapor-liquid interface that advances up through the textured surface to restore the Cassie state. These observations suggested to Patel and co-workers rational precepts for the design of resilient superhydrophobic surfaces to circumvent the classical Wenzel-Cassie free energy barrier by opening up more favorable non-classical routes. Specifically, they propose engineering the surface texture to contain highly confined nanoscopic regions that exploit nanoscale density fluctuations to nucleate vapor bubbles that can initiate spontaneous recovery of the Cassie state. The researchers devise an ingenious and experimentally realizable design satisfying these criteria by functionalizing the surface with spherical nanoparticles embedded between the surface features. Unbiased simulations confirm the spontaneous recovery of the Cassie state from the Wenzel, and INDUS calculations confirm that this design completely destabilizes the Wenzel state to make the Wenzel-Cassie transition a fully downhill and barrierless process.

This study by Patel and co-workers employs careful molecular simulation to furnish new fundamental insight into the thermodynamics of superhydrophobicity and design resilient superhydrophobic surfaces. More broadly, it stands as a quintessential example of the power of molecular simulation in revealing new microscopic physics, and the use of these insights to inform the rational design of new engineering technologies.

1. L. Oberli, D. Caruso, C. Hall, M. Fabretto, P.J. Murphy, and D. Evans "Condensation and freezing of droplets on superhydrophobic surfaces" *Adv. Colloid Interface Sci.* 210 47–57 (2014) doi:10.1016/j.cis.2013.10.018
2. P. Zhang and F.Y. Lv "A review of the recent advances in superhydrophobic surfaces and the emerging energy-related applications" *Energy* 82 1068-1087 (2015) doi:10.1016/j.energy.2015.01.061
3. S. Prakasha, E. Xia, and A.J. Patel "Spontaneous recovery of superhydrophobicity on nanotextured surfaces" *PNAS* 113 20 5508–5513 (2016) doi:10.1073/pnas.1521753113
4. A.J. Patel, P. Varilly, D. Chandler, and S. Garde "Quantifying density fluctuations in volumes of all shapes and sizes using indirect umbrella sampling" *J. Stat. Phys.* 145 2 265-275 (2011) doi:10.1007/s10955-011-0269-9

CoMSEF Logo Contest

CoMSEF is over 15 years old but still doesn't have a logo. Let's fix that! The CoMSEF Executive Committee would like to challenge the student members of CoMSEF to create a CoMSEF logo.

Logo Requirements:

- Must be a PNG file with transparent background
- Must be square in shape with resolution of 300 dpi or higher
- Must contain the CoMSEF acronym

Prizes for the winner:

- $100
- a copy of "Introduction to Scientific and Technical Computing" edited by Frank Willmore, Eric Jankowski, and Coray Colina.

Submissions are due by September 1, 2017 by email to admin@comsef.org

The winner will be selected by vote of the membership during the 2017 CoMSEF elections.

Where are They Now?

Now that CoMSEF has been giving the graduate student awards for more than 10 years, we've started including a "where are they now?" section in the newsletter, catching up with the winners from ~ 10 years ago.

Megha Surve
2006 Grad Student Award winner (University of Texas, Austin, Advisor: Venkat Ganesan)
Poster Title: A Multiscale Approach for Phase Behavior, Structure and Macroscopic Properties of Colloidal Suspensions in Polymeric Fluids

Megha received her Ph.D. in Chemical Engineering from The University of Texas at Austin in 2006. Soon thereafter, she joined Shell Exploration and Production company as an R&D Engineer and worked on Shell's Novel Thermal Recovery processes. During her 10-year tenure with Shell, she has undertaken a broad range of technology development and reservoir engineering assignments, working with Shell's Unconventional Oil, Onshore Gas, and Deep Water Waterflood portfolio. She is currently Lead Reservoir Engineer for Shell's Perdido Deepwater Asset in the Gulf of Mexico. Megha lives in Houston with her husband and two children.

