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

July 2016

Ortiz and Getman elected as CoMSEF Liaison Directors

Congratulations to Vanessa Ortiz (Columbia) and Rachel Getman (Clemson) who were elected as CoMSEF Liaison Directors in the fall of 2015. Thanks to Karl Johnson and Lev Gelb who have completed their terms!

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.

In This Issue

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.

2015 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering were 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. 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.

The 2015 student winners were:

- Abhiram Muralidhar (University of Minnesota, advisor: Kevin Dorfman)
- Christopher Paolucci (University of Notre Dame, advisor: William Schneider)

From left: Prof. Coray Colina (CoMSEF Chair) , Adhiram Muralidhar (U. Minnesota), Christopher Paolucci (U. Notre Dame), and Prof. Jeff Errington (CoMSEF Vice Chair)

Annual Meeting Sessions

CoMSEF has an exciting range of programming at the upcoming 2016 AIChE Annual Meeting in San Francisco. 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/2016/webprogram/Symposium4231.html

Day	Time	Session
Sun	1:00 PM	Poster Session: Meet the Faculty Candidate - CoMSEF (co-sponsor)
Sun	3:30 PM	The Industrial Fluid Properties Simulation Challenge
Mon	8:00 AM	Applications of Molecular Modeling to Study Interfacial Phenomena I
Mon	12:30 PM	Data Mining and Machine Learning in Molecular Sciences I
Mon	12:30 PM	In Honor of Carol Hall I (co-sponsor)
Mon	3:15 PM	In Honor of Carol Hall II
Mon	3:15 PM	Altsep - Sustainable Separation Processes Roadmap Review (co-sponsor)
Mon	6:00 PM	CoMSEF Poster Session
Tues	8:30 AM	Molecular Simulation of Protein Adsorption and Molecular Recognition Processes
Tues	12:30 PM	Software Engineering in and for the Molecular Sciences
Tues	3:15 PM	Recent Advances in Molecular Simulation Methods I
Wed	8:30 AM	Industrial Applications of Computational Chemistry and Molecular Simulation
Wed	12:30 PM	Plenary Session: Computational Molecular Science and Engineering Forum
Wed	3:15 PM	Making Molecular Simulation a Mainstream Chemical Engineering Tool: Reproducibility, Robustness, and Usability
Thu	8:30 AM	Molecular Modeling of Industrially Relevant Interfacial Phenomena
Thu	12:30 PM	Data-Driven Screening of Chemical and Materials Space
Thu	3:15 PM	Recent Advances in Molecular Simulation Methods II
Fri	8:30 AM	Applications of Molecular Modeling to Study Interfacial Phenomena II
Fri	12:30 PM	Data Mining and Machine Learning in Molecular Sciences II

Research Highlight: Guiding Materials Design with Machine Learning

Rachel B. Getman, Department of Chemical and Biomolecular Engineering, Clemson University

In the computationally driven approach to materials design, materials are assessed based on the values of their "descriptors," which are electronic-, atomic-, or microscopic-level quantities that predict macroscopic performance.[1] This is done by calculating a relevant thermodynamic or kinetic quantity, which has been functionalized in terms of the descriptors.

Catalysts are examples of materials that have been developed through computationally-driven design. For example, a catalyst comprised of Fe and Ni was developed for the methanation reaction ($CO + 3H_2 \rightarrow CH_4 + H_2O$).[2] In this case, the descriptor was determined to be the reaction energy for catalytic CO dissociation ($CO + 2^* \rightarrow C^* + O^*$, where the *'s are active sites on the catalyst). This energy, which was calculated on many potential catalyst materials using density functional theory (DFT), was linearly correlated to the activation energy for the reaction, allowing a relatively quick assessment of the catalytic rate (since it is the only quantity that needed to be calculated on a potential catalyst).

One drawback to this approach is that it can lack accuracy, for example, if a single descriptor and/or a linearized function lack certain information. Metal alloy catalysts are a class of materials that require more descriptors and more detailed functional relationships.

Recently, Hongliang Xin's group (Virginia Tech) made a breakthrough on this front.[3-4] Endeavoring to improve the ability of DFT to identify metal alloy catalysts for CO2 electroreduction, they considered five descriptors (all of them are electronic properties that can be obtained in just one DFT calculation) and used machine learning to functionalize their relationship to catalytic performance. In the machine learning approach, a detailed, non-linear function of the five descriptors was generated, with the aim of minimizing the root mean square error (RMSE) between the results predicted by the model and those calculated explicitly from DFT. Xin and co-workers considered ~250 randomly chosen bimetallic catalysts for this study. The RMSE of 0.33 eV using a single descriptor and a linear model was decreased to 0.13 eV using five descriptors and a model built through machine learning.

