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
May 2019

## In This Issue



## CoMSEF Executive Committee Elections

Congratulations to Sapna Sarupria (Vice Chair, Clemson), Rebecca Lindsey (Liaison Director, Lawrence Livermore), and Neeraj Rai (Liaison Director, Mississippi St.) who were elected to the CoMSEF Executive Committee in the fall of 2018! Thanks to Christy Payne (Liaison Director, NSF) who completed her term and to Andrew Ferguson (Liaison Director, Chicago) who has agreed to serve an extra year to fill the gap created by Sapna'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. A Vice Chair is elected once every two years and leads the programming activities before serving an additional two-year term as Chair.

## 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.

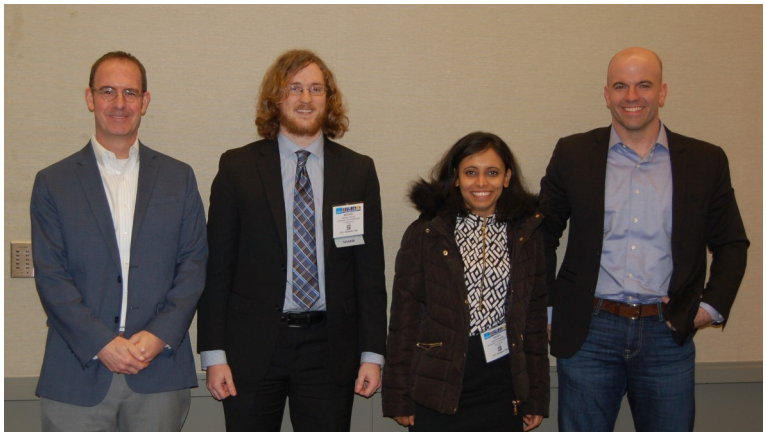
Nominations should consist of a **nominating letter** from the student's research advisor and the **curriculum vitae** of the nominee. These should be sent by the advisor via e-mail in pdf format to the CoMSEF co-Chair (co-chair@comsef.org) by **October 1.**

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.

## 2018 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.

- **Arushi Prakash** (PNNL/Washington, Advisors: Chris Mundy and Jim Pfaendtner)
- **Michael Taylor** (Pittsburgh, Advisor: Giannis Mpourmpakis)



From left: Prof. Jeff Errington (CoMSEF Chair), Michael Taylor (Pittsburgh), Arushi Prakash (PNNL/Washington), and Prof. Jim Pfaendtner (CoMSEF Vice-Chair)

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

## Research Highlight: Plasma catalysis: overcoming barriers for thermodynamically difficult chemical transformations

Neeraj Rai, Chemical Engineering, Mississippi St.

Plasma catalysis refers to coupling non-thermal plasma to catalytic materials to achieve the desired chemical transformation (1). Combining plasma with catalytic materials can potentially lead to improvements that are often not possible by either plasma or traditional catalytic systems alone (1). It is believed that Devins and Burton were the first to apply plasma catalysis (in 1954) for the synthesis of hydrazine from ammonia using platinum coated discharge tubes (1,2). In the recent past, plasma catalysis is fast gaining popularity to drive thermodynamically difficult reactions at relatively low temperatures and pressures (3). The chemical transformations that can benefit from plasma catalysis are reactions such as ammonia formation from $N_2$, volatile organic compound decomposition, and conversion of $CO_2$ and methane into value-added chemicals and fuels (3).

Atmospheric pressure, non-thermal plasma is traditionally generated using dielectric barrier discharges (DBD), corona, packed-bed, and surface discharge reactors and is driven by pulsed power sources (1). The high-energy electrons generated in this process collide with the atomic and molecular species present in the gas phase and lead to ionic species and molecular fragments that may be in the electronic and vibrationally excited states or in the ground state while the atoms and molecules remain cold (near ambient temperature) (1). Although plasma makes the gas mixture very reactive, there is little control over which part of the molecule or which molecules get activated. Thus, the coupling of plasma with the catalyst can potentially address the selectivity issue.