Harish Vashisth
2007 Grad Student Award winner (Drexel University, Advisor: Cameron Abrams)
Poster Title: Molecular Dynamics (MD) Study of T to R Transition in 2ZN-Insulin Hexamer
Web site: https://ceps.unh.edu/faculty/vashisth
Google Scholar: https://scholar.google.com/citations?user=haC2t6QAAAAJ

After winning the CoMSEF award in 2007, Harish finished his PhD in Chemical and Biological Engineering from Drexel University in June 2010. Thereafter, he worked until Summer 2013 as a postdoctoral research fellow in Theoretical Chemistry and Biophysics with Prof. Charles L. Brooks III at the University of Michigan, Ann Arbor. In Fall 2013, he started as a tenure-track Assistant Professor in Chemical Engineering at the University of New Hampshire, Durham, NH, where he has been directing a research group of undergraduate and graduate students with a focus on problems in computational biophysics domain. Specifically, his group studies dynamics of proteins and nucleic acid molecules and their applications in therapeutic and drug-discovery fields. He currently serves on the editorial board of journal *Frontiers in Endocrinology* (Section: Molecular and Structural Endocrinology), and is also a winner of 2016 CAREER Award from the National Science Foundation.

The 9th Industrial Fluid Properties Simulation Challenge

There is increasing interest in high temperature and pressure processing of emulsions. Typical conditions of interest are > 100 °C and > 1 bar (pressurized process to maintain liquid state). Dynamic drop tensiometer techniques are available for measuring interfacial tension (IFT) from droplet curvature at high T and P up to 200 °C and 200 bar.

The 9th Challenge aimed to test the ability of molecular modeling approaches to predict water/oil IFT at elevated T and P for three different oils:

- n-dodecane
- toluene
- 50:50 mixture of n-dodecane and toluene

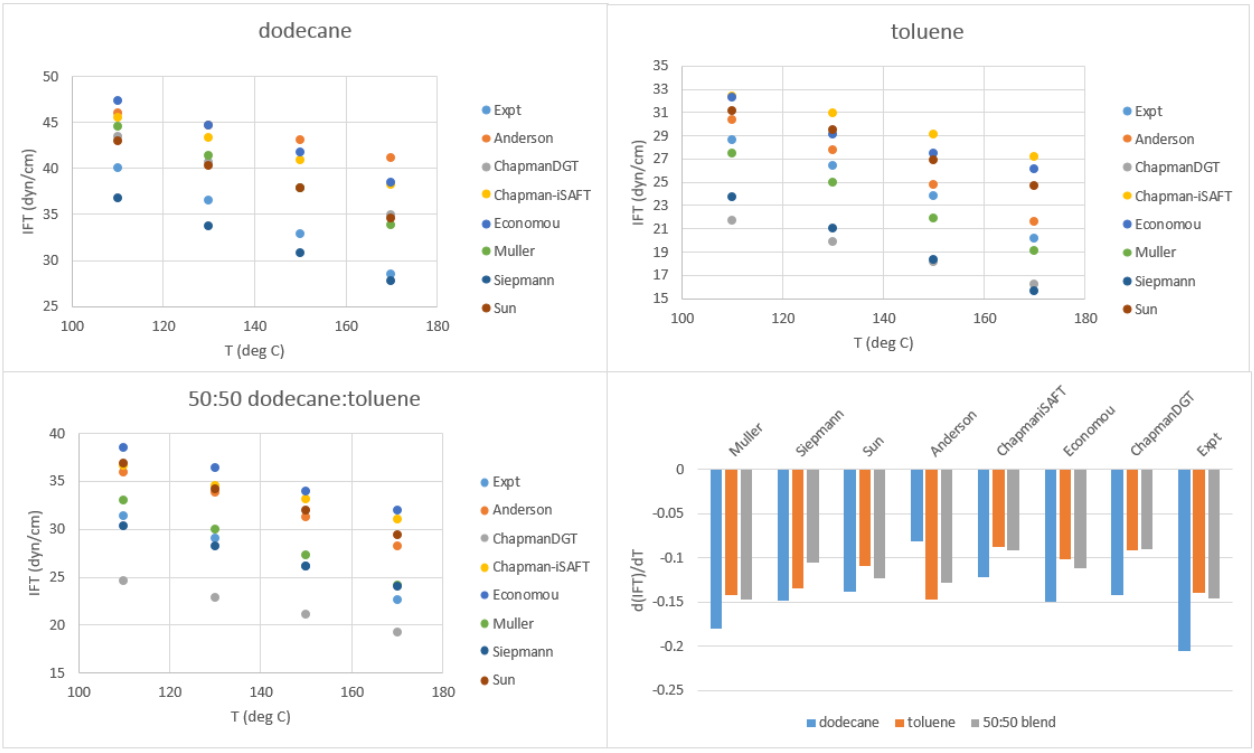
Challenge entrants were asked to make a total of 12 predictions of interfacial tension (3 oil phases and 4 temperatures). The pressure for all state points is 250 psig. The 4 temperatures are 110, 130, 150, and 170 °C.

