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 2018

In This Issue

CoMSEF Executive Committee Elections

Congratulations to Heather Mayes (Liaison Director, Michigan) and Sapna Sarupria (Liaison Director, Clemson) who were elected to the CoMSEF Executive Committee in the fall of 2017! Thanks to Rachel Getman (Liaison Director, Clemson) who completed her term and to Michael Shirts (Liaison Director, Colorado) who served an extra year to fill a gap!

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 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.

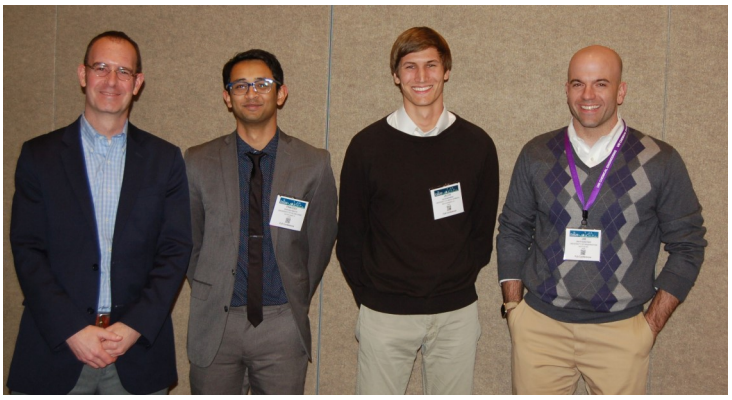
Nominations should consist of a **nominating letter** from the student's research advisor and the **curriculum vitae** of the nominee. These should be sent by the advisor via e-mail in pdf format to the CoMSEF co-Chair (co-chair@comsef.org) by **October 1.**

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.

2017 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.

- Jacob Monroe (California-Santa Barbara, Advisor: M. Scott Shell)
- Prateek Mehta (Notre Dame, Advisor: Bill Schneider)



From left: Prof. Jeff Errington (CoMSEF Chair), Prateek Mehta (Notre Dame), Jacob Monroe (Cal-Santa Barbara), 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.

Annual Meeting Update

AIChE 2018 is just around the corner, and we are looking forward to seeing you in Pittsburgh. We are currently working with AIChE to determine the final list of sessions but would like to note the following about the annual meeting.

1) This year, the plenary session and business meeting will be held on Tuesday instead of Wednesday. We anticipate returning to the usual schedule in 2019.
2) We received an increase of around 15% of contributed abstracts for oral presentations. Even though AIChE may grant us additional sessions, we will not be able to accommodate everyone. Our session chairs are hard at work reviewing your abstracts and we will make every effort to be inclusive of as many research groups as possible as well as follow the recommended guideline that emerged from our 2017 business meeting (i.e., one talk per person across all CoMSEF sessions).
3) If you have any suggestions for honorary sessions for AIChE 2019 or beyond, please send them to CoMSEF vice chair Jim Pfaendtner (jpfaendt@uw.edu)

Research Highlight: Bringing Machine Learning into Computational Molecular Science and Engineering

Heather Mayes, Chemical Engineering, U. Michigan

Data science (DS) and machine learning (ML) have permeated our day-to-day lives, from suggesting articles to read to reducing inbox spam, while its application to molecular simulation has been relatively slow. The CoMSEF sessions on "Data Mining and Machine Learning in Molecular Sciences" began in 2015, with strong interest resulting in two sessions on the topic from that year forward. Andrew Ferguson has been a leader in using ML to advance the understanding of a range of soft and biological materials by extracting low-dimensional free energy landscapes from molecular dynamics simulations.[1–3] Recently, Ferguson reviewed the progress at the intersection of ML and computational simulation of soft materials,[4] laying out the specific challenges, demystifying the jargon of this growing field, and providing an outlook on how this work will shape the future of soft materials engineering. Specifically, the biological and soft materials community works on problems that vary greatly in time and length scales, resulting in highly heterogeneous data, created to answer different sets of questions. However, the defining features of these materials—their conformational flexibility and responsiveness to interactions with their environment—present a common simulation challenge that machine learning can help address.

