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

October 2018

In This Issue

Mittall Winner of 2018 CoMSEF Impact Award

Professor Jeetain Mittal from the Department of Chemical and Biomolecular Engineering at Lehigh University is the winner of the 2018 CoMSEF Impact Award. He is cited, "***For development of atomistic and coarse-grained models to study biological self-assembly processes for a fundamental understanding of the cellular organization and design of novel materials***". Jeetain has been a member of the faculty at Lehigh since 2009. Prior to this appointment, he served as a Postdoctoral Fellow at the National Institutes of Health and earned a Ph.D. degree from the University of Texas at Austin, a M.Tech. degree from the Indian Institute of Technology Kanpur, and a B.Tech. degree from Punjab Technical University. All of Jeetain's degrees are in the field of chemical engineering. Jeetain will receive his award during the CoMSEF Plenary Session at the 2018 AIChE Annual Meeting, where he will also deliver a presentation describing his research. The CoMSEF Impact Award is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

Shukla Winner of the 2018 CoMSEF Young Investigator Award

Professor Diwakar Shukla from the Department of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign is the 2018 winner of the CoMSEF Young Investigator Award. He is cited, "***For development and application of computational methods to understand protein conformational dynamics and stability***". Diwakar has been a member of the faculty at Illinois since 2015, where he is now the Blue Waters Assistant Professor. Prior to this appointment, he served as a Postdoctoral Fellow at Stanford University and earned Ph.D. and M.S. degrees from the Massachusetts Institute of Technology as well as M.Tech. and B.Tech. degrees from the Indian Institute of Technology Bombay. All of Diwakar's degrees are in the field of chemical engineering. Diwakar will receive his award during the CoMSEF Plenary Session at the 2018 AIChE Annual Meeting, where he will also deliver a presentation describing his research. The CoMSEF Young Investigator Award is given annually to a CoMSEF member who is within 7 years of completion of their highest degree.

2018 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be 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. The awardees will be selected based on the nomination letters received from each student's advisor, their CV, and a poster presented during the CoMSEF poster session, which will be held Monday afternoon from 3:30 to 5:00 PM in Exhibit Hall B of the David L. Lawrence Convention Center. The winners will be announced at the CoMSEF/Area 1a General Meeting (Tuesday, from 6:15-7:15 pm).

CoMSEF General Meeting in Pittsburgh

CoMSEF will hold its annual General Meeting on Tuesday October 30 from 6:15-7:15 pm in room 308 of the David L. Lawrence Convention Center during the 2018 AIChE Annual Meeting. *Please note the shift to Tuesday. We anticipate returning to the usual Wednesday schedule in 2019.* As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend. The winners of the CoMSEF Graduate Student Awards and the Vice Chair and Liaison Directors election results will be announced. Programming for future AIChE meetings will also be discussed.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year we will elect a Vice Chair, a Secretary/Treasurer, and two Liaison Directors and select a logo for CoMSEF. Information about the candidates and the duties of the office can be found at http://comsef.org/elections-2018. You should have received voting instructions by email. If you didn't receive the email or lost it, contact admin@comsef.org for help. The deadline for casting your vote is Monday October 26th.

A Broader View: Getting the Most Out of Faculty Hiring Season

Jim Pfaendtner, Chemical Engineering, U. Washington

Along with the excitement and thrill of a new academic year, comes the inevitable requests from our colleagues to serve on various committees and participate in operations within our departments, universities and institutions. I personally believe that the decision of which new faculty members to hire, followed closely by the selection of new PhD students to admit, is at or near the top of the most impactful decisions we make as a faculty team. I would like to enthusiastically echo the call by Scott Shell [1] to promote a climate of diversity and inclusion in our departments, and one important way to do so is the application of evidence-based best practices to promote diversity in our faculty hiring process. [2]

Some key pieces of research that motivate the need to emphasize diversity and inclusion at the onset of faculty hiring have shown the need to take care at all phases of the faculty search. In the evaluation of CVs, research continues to show that science faculty of all genders from research-intensive schools rate job applicants significantly higher (i.e., more competent and hirable) when the applicants are labeled with a male name [3]. Once letters of recommendation have been requested, we know that there are differences in the way writers describe male and female applicants. For example, research has shown [4] that writers tend to describe males in a more agentic sense (i.e., they convey an individual who is assertive and capable of influencing others) in contrast to a tendency to describe women in a communal sense (examples include “kind”, “sensitive”, “nurturing”). The use of such communal terms in letters of reference has been negatively correlated with an applicant's ability to get hired for faculty jobs [4]. A final example (there are many more to be found in the literature) documented that faculty search committees much more actively considered a female candidates relationship status (i.e., the 2-body problem) when selecting hires [5].