The n-dodecane (Sigma Aldrich, ReagentPlus >99% purity) was further purified by passing through an alumina column to remove surface-active impurities. The n-dodecane had a final purity of 99.55%. The major impurities remaining consisted of isomers of undecane (0.32 %) and isomers of tridecane (0.13 %). The toluene (Fisher Scientific, HPLC grade) had a purity of 99.95%. Deionized water was used in this study.

IFT data for n-octane up to 150 °C (Flock et al., 1986), for n-decane up to 120 °C (Michaels et al., 1951), and for toluene up to 125 °C (Yu et al., 2014) are available in the literature.

Seven entries were received from: a) Andersson, Eckert, Reinisch, Klamt, and Stipp (U. Copenhagen, COSMOlogic, U. Regensburg); b) Papavasileiou,Moultos, and Economou (National Center for Scientific Research, Greece; Texas A&M at Qatar); c) Herdes, Ervik, Mejíac, and Müller (U. Bath, NTNU, U. Concepcion, Imperial College); d) Mu and Chapman (Rice); and e) Wang, Haghmoradi, and Chapman (Rice); f) Chen, Xue, Harwood, Chen, and Siepmann (Minnesota); and g) Shen and Sun (Shanghai Jiao Tong U., Jilin U.). Most of these teams were able to present their work at the IFPSC session (sponsored by CoMSEF) at the AIChE Annual Meeting in San Francisco. A summary of the predictions compared to experiment is provided in the figures below.

Based on the performance of their predictions using the coarse grained SAFT-γ Mie force field, Herdes, Ervik, Mejíac, and Müller were declared



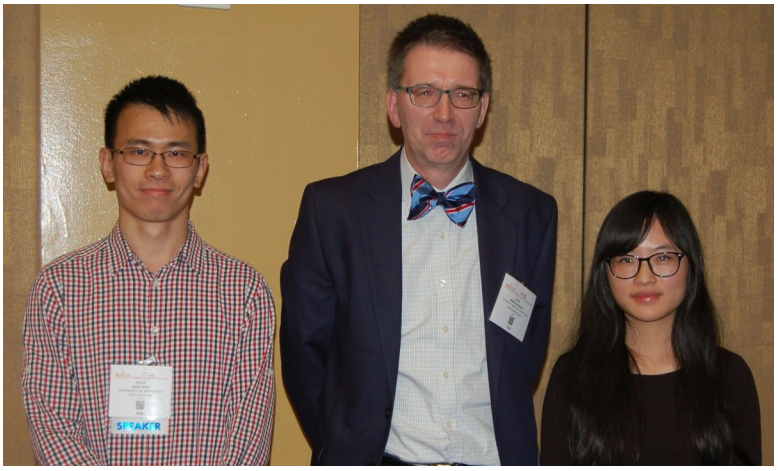
the Champions of the 9th Challenge.

Chen, Xue, Harwood, Chen, and Siepmann earned the award for second place for their predictions using Monte Carlo Methods.

Journal articles summarizing the challenge, benchmark data, and the challenge entries will be published in Fluid Phase Equilibria later this year.

More details about the challenge are available at http://fluidproperties.org/.

Planning for the 10th Challenge is currently underway. The tentative plan is to announce a challenge this summer to conclude in October to test predictions of the effect of a small-molecule additive at low concentration on water/oil IFT at high T and P.