Key terminology is introduced with examples relevant to computational molecular science, such as protein folding as an example of an unsupervised learning problem (the output is to be discovered) and classification of the binding affinity of an ensemble of aptamers that has a subset with known affinity (semi-supervised learning). The article highlights several methods that are particularly useful in modeling soft materials, including diffusion maps (dMaps) and methods based on relative entropy. dMaps are a type of manifold learning that can identify and parameterize reduced dimensional space, and have been used by Ferguson and others to advance the notoriously difficult task of modeling protein folding. Importantly, dMaps employ curvilinear manifolds (in contrast to the linear hyperplanes of principal component analysis) which are better able to capture many-body couplings typical of these problems. Spectral decomposition of a random walk is performed to reveal slowly-relaxing collective coordinates that govern the evolution of the walk. In addition to revealing interconversion pathways of peptide configurations, dMaps have been used to understand the free energy landscapes of colloidal and molecular self-assembly.

Measuring relative entropy is not always labeled as machine learning, yet it qualifies as an algorithm "that can learn from experience without explicit human instructions." Scott Shell's application of this information theory concept to calculate the maximum likelihood estimate of parameters for a coarse-grained model[5] has provided a robust framework for modeling systems at longer time- and length-scales than is feasible with atomistic molecular modeling.

Ferguson's outlook points to inherent challenges in these fields, including the proper accounting of entropy, environmental interactions, and non-equilibrium systems, and the coupling of disparate time and length scales. These factors prevent a concerted, focused effort from the community around a unifying question. The introduction to machine learning methods provided in this review will constitute a valuable resource in our endeavors.

(1) Wang, J.; Gayatri, M. A.; Ferguson, A. L. Mesoscale Simulation and Machine Learning of Asphaltene Aggregation Phase Behavior and Molecular Assembly Landscapes. *J. Phys. Chem. B* **2017**, *121*, 4923–4944 DOI: 10.1021/acs.jpcb.7b02574.
(2) Lee, E. Y.; Wong, G. C. L.; Ferguson, A. L. Bioorganic & Medicinal Chemistry Machine Learning-Enabled Discovery and Design of Membrane-Active Peptides. *Bioorg. Med. Chem.* **2017**, 1–11 DOI: 10.1016/j.bmc.2017.07.012.
(3) Thurston, B. A.; Ferguson, A. L. Machine Learning and Molecular Design of Self-Assembling Pi-Conjugated Oligopeptides. *Mol. Simul.* **2018**, *7022* (May), 1–16 DOI: 10.1080/08927022.2018.1469754.
(4) Ferguson, A. L. Machine Learning and Data Science in Soft Materials Engineering. *J. Phys. Condens. Matter* **2018**, *30*, 43002 DOI: 10.1088/1361-665X/aa8886.
(5) Shell, M. S. The Relative Entropy Is Fundamental to Multiscale and Inverse Thermodynamic Problems. *J. Chem. Phys.* **2008**, *129*, 144108 DOI: 10.1063/1.2992060.

CoMSEF Logo Contest Update

CoMSEF is over 15 years old but still doesn't have a logo...so CoMSEF leadership challenged the student members of CoMSEF to create CoMSEF logos as part of a contest during the 2017 officer elections. 19 logo entries were received and voted on by the membership.

During the election, the entry by Alex Yang from Vanderbilt University received the most votes. As a result, he won $100 and a copy of the book "Introduction to Scientific and Technical Computing" edited by Frank Willmore, Eric Jankowski, and Coray Colina.

Another entry by Arushi Prakash from the University of Washington caught the attention of the CoMSEF Executive Committee and will likely become the official forum logo after a few adjustments.

Thanks to all who participated!

Entry by Alex Yang

Entry by Arushi Prakash

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.