Over the last two decades, there has been a significant effort (primarily experimental) devoted to the design of plasma catalytic systems and to rationalize plasma catalysis. However, due to the complex parameter and chemical space it is difficult to establish one to one cause and effect (4,5). This presents a unique opportunity for the modeling community to contribute to plasma catalysis and provide mechanistic insights into these processes. Given the length and timescales involved, there is a need to explore physical phenomena at different scales using appropriate computational tools. For example, the first principles approach can be used to understand the excited state manifolds of discharge gases and reactants while mesoscale simulations are necessary to understand the plasma modification of the catalyst surface morphology (4). In recent work, Mehta et al. developed a microkinetic model using DFT energetics and information on nitrogen vibrational states derived from optical emission spectroscopy experiments (6). This model shows that the optimal catalysts and active sites in plasma catalysis tend to be different than thermal catalysis. For the catalysts considered in the work (Co, Ni, Ru, Pt, Fe), the authors find that experimentally observed activity trends are in good agreement with the computational predictions (6). More importantly, plasma catalysis can approach rates for ammonia synthesis that are observed at a much higher temperature and pressure in the Haber -Bosch process (6). This work shows how well-designed experiments and modeling can provide useful information to develop optimal catalysts. Readers are encouraged to read recent reviews on this subject to learn how modeling can contribute to this exciting sub-discipline of heterogeneous catalysis (4,7).

1. J. C. Whitehead *J. Phys. D: Appl. Phys*. **2019**, *49* 243001
2. J. C. Devins, M. Burton J*. Am. Chem. Soc*. **1954**, *76*, 2618–26
3. A. Bogaerts *Catalysts* **2019**, *9*, 196
4. E. C. Neyts, A. Bogaerts J*. Phys. D: Appl. Phys*. **2014**, *47*, 224010/1–18
5. A. Bogaerts, E. C. Neyts, A. Rousseau *J. Phys. D: Appl. Phys*. **2014**, *47*, 220301
6. P. Mehta, P. Barboun, F. A. Herrera, J. Kim, P. Rumbach, D. B. Go, J. C. Hicks, W. F. Schneider *Nature Catal.*, **2018**, *1*, 269-275
7. P. Mehta, P. Barboun, D. B. Go, J. C. Hicks, W. F. Schneider *ACS Energy Lett*. **2019**, *4*, 1115−1133

---

## 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.

**Gloria A. E. Oxford**
2009 Grad Student Award winner (Northwestern, Advisors: Randall Snurr and Linda Broadbelt)
Poster Title: Modeling Electronic and Steric Effects On An Immobilized (salen)Mn Catalyst

After winning the CoMSEF graduate student award in 2009, Gloria Oxford finished her PhD work in the area of computational catalysis under Professors Linda Broadbelt and Randall Snurr at Northwestern University in June 2010. She was awarded an NRC postdoctoral fellowship to study chromium adsorption on manganese oxide surfaces with advisor Anne Chaka at the National Institute of Standards and Technology in Gaithersburg, MD. After her fellowship ended in July 2012, Dr. Oxford completed a six-month contract to simulate terahertz spectra of drugs at NIST. During her time at NIST, she began to work as a contract editor for American Journal Experts in May 2012 and continues in this work today.

## A broader view: Creating an inclusive academic and work environment through our classroom and research lab interactions

**Arthi Jayaraman, University of Delaware**

I am excited to author this edition of "A broader view" column that started in the Summer 2018 COMSEF newsletter with the first article by Prof. Scott Shell.[1] In that article, Prof. Shell highlighted many institutional and department efforts that help create an inclusive academic environment for everyone, regardless of gender identity, age, race, ethnicity, nationality, religion, sexual orientation, etc. Having experienced the university-life as a female faculty member and prior to that as an international graduate student, I have personally valued every single constructive step that institutions, departments and individuals have taken and continue to take towards creating a truly equal-opportunity and inclusive academic environment. In the CoMSEF Fall 2018 newsletter, Prof. Jim Pfaentdner highlighted one such practice adopted by many institutions in the context of faculty search and hiring, to ensure unbiased hiring and improvement in diversity in the university faculty.[2] In contrast to these previous articles that have beautifully highlighted larger-scale institutional, college, and departmental efforts, in this article I choose to focus on some easy steps that we as *individuals* can take in the university to foster inclusion in the classrooms and labs.