Hands-On with Molecular Simulation

Network with your CoMSEF colleagues while learning to use and develop open-source software to assist your research! This dedicated forum to work with scientific package developers provides a unique opportunity to get hands-on experience with software for managing simulation data, advanced sampling techniques, and fundamental tools that cross-cut scientific computation. Hands-on with Molecular Simulation will be held in in conjunction with the AIChE Annual Meeting at the Minneapolis Hilton and Convention Center on October 29th 2017. Mark your calendar!

This all-day workshop targets students looking to expand their computational toolbox and would be beneficial for postdocs and faculty eager to do the same. Each ~1-hour session of the workshop is designed to be an on-ramp for open-source software projects (e.g., Cassandra, HDF5), led by expert developers and teachers familiar with inclusive programming pedagogy.

Workshop registration fees are $75, and can be added to your cart when registering for the AIChE Annual meeting. Seating will be limited. Graduate students can apply for registration discounts and travel support by emailing ericjankowski@boisestate.edu with their CV and brief statement of how the workshop would facilitate their research. Support for Hands-On with Molecular Simulation is provided by The HDF Group and CoMSEF.

Contact the chairs: Eric Jankowski (ericjankowski@boisestate.edu) Coray Colina (colina@chem.ufl.edu) Frank Willmore (frank.willmore@hdfgroup.org)

The HDF Group

Upcoming Conferences of Interest to CoMSEF Members

Hands-on Workshop on Computational Biophysics
Urbana, IL
April 17-21, 2017
http://www.ks.uiuc.edu/Training/Workshop/Urbana2017a/

Exploiting finite-size effects in simulations
CECAM-FR-MOSER
April 18-21, 2017
https://www.cecam.org/workshop-1416.html

13th International Conference of Computational Methods in Sciences and Engineering
Thessaloniki, Greece
April 21-25, 2017
http://www.iccmse.org/

SAFT 2017
Heidelberg, Germany
May 11-13, 2017
http://www.saft2017.com/

European Symposium on Applied Thermodynamics
Bucharest, Romania
May 18-21, 2017
https://www.esat2017.ro/

14th Joint European Thermodynamics Conference
Budapest, Hungary
May 21-25, 2017
http://jetc2017.hu/

Theoretical Chemistry for Extended Systems: systematically improvable electronic structure methods
CECAM-FR-GSO
May 22-24, 2017
https://www.cecam.org/workshop-1442.html

State of the art in mesoscale and multiscale modeling
CECAM-IRL
May 29-31, 2017
https://www.cecam.org/workshop-1487.html

Hands-on Workshop on Computational Biophysics
Pittsburgh, PA
May 30-June 2, 2017
http://www.ks.uiuc.edu/Training/Workshop/Pittsburgh2017/

The future of biomembrane simulations: hidden pitfalls and future challenges
CECAM-FR-RA
June 6-9, 2017
https://www.cecam.org/workshop-1470.html

Gordon Conference: Polymers
South Hadley, MA
June 11-16, 2017
https://www.grc.org/programs.aspx?id=11997

Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics
CECAM-IT-SIDE
June 14-30, 2017
https://www.cecam.org/workshop-1385.html

Ulam Computer Simulations Workshop: Challenges & Opportunities in Molecular Simulations
Lviv, Ukraine
June 21-24, 2017
http://icmp.lviv.ua/ucsw2017/index.html

Extended Software Development Workshop in meso and multiscale methods
CECAM-ES
July 3-14, 2017
https://www.cecam.org/workshop-1488.html

Frontiers of Quantum and Mesoscopic Thermodynamics
Prague, Czech Republic
July 9-15, 2017
https://fqmt.fzu.cz/17/

17th European Seminar on Computational Methods in Quantum Chemistry
Shropshire, England
July 11-14, 2017
http://www.ccpbiosim.ac.uk/events/eventdetail/89/-/17th-european-seminar-on-computational-methods-in-quantum-chemistry

Building links between experiments and computer simulations of crystallisation
CECAM-HQ-EPFL, Lausanne, Switzerland
July 12-14, 2017
https://www.cecam.org/workshop-1379.html

Gordon Conference: Computer Aided Drug Design
West Dover, VT
July 16-21, 2017
http://www.grc.org/programs.aspx?id=12081