Rachel B. Getman
2008 Grad Student Award winner (University of Notre Dame, Advisor: Bill Schneider)
Poster Title: A Quantum Chemical Approach to Understanding How Gas Phase Conditions Affect the Thermodynamics and Kinetics of Oxidation Catalysis
Web site: http://computationalcatalysis.sites.clemson.edu/
Google Scholar: https://scholar.google.com/citations?user=_F6kuNEAAAAJ&hl=en

Rachel B. Getman is an Associate Professor of Chemical and Biomolecular Engineering at Clemson University and the first woman to be tenured and promoted in her department. Dr. Getman's research is in computational catalysis. Specifically, her group uses quantum chemical calculations and Monte Carlo and molecular dynamics simulations to investigate molecular-level phenomena at catalyst surfaces. Her group is particularly interested in elucidating catalytic mechanisms of aqueous phase heterogeneously catalyzed reactions and in developing design criteria for atomically dispersed catalysts. Dr. Getman holds a CAREER award from the National Science Foundation studying how the structure of liquid water influences the free energies of catalytic surface intermediates at water/metal catalyst interfaces and a Clemson University College of Engineering, Computing and Applied Sciences Dean's Faculty Fellows Award. She has given 17 invited lectures and published 24 journal articles. In service, Dr. Getman is the Vice President and President Elect of the Southeastern Catalysis Society. She has also served as the Programming Chair of the Catalysis Division (Area 20A) of the AIChE and as a Liaison for CoMSEF. At Clemson, Dr. Getman is a member of the Clemson Tigers ADVANCE Trailblazers initiative, which strives to improve diversity and equity for under-represented groups on campus by developing and implementing structured mentoring programs. After graduating from the University of Notre Dame in 2009 under the advisement of William F. Schneider, Dr. Getman worked as a Postdoctoral Research Fellow with Randall Q. Snurr at Northwestern University. Dr. Getman started her independent career in August 2011, just three months after the birth of her first child, a daughter. Her son was born two years later, just three days before Dr. Getman was awarded her first grant. Dr. Getman lives with her husband and their two children in Six Mile, SC.

New Newsletter Section Launched: “A Broader View”

We are excited to announce a new column for the CoMSEF newsletter titled, "A Broader View". The purpose of this initiative 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.

Our inaugural contribution is authored by M. Scott Shell of UC Santa Barbara. Scott addresses the importance of diversity and inclusion in our profession. He makes a persuasive argument that we should make stronger efforts to enhance diversity within all aspects of our community (faculty, staff, students, employees) and create environments that allow all members to feel comfortable and achieve their maximum potential.

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.

A Broader View
M. Scott Shell

I am excited to see the addition of this new column as a forum for broader discussions in our community, and I am particularly honored to author the inaugural article. I will use this opportunity to make an appeal for creating climates of inclusion for diverse groups in chemical engineering, such as women, minorities, LGTBQ individuals, international researchers, those with disabilities, and more. I spoke on this topic at the 2017 AIChE CoMSEF plenary session based on my increasing involvement in diversity and climate efforts at UCSB, at both the department and campus levels. The latter have become a central focus of our Graduate Division, which has created an extensive yearly “Diversity Matters” program of workshops, invited speakers, and faculty training. I have been involved in a number of these and sit on our Graduate Dean’s Advisory Board for Diversity. While I could talk about many aspects of diversity, including pipeline issues that are extraordinarily important, here I will focus on climate specifically and share some of my experiences and thoughts.

Why should we care about diversity and climate? Moreover, why should we *all* care and *all* be involved, beyond a few “diversity champions” in each department? One reason is that diversity is part of our core professional values. The AIChE Code of Ethics compels us to “treat all colleagues and co-workers fairly and respectfully, recognizing their unique contributions and capabilities by fostering an environment of equity, diversity and inclusion.” In 2015, AIChE went further to release a formal Diversity Statement that reads “AIChE is committed to creating an environment in the Institute and profession in which all members, regardless of characteristics such as gender, race, religion, age, physical condition, sexual orientation, nationality or ethnicity, are valued and respected.” A recent excellent article in Chemical Engineering Progress also highlights the importance of diversity in our field, to which the reader is enthusiastically referred [1].