Since they explore detailed functional forms, machine learning approaches should significantly widen the compositional and

configurational spaces that can be reliably screened when designing catalysts and other materials. They will likely expand the already great predictive capabilities of molecular simulations in guiding the development of novel materials in a variety of research fields.

1. Curtarolo, S.; Hart, G. L. W.; Nardelli, M. B.; Mingo, N.; Sanvito, S.; Levy, O., The High-Throughput Highway to Computational Materials Design. Nature Materials 2013, 12, 191-201.
2. Norskov, J. K.; Bligaard, T.; Rossmeisl, J.; Christensen, C. H., Toward the Computational Design of Solid Catalysts. Nature Chemistry 2009, 1, 37-46.
3. Ma, X.; Li, Z.; Achenie, L. E. K.; Xin, H., Machine-Learning-Augmented Chemisorption Model for CO_2 Electroreduction Catalyst Screening. The Journal of Physical Chemistry Letters 2015, 6, 3528-3533.
4. Li, Z.; Ma, X.; Xin, H., Feature Engineering of Machine-Learning Chemisorption Models for Catalyst Design. Catalysis Today 2016, in press. DOI: 10.1016/j.cattod.2016.04.013.

Research Highlight: Coarse-graining with the Relative Entropy

Erik Santiso, Chemical & Biomolecular Engineering, N.C. State

The development of coarse-grained (CG) models to study complex systems continues to be a very active area of research in our field. Both bottom-up and top-down coarse-graining methods have been proposed and tested in recent years, increasing our understanding of the advantages and limitations of CG approaches. In a recent contribution to Advances in Chemical Physics, M. Scott Shell presents a detailed overview of the Relative Entropy (S_{rel}) approach for building CG models [M.S. Shell, Advances in Chemical Physics, A. Dinner and S.A. Rice (Eds.), in press]. The relative entropy is a measure of the loss of information in mapping a system onto a model with fewer degrees of freedom, as defined by a mapping function. By minimizing S_{rel}, the method produces the best possible CG model corresponding to a predetermined mapping. This approach has the advantage of providing a quantitative measure of the quality of a CG model (the relative entropy itself), which can be readily used to compare different models. This paper covers the theoretical framework behind the S_{rel} approach, its relationship to other coarse-graining methods, and algorithms for the numerical minimization of the relative entropy, as well as applications including CG models for water and peptides, and ways to construct optimal mapping functions such as maximizing the per-site information content. The paper is an excellent introduction not only to the S_{rel} method, but also to the theoretical basis behind bottom-up coarse-graining approaches.

A pre-print of the review is available here: http://www.engr.ucsb.edu/~shell/papers/2016_preprint_ACP_review_Shell.pdf

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From CoMSEF Sessions to a Teaching Text

In 2014, Frank Willmore, Eric Jankowski, and Coray Colina organized a group of sessions on software engineering for the molecular sciences at the annual meeting of the American Institute of Chemical Engineers. Soon thereafter, they received an inquiry about producing a book on the topic. Understanding the need for such training material from conversations with the molecular modeling community, they agreed to create a new volume to help scientists and engineers create, test, and share computer code. This practical book addresses the tools and techniques necessary for scientific computing but which are not yet commonplace in university curricula.

Several of the book's contributed chapters were written by CoMSEF members. Each chapter focuses on a specific tool or skill, providing the content needed to cover fundamentals of software engineering practice. The book includes sample code that readers can obtain with 'git', allowing them to experiment and modify according to their needs. It provides an on-ramp for new students to begin coding with Python, OpenMP, MPI, and Bash. Tutorials for important tools provide introductions to CMake, git, HDF5, and debuggers. Building on top of coding fundamentals, the book discusses key higher-level topics including parallel programming, testing and verification, and software licensing and distribution.