The above examples are meant to underscore that there are documented biases in our faculty hiring process. Beyond ethical and legal concerns, there is abundant evidence in the value of diversity and inclusion in our ranks [1], which begs the question of how should we take action? As your search committees are ramping up this year I recommend that you first look within your own institution. A quick search of recent and current CoMSEF officers’ home universities showed me that at least ⅔ of the schools provide literature on promoting diversity and inclusion in the faculty hiring process. A next best step is to use the NSF ADVANCE programs at many universities around the nation. The ADVANCE program’s purpose is to increase participation of women in STEM academic careers. A web search for “advance faculty recruiting toolkit” provided guidance from ADVANCE programs at eight different institutions. Another great starting point can be found from Science Careers, with a mini-primer on tips for combating unconscious bias in our faculty recruitment process.[6]

In closing, I think that the decision to hire new faculty is too important to leave to chance. All of CoMSEF will be enriched if we are proactive in bringing a broadly inclusive slate of candidates to our colleagues in consideration for hiring for academic positions. I encourage you to find an ally in your department (or within CoMSEF!) and help your departments reduce bias in the hiring process using all of the available tools and best scientific research.

References and notes

[1] M. S. Shell, “A Broader View”, Summer 2018 CoMSEF Newsletter.
[2] JP would like to acknowledge the contribution of Dr. Joyce Yen (UW ADVANCE) in preparing this document both through many individual discussions and mentorship as well as providing much of the source material that is credited within, in particular the UW LEAD-It- Yourself! Primer document on Diversity in Faculty Recruitment. More information is available from the LiY! website: https://advance.washington.edu/liy
[3] C. A. Moss-Racusin et al., “Science faculty’s subtle gender biases favor male students,” PNAS (2012).
[4] J. M. Madera et al., “Gender and Letters of Recommendation for Academia: Agentic and Communal Differences,” J. Appl. Psych. (2009).
[5] L. A. Rivera, “When Two Bodies Are (Not) A Problem: Gender and Relationship Status Discrimination in Academic Hiring,” Am. Soc. Rev. (2017).
[6] M. Kuo, “Consciously combatting unconscious bias,” Science Careers blog post 1/30/17

Research Highlight: Strength in heterogeneity – surface patterning as a design factor in solid-water interfaces

Sapna Sarupria, Associate Professor, Chemical and Biomolecular Engineering, Clemson University

In a recent paper, Monroe and Shell[1] explored water dynamics near model surfaces – Lennard Jones based surfaces made of two particle types with weak and strong interactions with water, mixed self-assembled monolayers (SAM) comprising -CH_3 and -OH terminated groups and silica surfaces with varying density of silanol groups. Specifically, they focused on studying water diffusivity as the surface coverage and patterns of the hydrophilic groups on the model surfaces were varied. Instead of searching through randomly generated surface patterns, Monroe and Shell employed a genetic algorithm to find the surface patterns on each of these model surfaces that maximized and minimized water diffusivity for a given value of surface coverage. Interestingly, while surface patterning did not affect water dynamics much in the case of LJ surfaces, it had a significant effect on SAM and silica surfaces – both interact through directional hydrogen bonding with water. It was found that clustering of hydrophilic groups resulted in higher water diffusivity. Strong correlations were identified between water diffusivity at these surfaces and orientation-

al entropy. Such correlations between entropy and dynamics have also been observed in bulk fluids! These findings highlight the fundamental relations between thermodynamics and water dynamics.

This study showcases the role of surface chemical patterning in governing water dynamics and hence various processes driven at the water-surface interfaces. However, it also highlights some challenges in studying solid-water interfaces. For example, in a related study Schrader et al.[2] used Overhauser dynamic nuclear polarization and surface forces apparatus to study water diffusivity near silica surfaces as a function of silanol groups. Indeed, they observed a dependence on silanol coverage but more interestingly, a steep drop in diffusivity was observed at silanol coverage corresponding to contact angle of 26°. While it may be hypothesized that this change occurs from clustering of silanol groups at some coverage based on computational results, a direct comparison cannot be made. The bridging (and direct comparison) of experimental and simulation results for interfacial phenomena continues to remain a challenge. In addition to chemical patterns, surface heterogeneity can also appear in the form of topology and/or defects. This vastly increases the parameter space available to engineer surface-water interactions. These challenges also present opportunities – from developing novel experimental techniques to new algorithms (perhaps, machine learning based)– to continue to unravel the complexities of surface-water interactions!