The classroom is the perfect platform with a captive audience where we as instructors get to shape the way young students think and influence the way they behave. We as instructors can directly influence the classroom climate by being cognizant of the diversity in the classroom (by getting to know our students) and by interacting with fellow instructor(s) and students in a respectful manner. How we communicate course objectives and conduct in-class activities can also create a more inclusive environment. For example, when we explain course policies, we should describe these policies in terms of how students will benefit from them, rather than how they will be penalized if they do not comply; this has been shown to improve student success especially among under-represented minority student groups.[3] We can embed in-class activities like "*think-pair-share*" where students first tackle the given problem on their own (*think*), then compare their thoughts with a partner (*pair*) and derive a collaborative solution to share with the class (*share*). Besides creating a *cooperative learning* environment for *all*, such activities are valued by first-generation college students and non-native English speakers who will have questions addressed early and often so as to not fall behind in class.

There are other more *subtle*, *yet impactful,* changes we can make to our classroom etiquette. For example, in our quest to make abstract, difficult technical concepts easier to grasp, we often give every-day, practical examples relevant to the concepts so that students can better relate to the concept through that example. We should be vigilant in the types of examples and the language we use when giving those examples. For example, statements like "any engineer… *he* will …" suggest engineers are male in general; this should be avoided. Unless it is a religious studies course, instructors should not choose examples pertaining to experiences related to a specific religion. Similarly, images used in the class lectures should not foster stereotypes, biases towards/against certain population of students, and instead, should be chosen intentionally to convey lack of bias and prejudice. Older Engineering textbooks may have photos of women doing household activities to describe a home product or photos of men in hard hats at a plant, but these can easily be avoided in lectures. In general, we can choose to use inclusive images and language during lectures, and in homework and exam problems.[4] By correcting *unintentional* bias (e.g., by *gently* correcting a student who may use a gender-specific pronoun, say) we are able to bring awareness to these issues in the classroom. By bringing awareness to such issues we are already taking a large step towards a solution. Teaching assistants, who themselves may be unaware, should be explicitly trained by faculty members so that the above inclusive practices are also prevalent in the office hours, review sessions and other spaces where students interact with their instructional team. If these practices are followed throughout the curriculum, it will become common practice and the 'norm' for the students. This then translates to inclusive practices in the workplaces that these students join after graduation.

Faculty members as principal investigators (PIs) can also show their group members that their research lab space is an inclusive and equal environment for all. The above examples of our efforts in classroom are also relevant in the research lab. In fact, it is encouraging that the science and engineering fields are becoming increasingly aware of gender identity biases in research labs (faculty towards students and students toward faculty) but there is still a long way to go.[5] As thesis advisors, we can encourage equality and inclusivity in our groups by being clear and explicit in our research expectations (e.g., number of papers required to graduate, specific guidelines for what constitutes authorship, etc.) as studies have shown that outlining clear expectations resulted in higher degrees of achievement for women and underrepresented minority graduate students.[6] As PIs of our labs, we can ensure that group service responsibilities (e.g., lab safety, lab clean up, purchasing, systems administration, etc.) are assigned in an unbiased manner among all group members.

Another current issue relevant to inclusion is the increasing incidents of hate crimes or intentional bias/prejudice against under-represented minority researchers, international students/researchers or those who are first generation US citizens.[7] It is vital that we take all appropriate steps to create a *safe,* inclusive environment for all, regardless of race, nationality, sexual orientation, etc. Of course, creating a physically safe environment in the labs for *all* researchers is our responsibility. If we witness any incidents in our lab that may indicate a bias towards/against one group of people we should take *appropriate* actions (e.g., talking to the student/postdoc or reporting to superiors or reporting to police depending on intensity of the incident). As PIs we should be aware of our university support groups that can help our group members who are victims of such incidents.

We should also be aware of challenges unique to one group of students that could impact their lives during their graduate education. For example, for international students with the increasing uncertainty in visa renewal times [8], we should try to

make appropriate accommodations in research expectations, if at all possible. Faculty members in the role of graduate program directors should remain well-informed of the current challenges that uniquely impact international graduate students (e.g., certain nationality students may have visa renewal dates coinciding with qualifying exams, students may be unable to attend TA-training sessions prior to their first semester as new graduate students, etc.) and accommodate as needed. Lastly, as PIs or directors, we can organize group recreational activities or team-building group exercises which allow researchers to learn about one another's culture, practices, backgrounds, strengths and weaknesses making it a positive bonding experience for all, students, postdocs and PIs.

