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/

Newsletter

AIChE®
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In This Issue

CoMSEF Executive Committee Elections

Congratulations to Heather Kulik (Liaison Director, MIT) and Jindal Shah (Liaison Director, Oklahoma State who were elected to the CoMSEF Executive Committee in the fall of 2019! Thanks to Heather Mayes (Liaison Director, Michigan) who completed her term and to Andrew Ferguson (Liaison Director, Chicago) who served an extra year to fill the gap created by Sapna Sarupria's election to Vice Chair!

Two Liaison Directors are elected each year and serve two-year terms. Their responsibilities include identifying opportunities for co-sponsorship and communicating and advocating CoMSEF activities with other organizations. Liaison Directors also aid 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.

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.** The student should have already submitted an abstract to the CoMSEF poster session at the AIChE annual meeting.

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.

2019 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering were awarded at the annual AIChE Meeting in Pittsburgh. 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.

- **Yasemin Basdogan** (Pittsburgh, Advisor: John Keith)
- **Kaihang Shi** (North Carolina St., Advisors: Erik Santiso and Keith Gubbins)

From left: Prof. Jim Pfaendtner (CoMSEF Chair), Kaihang Shi (North Carolina St.), Yasemin Basdogan (Pittsburgh), and Prof. Sapna Sarupria (CoMSEF Vice-Chair)

* Opinions presented in the newsletter are the authors' and do not necessarily represent the view of the CoMSEF organization.

Research Highlight: Machine Learning Meets Ionic Liquids

Jindal Shah, Chemical Engineering, Oklahoma State University

Ionic liquids are an intriguing class of solvents comprising entirely of molecular ions. The often bulky and asymmetric nature of these ions frustrates crystal packing rendering many to exist as liquids under ambient conditions. The research in the past two decades has focused on exploiting the beneficial properties of ionic liquids such as negligible vapor pressures, nonflammability, polar and nonpolar solvation, and electrochemical stability. The continued excitement for ionic liquids to serve as solvents in a number of applications stems primarily because they are 'designer solvents': altering the cation, anion, or substituents on the ions is expected to yield approximately a billion ionic liquids.[1]

Although promising, such a vast chemical space is almost impossible to navigate experimentally or even computationally with atomistic simulation methods. However, the magnitude of the apparent problem also presents an opportunity to apply machine learning-based approaches for their design. Some progress has occurred in the past few years in this direction, primarily for the purpose of developing artificial neural network (ANN) models for correlating properties with chemical structures.[2-6] As the predictive capability of models improves, it is conceivable that new ionic liquids with desired properties will emerge. A recent article by Beckner and Pfaendtner is a step in this direction.[7]

In this article, the authors elegantly combines ANN model formulation with what they term as 'adaptive learning and design' (AL&D) to develop novel ionic liquids *in silico*. As the first step, the authors develop an ANN model from the data collected on density and constant pressure heat capacity from the NIST ILThermo Database.[8] Genetic algorithm (GA) is then applied to generate ionic liquids from the pool of cations and anions that form ionic liquids exceeding the target density and constant pressure heat capacity values. After examining these ionic liquids for proper valences and potential for exceeding the thresholds of properties of interest, quantum mechanical calculations are performed for assessing the chemical stability. If found suitable, molecular dynamics simulations are carried out which serve as a screen for the liquid-like behavior and generators for properties. New ionic liquid cations and anions are then appended to the original dataset for the next round of ANN development and guide the GA search. The process of search, verify, and model is repeated four times, which results in ANN model refinement and a systematic reduction in the error between atomistic simulation predictions and ANN models. The results from the article also show that new ionic liquids that exceed the targets for density and constant pressure heat capacity can be developed. For the future research direction, it is suggested that a continuous chemical representation of ionic liquids using generative adversarial networks, variational autoencoders, or reinforcement learning should be explored to solve harder design problems.

Outcomes from the research article are very encouraging: (a) They indicate that the error in the prediction of properties from ANN can be systematically improved by data generated using a combination of quantum mechanics calculations and molecular dynamics simulations; (b) it is possible to carry out a dual-objective search in the chemical space of ionic liquids, which is exciting as many ionic liquids exhibit competing properties (e.g., toxicity vs. biodegradability); (c) the primary hurdle for ionic liquid synthesis and subsequent measurements of property of interest can be overcome by acquiring data for *in silico*-designed ionic liquids *in silico*!

As ionic liquids find industrial applications,[9,10] the time is ripe for such machine learning approaches to bear on the design and development of next generation of ionic liquids. Such a confluence of the two fields has the potential to strengthen existing collaborations and catalyze new ones between the molecular modeling community and experimentalists as the computing power continues to increase and high-throughput synthesis and property measurements enter the ionic liquid world.