ESDW7: Quantum MD
CECAM-IRL
July 17-28, 2017
https://www.cecam.org/workshop-1407.html

Liquids 2017 - 10th Liquid Matter Conference
Ljubljana, Slovenia
July 17-21, 2017
http://liquids2017.ijs.si/

Designing forcefields in an age of cheap computing
CECAM-UK-HARTREE
July 26-28, 2017
https://www.cecam.org/workshop-1374.html

Gordon Conference: Liquids, Chemistry & Physics of
Holderness, NH
August 6-11, 2017
https://www.grc.org/programs.aspx?id=11490

Gordon Conference: Soft Condensed Matter Physics
New London, NH
August 13-18, 2017
https://www.grc.org/programs.aspx?id=11149

ESDW6: Classical MD
CECAM-NL
August 14-25, 2017
https://www.cecam.org/workshop-1406.html

ACS Fall Meeting
Washington, DC
August 20-24, 2017
https://www.acs.org/content/acs/en/meetings/fall-2017.html

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

Addressing metastability in interfacial phenomena across multiple time and length scales
CECAM-HQ-EPFL, Lausanne, Switzerland
August 29, 2017 - September 1, 2017
https://www.cecam.org/workshop-1398.html

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

Thermodynamics 2017
Edinburgh, UK
September 5-8, 2017
http://www.thermodynamics2017.efconference.co.uk/

Big-Data driven Materials Science
CECAM-HQ-EPFL, Lausanne, Switzerland
September 11-13, 2017
https://www.cecam.org/workshop-1437.html

5th Annual CCP-BioSim Conference: Frontiers of Biomolecular Simulation
Southampton, UK
September 13-15, 2017
http://www.ccpbiosim.ac.uk/ccpbiosim2017

ESDW8: Meso- and Multiscale Modelling
CECAM-DE-MMS
September 18-29, 2017
https://www.cecam.org/workshop-1408.html

27th International Workshop on Computational Mechanics of Materials
Leuven, Belgium
September 20-22, 2017
http://iwcmm27.be/index.php

AIChE Annual Meeting
Minneapolis, MN
October 29 - November 3, 2017
https://www.aiche.org/conferences/aiche-annual-meeting/2017

Quantum-chemistry methods for materials science
CECAM-HQ-EPFL, Lausanne, Switzerland
November 8-10, 2017
https://www.cecam.org/workshop-1387.html

Supercomputing 2017
Denver, CO
November 12-17, 2017
http://sc17.supercomputing.org/

MRS Fall Meeting
November 26-December 1, 2017
Boston, Massachusetts
http://www.mrs.org/fall-2017-exhibit

Physics and Chemistry at Fluid/Fluid Interfaces
CECAM-AT
December 11-13, 2017
https://www.cecam.org/workshop-1459.html

MolSim-2018
CECAM-NL
January 8-19, 2018
https://www.cecam.org/workshop-1494.html

Anharmonicity and thermal properties of solids
CECAM-FR-MOSER
January 10-12, 2018
https://www.cecam.org/workshop-1397.html

2018 AIChE Spring Meeting
April 22-26, 2018
Orlando, FL
https://www.aiche.org/conferences/aiche-spring-meeting-and-global-congress-on-process-safety/2018

Tenth Liblice Conference on the Statistical Mechanics of Liquids
Cesky Krumlov, Czech Republic
June 17-22, 2018
http://liblice.icpf.cas.cz/2018/2018.php

Symposium of Thermophysical Properties
Boulder, CO
June 24-29, 2018
http://fomms.org

FOMMS 2018
Delavan, WI (Lake Lawn Resort)
July 15-20, 2018
http://fomms.org

XXVII International Materials Research Congress
Cancun, Mexico
August 19-24, 2018
https://www.mrs.org/imrc-2018

AIChE Annual Meeting
Pittsburgh, PA
October 28 - November 2, 2018
https://www.aiche.org/conferences/aiche-annual-meeting/2018

PPEPPD 2019
The 15th International Conference on Properties & Phase Equilibria for Product and Process Design
Vancouver, Canada
May 12-16, 2019

Why CoMSEF?

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. Our 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!