[1] Jacob I. Monroe and M. Scott Shell, "Computational discovery of chemically patterned surfaces that effect unique hydration water dynamics", Proc. Natl. Acad. Sc., 2018, https://doi.org/10.1073/pnas.1807208115
[2] Alex M. Schrader, Jacob I. Monroe, Ryan Sheil, Howard A. Dobbs, Timothy J. Keller, Yuanxin Li, Sheetal Jain, M. Scott Shell, Jacob N. Israelachvili, and Songi Han, "Surface chemical heterogeneity modulates silica surface hydration", Proc. Natl Acad. Sc., 2018, DOI:10.1073/pnas.1722263115

2nd Annual Hands-On with Molecular Simulation Workshop

2nd Annual Hands-On with Molecular Simulation
8am-6pm October 28 at the 2018 AIChE Annual Meeting

Join CoMSEF developers for our annual workshop dedicated to collaborating on open-source tools used by the molecular simulation community for understanding chemical behaviors. This year we are pleased to showcase tutorials on MoSDeF, HOOMD, Ssages, GOMC, physical validation, and a suite of tools for biomolecular simulations.

The full lineup can be seen online here: https://aiche.confex.com/aiche/2018/meetingapp.cgi/Session/40345
(note that the lunch break was omitted by confex, so the afternoon timings are off)

Registration is limited to 35 seats, so sign up fast! Seat reservations are made during AIChE registration (the first "ticketed event"). We are pleased to offer discounted registration of $50 for academic participants and $200 for industrial participants.

For questions about participating, please email the session chairs: Eric Jankowski <ericjankowski@boisestate.edu> and Sapna Sarupria <ssarupr@g.clemson.edu>.

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.

Jeremy Purvis
University of Pennsylvania, Advisor: Scott Diamond
2008 Poster Title: Reverse Engineering the Human Platelet: A Computational Framework for Predicting Platelet Activation

Jeremy Purvis is an Assistant Professor of Genetics at the University of North Carolina at Chapel Hill and a member of the Lineberger Comprehensive Cancer Center. He received a Ph.D. in Computational Biology from the University of Pennsylvania where he developed computational models of cell signaling with Scott Diamond and Ravi Radhakrishnan. He completed his postdoctoral training at Harvard Medical School under the mentorship of Galit Lahav, where he studied the role of p53 dynamics in the DNA damage response. As an independent investigator, his group seeks to understand how individual cells make fate decisions and how groups of interacting cells give rise to emergent properties. Their work focuses primarily on early differentiation decisions in human embryonic stem cells and cell cycle arrest decisions in the context of cancer.

The Tenth Industrial Fluid Properties Simulation Challenge

The Industrial Fluid Properties Simulation Challenge is an open competition organized by employees of the Army Research Lab, the National Institute of Standards and Technology (NIST), The Dow Chemical Company, 3M, and United Technologies Research Center with support from CoMSEF and the ACS. The goals of the competition are to drive improvements in the practice of molecular modeling, formalize methods for the evaluation and validation of simulation results with experimental data, and ensure relevance of simulation activities to industrial requirements. The Simulation Challenge was initiated by the workshop on "Predicting the Thermophysical Properties of Fluids by Molecular Simulation" held at NIST in 2001.

The 10th Industrial Fluid Properties Simulation Challenge will test the capability of molecular dynamics simulation to provide the property of liquids most important to elastohydrodynamic lubrication (EHL), the pressure-viscosity relation. The temperature dependence at elevated pressure could be the subject of a future challenge.

More details about the 10th challenge are here: http://fluidproperties.org/10th

Seven entries have been received, and the authors will present their work at the IFPSC session on Wednesday, October 31, 2018 03:30 PM - 06:00 PM David L. Lawrence Convention Center - 308. The champions of the current challenge and info about the next challenge will be announced.

Upcoming Conferences of Interest to CoMSEF Members

PPEPPD 2019
The 15th International Conference on Properties & Phase Equilibria for Product and Process Design
Vancouver, Canada
May 12-16, 2019
http://ppeppd2019.org/