The examples I give above are *individual* efforts that can contribute to a large scale positive change in our community. I cannot help but compare this to molecular modeling and simulations where many molecular (microscopic) changes to the system can lead to macroscopic changes in structure and dynamics of the system. Similarly, each and every small step that we as individuals take consciously to improve diversity and inclusion will collectively bring about macroscopic changes towards a more inclusive, diverse academic environment and workforce.

REFERENCES


1. M. Scott Shell, A Broader View, http://comsef.org/sites/comsef.org/files/2018-07-CoMSEF.pdf
2. Jim Pfaendtner, A Broader View: Getting the Most Out of Faculty Hiring Season,
3. http://comsef.org/sites/comsef.org/files/2018-10-CoMSEF.pdf
4. C. Staats, et al., Race and Ethnicity: Views from Inside the Unconscious Mind. 2017, http://kirwaninstitute.osu.edu/wp-content/uploads/2017/11/2017-SOTS-final-draft-02.pdf
5. Tips and Tools for using Gender Inclusive Language,
6. https://writingcenter.unc.edu/tips-and-tools/gender-inclusive-language/
7. Teaching Beyond the Gender Binary in the University Classroom,
8. https://cft.vanderbilt.edu/guides-sub-pages/teaching-beyond-the-gender-binary-in-the-university-classroom/
9. Aleksandra Cislak et al., Bias against research on gender bias. Scientometrics vol. 115,1 (2018): 189-200. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5838121/;
10. WIRED article on gender bias in science https://www.wired.com/story/why-men-dont-believe-the-data-on-gender-bias-in-science/
11. Rodolfo Mendoza-Denton et al., Go beyond bias training, https://www.nature.com/articles/d41586-018-05144-7
12. Hate Crimes on Campus https://www.insidehighered.com/news/2019/02/25/hate-incidents-still-rise-college-campuses; https://www.chronicle.com/article/Hate-Crimes-on-Campuses-Are/245093
13. Jeffrey Mervis, More restrictive U.S. policy on Chinese graduate student visas raises alarm https://www.sciencemag.org/news/2018/06/more-restrictive-us-policy-chinese-graduate-student-visas-raises-alarm
14. I am thankful to Prof. Joshua Enszer, my colleague and co-instructor for multiple undergraduate courses at University of Delaware, for teaching me about many valuable active and cooperative learning in-class activities. I am also thankful to the students and postdocs in my group who gave me valuable feedback on this article.


*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 2019 Annual Meeting

| | |
|---|---|
| Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks) | Jeffrey R. Errington<br>Jim Pfaendtner |
| Industrial Applications of Computational Chemistry and Molecular Simulation (Invited talks) | Phillip R. Westmoreland<br>Joseph Golab<br>Martin Sanborn<br>Jonathan Moore |
| Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF) | Sapna Sarupria<br>Andrew Ferguson |
| Applications of Molecular Modeling to Study Interfacial Phenomena I and II | Harold W. Hatch<br>Vance Jaeger |
| Making Molecular Simulation a Mainstream Chemical Engineering Tool | Michael R. Shirts<br>Heather Mayes |
| Practical Applications of Computational Chemistry and Molecular Simulation I and II | Phillip R. Westmoreland<br>Joseph Golab<br>Martin Sanborn<br>Jonathan Moore |
| Recent Advances in Molecular Simulation Methods I and II | Harish Vashisth<br>Andrew White<br>Jindal Shah |
| Software Engineering in and for the Molecular Sciences | Eric Jankowski |
| Recent advances in interfacial and Nano particle simulation methods | Harold Hatch |
| The Industrial Fluid Properties Simulation Challenge | Jonathan Moore<br>Daniel W. Siderius |

Co-sponsored sessions:

18A01 CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education
T3001 Applications of Data Science in Catalysis and Reaction Engineering
T3002 Applications of Data Science in Molecular Sciences
26007 Computational Solid State Pharmaceutics
T3003 Data-Driven Design and Modeling of Biomaterials
01A06 Faculty Candidates in CoMSEF/Area 1a
01A07 Gas Hydrates Science and Engineering
01A08 Inverse Design of Soft Materials
01A01 Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)
01A09 Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction
01A00 New Frontiers of Molecular Thermodynamics (Invited Talks)
T3000 Plenary: Topical Conference in Molecular and Materials Data Science
T3005 Reaction Path Analysis Using Advanced Data Science Methods
01A13 Thermodynamics Needs of the Chemical Industry
08A03 Atomistic and Molecular Modeling and Simulation of Polymers
20031 New Methods and Developments in Computational Catalysis
20019 Confluence of Experimental and Theoretical Methods
08A10 Multiscale and Coarse-Grained Modeling of Polymers
20012 Catalysis for Biomass Upgrading

## Foundations Of Process Analytics and Machine learning (FOPAM) 2019

Raleigh NC – August 6 - 9, 2019

Foundations Of Process Analytics and Machine learning (FOPAM) http://fopam.org is a new CACHE-sponsored conference series that aims to be the premier forum for researchers from industry and academia to discuss the current status and future directions of data analytics and machine learning in the process industries. The first FOPAM conference will take place August 6–9, 2019 in Raleigh, North Carolina. Using a Gordon Conference-like format, the conference features an exciting program of invited speakers on wide-ranging topics that include:

- Process Monitoring
- Process Design
- Computational Materials Design
- Control Design
- Business, Scheduling, and Supply Chain
- Educating Students and Colleagues.

An optional workshop on "Process Data Analytics and Machine Learning", to be held on the two days before the conference, covers the major classes of methods as well as industrial case studies. Please see the FOPAM website http://fopam.org for a detailed workshop agenda. The early-registration deadline is June 7 and the reduced-rate room block deadline is July 12. Please direct any questions on the conference or extended abstract submission to the Conference Manager, Robin Craven at robin@fopam.org. We look forward to seeing you and your colleagues in North Carolina this summer!

Conference Co-chairs,
Richard D. Braatz
Thomas A. Badgwell
Phillip Westmoreland
LINK to FOPAM flyer

---

## Upcoming Conferences of Interest to CoMSEF Members

**Accelerating material discovery by smart high-throughput computations**
Liverpool, UK
July 3-5, 2019
https://www.cecam.org/workshop1771/

**StatPhys 27**
Buenos Aires, AR
July 8-12, 2019
https://statphys27.df.uba.ar/

**Combining Artificial Intelligence and Physics-Based Modeling for Small- and Macro-Molecular Drug Design**
West Dover, VT
July 13 - 14, 2019
https://www.grc.org/computer-aided-drug-design-grs-conference/2019/

**Integrating Big Data and Macromolecular Protein Structures into Small Molecule Design**
West Dover, VT
July 14 - 19, 2019
https://www.grc.org/computer-aided-drug-design-conference/2019/

**CPMD Meeting 2019 – Pushing the Boundaries of Molecular Dynamics**
Lausanne, Switzerland
July 22-24, 2019
https://www.cecam.org/workshop1738/

**European Conference on Thermophysical Properties**
Venice, IT
September 14-17, 2020
http://www.ectp2020.eu/

**Deep learning in materials science: interpretation, generalization, and the risk of overfitting**
Warth, Switzerland
September 23-25, 2019
https://www.cecam.org/workshop1777/

**WaterEurope: Multiscale simulations and coarse-grained models for water and aqueous systems**
Lausanne, Switzerland
October 21-23, 2019
https://www.cecam.org/workshop1798/

**AIChE Annual Meeting**
Orlando, FL
November 11-15, 2019
https://www.aiche.org/conferences/aiche-annual-meeting/2019

**Gordon Conference: Computational Chemistry**
Castelldefels, Spani
July 19-24, 2020
https://www.grc.org/computational-chemistry-conference/2020/

**Gordon Conference: Computational Materials Science and Engineering**
Newry, ME
August 2-7, 2020
https://www.grc.org/computational-materials-science-and-engineering-conference/2020/

## 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!