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A broader view: The need for better standards for etiquette and safety at conferences

Poornima Padmanabhan, Rochester Institute of Technology
https://www.rit.edu/engineering/compmatnucleus

Most members of the CoMSEF community look forward to the AIChE Annual meeting for several fantastic reasons: to be exposed to new content at scientific sessions, to forge new and strengthen existing connections at networking events and receptions, and to celebrate their own/group's hard work. It should be a rewarding and exciting experience for everyone. However, there is a fraction of us who undergo unpleasant experiences at the conference which overall impacts the culture, climate and has negative consequences to the academic community.[1] For some of us, the conference is not an inclusive space, we face unwanted and inappropriate social behavior, and we fear for our safety.[2] Traveling to a different geographical location carries its own risk; occasionally having resulted in extreme outcomes.[3] We each have several roles to play and must reflect on how our behaviors influence the atmosphere at AIChE – interrogating ourselves on our roles as participants, group leaders, and as a collective COMSEF community. NSF provides a list of promising practices[4] that includes having a code of conduct in place, setting standards for professional behavior, taking steps to prevent harassment, establishing effective means of reporting, and reporting findings to NSF.

It is good practice to familiarize yourself with the AIChE code of conduct[5] and sexual harassment policy,[6] and periodically review it before every conference you attend. Without a doubt, representatives from universities must adhere to Title IX policies that impact all university-related business including travel to conferences. Participants from industry who are not subject to Title IX will still have sexual harassment policies to adhere to. NSF funding requires appropriate handling and reporting of sexual harassment.[7] At conferences, please note that university receptions *are specified* in the AIChE booklet and are covered by the same code of conduct, regardless of the amount of alcohol being served. The level of intoxication at receptions is no excuse to lower standards of behavior or assume that one can behave in an inappropriate manner. Please remember that your intention behind the action may be friendly, but what really matters is the perception of your action and not your intention. Here are some questions one can think about to ensure that everybody has a safe and rewarding experience at the individual level, as a group leader, and as a community:

As an individual who is a conference participant, have you thought about how your behavior at conferences differs from your behavior at work? Are you aware of your alcohol intake and the threshold after which there is a change in behavior? Before you attend social events, do you know how many drinks you will limit yourself to? Have you thought about what you would do if you were a bystander and observed unprofessional behavior? While traveling to off-site events or receptions, will you be walking alone or taking a cab or have you and a buddy agreed to walk over together? If you are in an unsafe situation, do you have a plan for whom to contact if you need help getting out of the situation, and subsequently to offer you emotional support? Please remember that while traveling, we are often exposed to an unfamiliar environment and having a plan can help react to and manage an unpleasant situation.

As the leader of a research group, how would you manage discussions about etiquette and safety? Small actions can have an impact in promoting the climate at conferences. You likely hold group meetings where everybody prepares for the conference presentations. Do you have a group discussion about expectations regarding professional behavior? Do you know whether your group members have developed their plans for staying safe and/or support each other? Have you considered reminding everyone in your group that only the best behavior is expected *at all times* toward all other conference participants? Can you ensure that group members undergo Title IX training a few days or weeks prior to attending a conference? Have you reminded everyone that Title IX policy applies to conference travel as well? What is your policy regarding where group members stay at conferences? While balancing budgetary considerations, do you consider environment of the stay? How do you know that participants feel safe – whether it is the conference hotel, Airbnb, shared accommodation? Please think about having one-on-one conversations about what your group members feel about safety without bringing up the financial considerations of their choice of accommodation.

The CoMSEF community can work together and take actions to improve the conference experience. As a community, the AIChE code of conduct can be tweeted and shared by members during the conference. We can educate ourselves on effective bystander intervention techniques.[8] Policies for promoting safety are more effective when there is an effective means of reporting. One can report any incident to an AIChE staff member or to their own university's Title IX office, but staff members are seldom present during all events, which does not encourage effective reporting. We may wish to hold AIChE accountable in providing clear guidelines for reporting incidents and publishing statistics, following policies at other conferences.[9]

To conclude, the broader view segment of the CoMSEF newsletter has fostered a lot of communication and discussions on important topics. By being more reflective and prepared as individuals, opening up honest discussions and offering timely reminders within your research group, and holding each other and the broader AIChE community more accountable, I hope that the next conference season is a much more enriching experience for all participants.