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/

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

Annual Meeting Sessions

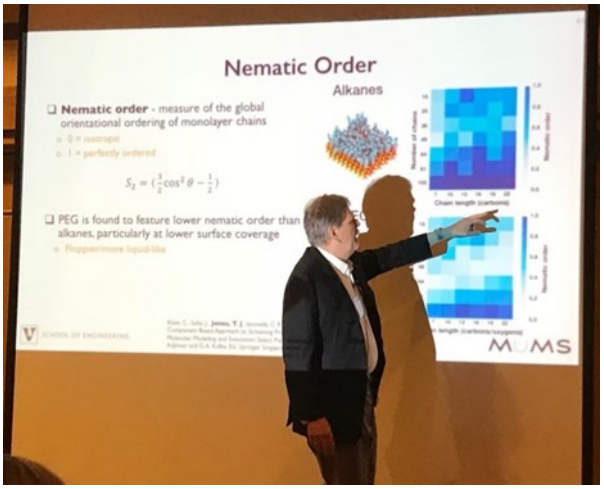
Day	Title	Time	Location (all CoMSEF sessions are in Convention Center)	Colisted w/ CoMSEF
Sunday	Workshop: Hands On With Molecular Simulation (Ticketed Event)	8 - 6	334	
Sunday	Applications of Molecular Modeling to Study Interfacial Phenomena I	3:30 - 6	308	
Monday	In Honor of Pablo Debenedetti I (Invited Talks)	8 - 10:30	308	
	Industrial Applications of Computational Chemistry and Molecular Simulation	12:30-3:00	308	
	In Honor of Pablo Debenedetti II (Invited Talks)	12:30-3:00	307	X
	New Developments in Computational Catalysis I	12:30-3:00	402	X
	Faculty Candidates in CoMSEF	3:30-6:00	308	
	New Developments in Computational Catalysis II	3:30-6:00	402	X
	Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	3:30-5:00	Exhibit Hall B	
Tuesday	Computational Catalysis I: Fundamentals	8:00-10:30	402	X
	Data Mining and Machine Learning in Molecular Sciences I	8:00-10:30	308	
	Applications of Molecular Modeling to Study Interfacial Phenomena II	12:30-3:00	308	
	Computational Catalysis II: Metal and Alloy Catalysis	12:30-3:00	402	X
	Computational Catalysis III: Electrocatalysis	3:30-6:00	402	X
	Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)	3:30-6:00	308	
	Tools for Product Design	3:30-6:00	319	X
Wednesday	Computational Catalysis IV: Biomass Chemistry and Chemicals Production	8:00-10:30	402	X
	Data-Driven Screening of Chemical and Materials Space	8:00-10:30	307	X
	Recent Advances in Molecular Simulation Methods I	8:00-10:30	308	
	Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, and Supported Catalysts	12:30-3:00	402	X
	Practical Applications of Computational Chemistry and Molecular Simulation	12-3:00	308	
	The Industrial Fluid Properties Simulation Challenge	3:30-6	308	
Thursday	Data Mining and Machine Learning in Molecular Sciences II	8:00-10:30	308	
	Atomistic and Molecular Modeling and Simulation of Polymers	12:30-3:00	330	X
	Data Science in Catalysis I	2:30-3:00	402	X
	Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction	12:30-3:00	307	X
	Software Engineering in and for the Molecular Sciences	12:30-3:00	308	
	Data Science in Catalysis II	3:30-6:00	402	X
	Making Molecular Simulation a Mainstream Chemical Engineering Tool	3:30-6:00		
Friday	Recent Advances in Molecular Simulation Methods II	8:00-10:30	305	X
	Recent Advances in Force Fields	12:30	306	

7th International Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2018)
Innovations for Complex Systems

The 7th triennial FOMMS conference was held July 15-20, 2018 at Lake Lawn Resort, located in Delavan, Wisconsin. Over 150 participants took part in the meeting, with approximately 10% of them from industry, 10% from national labs, and 22% from countries outside the U.S. CoMSEF served as one of the sponsors for the event.

The traditional FOMMS schedule was followed. The conference featured a keynote lecture from Prof. Sharon Glotzer (University of Michigan), 18 plenary lectures from leading figures in the field of molecular modeling and simulation, two contributed poster sessions with over 100 posters, four workshops, the FOMMS movie, and the FOMMS Medal lecture by Prof. Peter Cummings (Vanderbilt University).

There were also numerous networking opportunities, with nightly hospitality sessions, three group outings (Zip Line Canopy Adventure, Yerkes Observatory, and a boat tour of Lake Geneva), open afternoons to promote discussion and collaboration, and a banquet.



Peter Cummings delivers the FOMMS Medal lecture

We are grateful for the support of several sponsors. The generosity of the Department of Energy and the National Science Foundation enabled us to award 26 graduate student fellowships. Several participants were awarded poster prizes provided by the American Chemical Society and Springer. In addition to CoMSEF, ExxonMobil, Solvay, The Dow Chemical Company Foundation, Springer, the American Chemical Society, and the University of Minnesota also provided support.

Recipients of Department of Energy (left) and National Science Foundation (right) fellowships

Overall, FOMMS 2018 was a great success. Participants commented favorably on the location, the speakers, and the format. Participants seemed appreciative of the ample time scheduled into the program for informal meetings and interactions, the quality of the speakers and the poster sessions. Jeff Errington (University at Buffalo) agreed that, pending approval by CACHE, he would take on the role of Chair for FOMMS 2021 with co-Chairs Sabrina Pricl (University of Trieste) and Jim Pfaendtner (University of Washington).

J. Ilja Siepmann
University of Minnesota

Claire Adjiman
Imperial College London

Jeffrey Errington
University at Buffalo

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. Most recently we initiated the Young Investigator Award for Modeling and Simulation. This and our other 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!