Another motivation for caring is that many underrepresented groups continue to experience negative environments that impact their success, and hence the collective success of our field. For example, recent research shows that female students in STEM fields often face unwelcoming and even hostile environments, underscoring the importance of department-level support structures and resiliency training [2]. As another example, the American Physical Society recently conducted an extensive climate survey, finding that LGBTQ physics students feel highly isolated and an expectation to remain closeted, and are at significantly higher risk for leaving their workplace or school [3]. Barriers exist further down the career line too: a recent PNAS article found that women are less likely than men to be invited as colloquium speakers [4]. Studies support similar issues for many other underrepresented groups.

Beyond these ethical imperatives, we should also be fundamentally interested in diversity because it will improve our science, according to the research. Simply put, diversity drives innovation. A wide range of observational studies and controlled group experiments, spanning many disciplines, has consistently shown that diverse teams make fewer factual errors, reexamine/scrutinize ideas and assumptions more frequently, raise broader and more novel solutions to problems, are less susceptible to groupthink, and communicate more effectively [5-8]. These performance benefits occur even when the teams are merely socially diverse (i.e., a mix of race, ethnicity, gender, sexual orientation, etc.) as opposed to intellectually varied in expertise.

The business world, and particularly the consulting industry, is well aware of these facts. In many cases companies are aggressively improving diversity support structures to increase employee productivity and the bottom line. Statistics show that companies diverse with respect to gender, race, and ethnicity outperform non-diverse ones; they have higher sales revenues, more customers, and greater profits [9,10]. Diverse companies are also more likely to expand market share or capture new markets [11]. Moreover, companies that make diversity a core business strategy have a higher fraction of highly engaged workers [12]. Diversity also helps in recruiting talent; younger employees in particular prefer to work in an inclusive work environment [13].

All of these reasons should strongly motivate our collective efforts to improve climate, particularly in the research world. While chemical engineering has become a more diverse profession than historically, we must be careful not to assume that our

communities self-evolve towards an inclusive environment. Particularly in academic departments, we typically bring together researchers from all over the country and world, with very different backgrounds, cultural expectations, and awareness. Actively cultivating an inclusive climate, through student and faculty communication and training, should thus play a role in developing our research culture.

Data- and evidence-based activities are essential. The scientific community demands that we approach our research with precise and quantitative planning. Yet I am frequently surprised by the extent to which students and particularly faculty – everywhere – tend to be highly anecdotal and speculative in matters of personnel. "That school produces fantastic students; Jane Doe graduated from there and has done fabulously." "Our department climate is just fine. I have never heard of any issues." "Female graduate students tend to be more interested in bio-related research." These are just examples, but they exemplify a type of reckless statement that is not based on detailed investigation but rather stems from a haughty assumption that the status quo is operating without issue.

It is not difficult to collect the needed data and make informed assessments. At UCSB, our department initiated yearly surveys of our graduate students that includes several questions about climate (examples are given in Box 1), including all-important space for open-ended responses. We also chatted with individual students and groups, and interacted with on-campus diversity experts and workshops to learn best-practices. Not only did our surveys suggest several concrete areas for improvement, they also provided us with a mechanism to assess and continuously reevaluate progress in response to initiatives.