References and acknowledgement

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3. Title/content warning: assault, violence, death. Alison Abbott, “Biologist found dead during Crete conference”, https://www.nature.com/articles/d41586-019-02132-3
4. “Promising practices” https://www.nsf.gov/od/odi/promising_practices/index.jsp
5. Code of Conduct, AIChE volunteer and meeting attendee conduct guidelines https://www.aiche.org/resources/conferences/code-conduct
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10. The author would like to acknowledge input and resources provided by Stacey DeRooy (Title IX office, RIT), Dr. Obioma Uche (Assistant Professor, RIT), and Dr. Patricia Taboada-Serrano (Associate Professor, RIT)

The purpose of this newsletter feature is to provide members a forum to call attention to or report on matters of general importance to our community. We aim to provide a means to highlight aspects of our profession wherein action is perhaps needed. We invite members of our community to contribute to future CoMSEF newsletters. Please write to the CoMSEF Chair at chair@comsef.org to express your interest in providing an article. We welcome contributions that focus on a broad range of topics. We simply ask that you make some connection to our profession. Examples include topics related to human, political, social, and/or environmental elements that impact our field and the people who work in it.

CoMSEF Sessions at the 2020 Annual Meeting

Session CoMSEF	Chair(s) and co-chair(s)
Plenary Session: Computational Molecular Science and Engineering Forum	Sapna Sarupria & Jim Pfaendtner
Applications of Molecular Modeling to Study Interfacial Phenomena	Harold Hatch and Vance Jaeger & Mona Minkara
Recent Advances in Molecular Simulation Methods	Harish Vashisth and Diego Gomez
Practical Applications of Computational Chemistry and Molecular Simulation	Westmoreland and team
Software Engineering in and for the Molecular Sciences	Eric Jankowski and Utkarsh Kapoor
The Industrial Fluid Properties Simulation Challenge	Jonathan Moore and Daniel Siderius
Nanoscale Behavior of Sustainable Processes	Jindal Shah and Joshua Howe
Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)	Scott Shell
Data-Driven Design and Modeling of Biomaterials	Yi He and Qing Shao
Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	Sapna Sarupria and Yamil Colon
Applications of Data Science in Molecular Sciences	Andrew Ferguson, Andrew White, and Johannes Hachmann

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.

Diwakar Shukla
2010 Grad Student Award winner (Massachusetts Institute of Technology, Advisor: Bernhardt Trout)
Poster Title: Additives for Inhibiting Protein Aggregation: Mechanistic Understanding, Rational Design, and Performance Prediction

Diwakar Shukla won the CoMSEF graduate student award in 2010. He graduated with a PhD in Chemical Engineering from MIT in 2011 and joined the laboratory of Prof. Vijay S. Pande at Stanford University as a NIH distinguished postdoctoral fellow. His postdoctoral research pioneered large-scale distributed computing simulations of receptors and enzymes that play a key role in cancer. He collaborated with Google to develop the “exacycle” platform for distributed computing applications, achievements that were featured on the cover of Nature Chemistry. In 2015, Diwakar joined the Department of Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign as a Blue Waters Assistant Professor. At Illinois, his research has moved into a new interdisciplinary area at the interface of computational molecular sciences and plant biology. In particular, his research program focuses on understanding how plants sense and cope with stressful environmental conditions. These proteins play a key role in enhancing plant productivity under biotic (e.g. pests) and abiotic (e.g. drought, nutrient-deficiency) stress conditions. Both represent a key societal challenge due to the continued rapid rise in global population and the threat of the undesirable effects of climate change. Diwakar has received several young investigator awards including the NSF Early Career Award, Outstanding Junior Faculty in Computational Chemistry from American Chemical Society, Sloan Research Fellowship, New Innovator in Food & Agriculture Research and the CoMSEF young investigator award from AIChE. He has also been recognized as an excellent mentor and teacher. He has received the undergraduate advising award and Excellence in Teaching award from the University of Illinois.

Upcoming Conferences of Interest to CoMSEF Members

34th Molecular Modelling Workshop 2020
Erlangen, GER
Mar 8-10, 2021
https://mmws2020.mgms-ds.de/

21st Symposium on Thermophysical Properties
Boulder, CO, USA
June 20-25, 2021
https://thermosymposium.org/

31st European Symposium on Applied Thermodynamics
Paris, France
July 4-7, 2021
http://www.esat2020.com/

Molecular Simulation 2020
Erice, Sicily
July 5-9, 2021
https://bricabrac.fisica.unimo.it/ErcMlk80/

ICCT-2020: the 26TH International Conference on Chemical Thermodynamics
London, UK
July 18-22, 2021
https://www.icct2020.org/

11th Liquid Matter Conference
Prague, Czech Republic
July 18-23, 2021
http://www.lmc2020.cz/

13th European Congress of Chemical Engineering and 6th European Congress of Applied Biotechnology
Berlin, GER
Sep 19-23, 2021
http://ecce-ecab2021.eu/

PPEPPD
Tarragona, Spain
May 22-26, 2022
https://ppeppd.org/

FOMMS
Delavan, WI
July 2022 (postponed from 2021)
http://fomms.org

STATPHYS28
Yokohama, Japan
July 25-29, 2022

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!