You can find more information at:

https://www.crcpress.com/Introduction-to-Scientific-and-Technical-Computing/Willmore-Jankowski-Colina/p/book/9781498745048

Promo Code for 20 % discount: EMS16

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 aims 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

Timeline

- Monday, October 24, 2016 - challenge entries are due
- Sunday, November 13, 2016 - entrants present their work and champions are announced at the AIChE Annual Meeting

Challenge entrants are asked to make a total of 12 predictions of interfacial tension as summarized below (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.

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

Grad Student Award Winners: Where Are They Now?

2016 marks the 10-year anniversary of the Graduate Student Awards in Computational Molecular Science and Engineering that recognize excellence in research by graduate students. To celebrate this anniversary, we are beginning a new feature for the newsletter that provides a brief “where are they now?” highlight for a grad student award winner from 10 years ago.

This time we are highlighting Erik Santiso who won an award in 2006 for work done in collaboration with his advisor Prof. Keith Gubbins. After finishing his Ph.D., Erik worked as a postdoctoral associate at MIT with Bernhardt Trout for 4 years, and then spent one and a half years working at the Centre for Process Systems Engineering at Imperial College London. Since 2012, Erik has been working as an Assistant Professor in the Department of Chemical and Biomolecular Engineering at NC State University. His research is now focused on developing methods for automatic discovery of new materials.

The Road to Sustainable Separations Starts at the Molecular Level

Robert Giraud, Engineering Technology, The Chemours Company

Fluid separations are central to all chemical manufacturing, but conventional separation processes (e.g., distillation) account for 10% of global energy use [1]. That's why the American Chemical Society Green Chemistry Institute® Chemical Manufacturers Roundtable and the AIChE have teamed up to develop a NIST-funded innovation roadmap for sustainable separations. The overall goal of the roadmap is to enable significant further cuts in the energy intensity of the chemicals sector by accelerating industrial application of sustainable alternative separation (AltSep) processes.

Instead of continuing to rely on separation processes based solely on relative volatility, we are taking an integrated approach to identify and prioritize the research, development, and demonstration projects needed to solve technical challenges starting at the molecular level. Hence, roadmapping is guided by the concept that a molecular property-based system can efficiently guide selection, process simulation, and rational design of AltSep processes. Development of such a system would enable exploration of the range of intrinsic molecular properties (e.g., molecular shape, dipole moment, molecular volume) best utilized for more effective and energy-efficient separations.

Broad participation is critical to success in developing an effective roadmap. Among the industrial, federal, nonprofit, and research institutions involved, several CoMSEF members have contributed to roadmap development. Collaboration is also at the core of the robust ecosystem across the chemical enterprise needed to foster industrial implementation of sustainable alternative separation processes. Learn more and get involved by visiting http://altsep.org, or better yet come to the AltSep roadmap session in San Francisco on Monday afternoon November 14 at the 2016 AIChE Annual Meeting.

[1] D. Sholl and R. Lively, "Seven chemical separations to change the world," *Nature* **532** (2016) 435-437. http://www.nature.com/news/seven-chemical-separations-to-change-the-world-1.19799

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!

Upcoming Conferences of Interest to CoMSEF Members

Multiscale Simulation: from Materials through to Industrial Usage
CECAM-IRL
September 5-7, 2016
https://www.cecam.org/workshop-1255.html

Free Energy Calculation and Molecular Kinetics Workshop
King's College London
September 13-15, 2016
http://www.ccpbiosim.ac.uk/freeenergyandkinetics

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

3rd Workshop on High-Throughput Molecular Dynamics (HTMD) 2016
Barcelona
November 10-11, 2016
http://workshop.htmd.org/

AIChE Annual Meeting
San Francisco
November 13-18, 2016
http://www.aiche.org/conferences/aiche-annual-meeting/2016

MRS Fall Meeting
November 27th-Dec 2, 2016
Boston, Massachusetts
http://www.mrs.org

"Hands-on" Workshop on Computational Biophysics
December 12-16, 2016
San Francisco
http://www.ks.uiuc.edu/Training/Workshop/SanFrancisco2016/

Challenges across Large-Scale Biomolecular and Polymer Simulations
CECAM-AT
February 21-24, 2017
https://www.cecam.org/workshop-1295.html

2017 AIChE Spring Meeting
March 26-30, 2017
San Antonio, TX
http://www.aiche.org/conferences/aiche-spring-meeting-and-global-congress-on-process-safety/2017

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

Gordon Conference: Soft Condensed Matter Physics
New London, NH
August 13-18, 2017
https://www.grc.org/sites.aspx?id=1

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/