There are indeed many actions that departments can take to encourage a climate inclusive of diversity. For example, we created a faculty diversity committee – with representatives from undergraduate affairs, graduate affairs, and faculty hiring – to formalize a strategic and integrated department approach towards diversity initiatives. We created common student areas and provided funds for weekly coffee hours, acknowledging research showing that such community-wide areas and activities differentially benefit marginalized groups. We also incorporated a required diversity and sensitivity training workshop into our graduate student orientation, run by UCSB's Resource Center for Sexual and Gender Diversity. Extending this idea, we have begun to include a yearly seminar broadly focused on a diversity related topic; this year's was from a faculty expert on the science of team intelligence and performance. Our department chair also held a faculty meeting discussion on implicit bias in reference letter writing. These efforts have had a positive effect so far, as measured by the surveys, but we continue to evaluate new approaches and view this effort as an ongoing component of our department administration.

My challenge to our community is to think constructively about inclusion. Do you know what your department climate is like, for various groups? Have you measured it? Have you communicated your experiences to the department, particularly if you are a member of an underrepresented group? Do you send an explicit message of inclusion and expectations to your faculty, students, research group, peers, and/or colleagues? Do you rely on data and evidence-based strategies versus anecdote, speculation, and assumption?

It is particularly important that we become cognizant of problematic behavior, even if unintentional. Implicit bias describes a characteristic subconsciously attributed to a particular group. Examples include "Math comes easy to you because you're Asian." or "We need some women on the symposium food committee." We all have implicit biases, and so the point is really to become aware of and avoid them, and to be confident enough to apologize and course-correct when we offend. An excellent online resource, which includes an enlightening self-test activity, is Harvard's Project Implicit (implicit.harvard.edu). A related problem is microaggressions, which are casual but derogatory comments directed at a particular group. Examples include "He's a little too flaming to give a good presentation." or "She's such a bubbly faculty candidate." Training to increase awareness of these behaviors, as well as the skills necessary to cope with and interrupt them (even as bystanders), are important to the functioning of our research communities.

Part of working towards an inclusive climate is also acknowledging that there can be push-back, individuals that for various reasons see diversity efforts as fringe, non-essential, excessive, or political. There will be the folks who question why certain groups need "special treatment." My response has been that the issue is about eliminating the special *negative* treatment. Some will claim that it isn't their job to engineer the social environment. Actually, the academic research environment is subject to the same anti-harassment, anti-discrimination, and anti-bias legal protections as industry workplaces, which require us to ensure appropriate climates and report & address many kinds of problematic behaviors. Some can recoil from diversity initiatives with statements like "Don't brainwash me into what to think." For those, I emphasize that the efforts are about expectations for their professional conduct in the research environment, not their specific value systems. Others may want to argue the merits of diversity-related activities ("The only diversity that matters is intellectual diversity!") These individuals need referring to the extensive literature described above, as well as reminding of their professional responsibilities, including the AIChE code of ethics. Finally, there may be many that simply feel uncomfortable or untrained. The good news is that we are all intelligent, capable, and adaptable intellectuals, and can readily self-educate in diversity, even if it takes some time.

We have an opportunity to formulate our vision for a more inclusive chemical engineering community. I hold great admiration for the CoMSEF family and have many friends in it. We are a capable and talented group, and it just so happens that we collectively straddle a wide swath of the chemical engineering community. Thus, we have a unique potential to nucleate discussions, activities, and positive change widely. Let's keep taking a broader view.

1. Z. Otero Gephardt, V. G. Grassi, A. McCormic, O. Shelton, "Creating a Culture of Diversity," Chemical Engineering Progress, October 2016.

2. B. E. Rincón and C. E. George-Jackson, “Examining Department Climate for Women in Engineering: The Role of STEM Interventions,” J. College Student Development 57, 742, (2016).
3. “LGBT Climate in Physics,” report of the American Physical Society, (2016).
4. C. L. Nittrouer et al., “Gender disparities in colloquium speakers at top universities,” PNAS Early Edition (2017).
5. “Why Diversity Matters,” report of the Catalyst Information Center (2013).
6. K. W. Phillips, “How Diversity Makes Us Smarter,” Scientific American (2014).
7. A. Wooley, T. W. Malone, C. F. Chabris, “Why Some Teams are Smarter Than Others,” New York Times (Jan. 16, 2015).
8. D. Rock and H. Grant, “Why Diverse Teams Are Smarter,” Harvard Business Review (November 4, 2016).
9. V. Hunt et al., “Diversity Matters,” report of McKinsey & Co. (2016).
10. C. Herring, “Does Diversity Pay? Race, Gender, and the Business Case for Diversity,” Am. Soc. Rev. (2009).
11. “Innovation, Diversity, and Market Growth,” report of the New York Center for Talent Innovation (2014).
12. R. Anand, “How Diversity and Inclusion Drive Employee Engagement,” report of DiversityInc (2013).
13. D. Schawbel, “How Companies Can Benefit from Inclusion,” Forbes (2012).

Box – sample climate survey questions

Considering our department graduate student and postdoc culture, how supportive is it of the following groups?
Considering our department faculty culture, how supportive is it of the following groups?
Considering our campus culture, how supportive is it of the following groups?

	not particularly supportive	mostly supportive	supportive	very supportive
female students	○	○	○	○
international students	○	○	○	○
LGBT students	○	○	○	○
minority students	○	○	○	○

Where should the culture or support be improved? Please rate the overall department climate on the following scale.

	Highly	Somewhat	Neutral	Somewhat not	Not
Friendly (vs. hostile)	○	○	○	○	○
Welcoming (vs. cliquish)	○	○	○	○	○
Communicative (vs. reserved)	○	○	○	○	○
Interactive (vs. non-sociable)	○	○	○	○	○
Respectful (vs. disrespectful)	○	○	○	○	○
Cooperative (vs. uncooperative)	○	○	○	○	○
Competitive (vs. noncompetitive)	○	○	○	○	○
Improving (vs. worsening)	○	○	○	○	○
Non-racist (vs. racist)	○	○	○	○	○
Non-sexist (vs. sexist)	○	○	○	○	○
Non-homophobic (vs. homophobic)	○	○	○	○	○
Accessible to persons with disabilities (vs. non-accessible)	○	○	○	○	○

2nd Annual Hands-On with Molecular Simulation Workshop

8am-6pm October 28 at the 2018 AIChE Annual Meeting

This workshop is the dedicated forum for collaborating on open-source tools developed and used by the molecular simulation community for understanding chemical behaviors. It supports CoMSEF sessions focusing on molecular simulation reproducibility, usability, software engineering, machine learning, and methods advances, by providing a hands-on coding workshop where authors can guide learners through the tools they've developed, and where our community can more efficiently have the group conversations about library use, community standards, and reproducibility that we need.

Last year's 35 participants lauded the variety of topics and presenters and their helpfulness. This year we aim to resolve the two complaints from last year: Fixing the room's temperature and providing coffee.

Students looking for more expertise with computational sciences, students and faculty who wish to get practice with recent developments in molecular simulation tools, and investigators building software packages whose visibility would be mutually beneficial to their work and the molecular simulation community will all be served by this workshop. For questions about participating, please email the session chairs: Eric Jankowski ericjankowski@boisestate.edu and Sapna Sarupria ssarupr@g.clemson.edu.

Workshop registration fees will be under $100 for students and faculty and can be added to your cart when registering for the AIChE Annual Meeting. Seating will be limited to 35 participants.

Upcoming Conferences of Interest to CoMSEF Members

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

Hermes Summer School in Materials Modelling and Science Communication
Windsor, UK
July 19-23, 2018
http://hermessummerschool.org/

GRC: Towards Next-Generation Challenges in Computational Chemistry: From Quantum Chemistry and Molecular Simulation to Data Discovery and Quantum Computing
West Dover, VT
July 22-27, 2018
https://www.grc.org/computational-chemistry-conference/2018/

GRC: Polymer Physics
South Hadley, MA
July 22-27, 2018
https://www.grc.org/polymer-physics-conference/2018/

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

European Conference on Thermophysical Properties
Venice, IT
September 14-17, 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!