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

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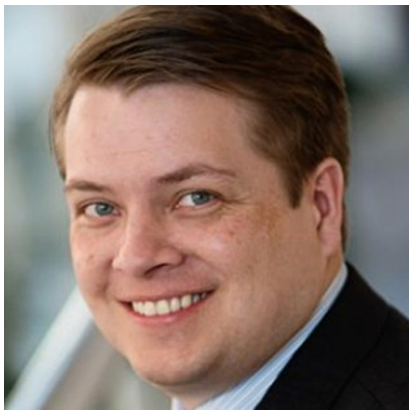
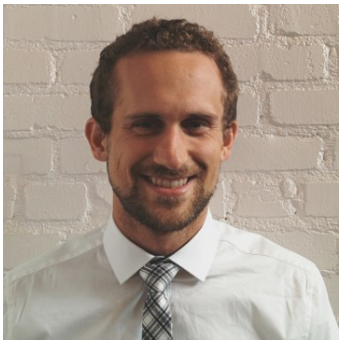
In This Issue

Shirts Winner of 2020 CoMSEF Impact Award



Professor Michael R. Shirts from the Department of Chemical and Biological Engineering at the University of Colorado Boulder is the winner of the 2020 CoMSEF Impact Award. He is cited "***for increasing the utility, power, and reliability of molecular simulation as a chemical engineering tool through development and improvement of statistical mechanics methods and programs***." Prior to joining the faculty at Colorado in 2016, Michael was a professor in the Department of Chemical Engineering at the University of Virginia. Shirts received his PhD from Stanford University in 2005 with Vijay Pandey. For his post-doctoral research, he worked with Richard Friesner at Columbia University. Michael will deliver a presentation describing his research during the CoMSEF Plenary Session at the 2020 AIChE Annual Meeting. The CoMSEF Impact Award is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

White Winner of the 2020 CoMSEF Young Investigator Award



Professor Andrew D. White from the Department of Chemical Engineering at the University of Rochester is the 2020 winner of the CoMSEF Young Investigator Award. He is cited "***for excellence in scholarly research in computational molecular science and engineering on the topics of multiscale modeling, molecular simulation methods and modeling of peptides***." Andrew joined the faculty at Rochester in 2015. Before that he worked with Professor Greg Voth at University of Chicago as a Post-doctoral fellow in the Institute for Biophysical Dynamics from 2013-2014. Andrew received his PhD in chemical engineering from the University of Washington in 2013. Andrew will deliver a presentation describing his research during the CoMSEF Plenary Session at the 2020 AIChE Annual Meeting. The CoMSEF Young Investigator Award is given annually to a CoMSEF member who is within 7 years of completion of their highest degree.

2020 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering were awarded to participants in the CoMSEF poster session at the virtual annual AIChE Meeting: **Sarah Alamdari** (Washington, Advisor: Jim Pfaendtner) and **Ryther Anderson** (Colorado School of Mines, Advisor: Diego Gomez-Gualdron). This year the forum also named two Honorable Mentions: **Andrew S. Rosen** (Northwestern, Advisor: Randall Q. Snurr) and **Karun Kumar Rao** (Houston, Advisor: Lars Grabow). The CoMSEF Graduate Student Awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. The awardees were selected based on the nomination letters received from each student's advisor, their CV, and a poster presented during the CoMSEF poster session.

CoMSEF Elections

The annual CoMSEF election recently concluded. Congrats to Jeetain Mittal who was elected Vice Chair, Joe Golab who was elected Secretary-Treasurer, and to Kayla Sprenger and Poornima Padmanabhan who were elected Liaison Directors! Information about the candidates and the duties of the office can be found at http://comsef.org/elections-2020.

A Broader View: Towards a culturally competent academic experience for all

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

Many research groups have students and postdocs from different countries. The data shows that international students make up a large fraction of graduate students in the US with most coming from India and China [1,2]. For these students, assimilating into a new culture while holding on to their identity and being successful in the academic pursuits is a challenging process. This process can be made smoother by simple considerations and fostering a practice of cultural competence (a term used often in healthcare, but yet to be made popular in engineering. [3]). Research has demonstrated that celebrating diversity and taking a multicultural, identity-affirming approach is more beneficial than taking a color-blind approach in which one ignores identity-based differences [4]. Thus, it is important that we create an environment in our groups and departments that celebrates the identities of the individuals coming from all backgrounds and ethnicities.

To begin with, I will share two anecdotes from my repository of (cultural) experiences. With these examples, I want to illustrate some ways in which we often fail to realize how subtle, yet impactful cultural differences can be, and the difference that even a little awareness can make in creating an inclusive vs a non-inclusive environment.

Anecdote 1: After moving to Clemson, I joined a small group of graduate students in a game of ultimate frisbee every Friday evening. The group comprised of mostly American students, of which one participant had moved from India to the US at a very young age. After the game, the students would all go out for dinner. I was also invited, but I declined. On each occasion they asked me once which I interpreted as them asking out of courtesy. However, the student familiar with both the Indian and American social contexts explained to me that while in the Indian concept of hospitality, extending oral invitations multiple times is the norm and accepting the invitation immediately is often considered impolite, the American way is more explicit and direct; they usually just ask once. Needless to say, after this I was less concerned about my inclusivity in the group and joined them for dinner whenever I could. This cultural awareness helped me become better assimilated into this group of wonderful folks.

Anecdote 2: My colleague had recently purchased a home previously owned by an Indian family. In a casual conversation with them, I asked about their experience settling into the new house. They remarked about the tendency of Indians to decorate their houses with gaudy things and having to redo several things in the house as a result. Note that my colleague had not explicitly stated something charged, insensitive or offensive, nor had they attacked me with their statement. However, by invoking a generalization and being offhanded about the cultural practices of an entire group of which I was a member, they had instantly made me feel unwelcome and out-of-place. A slight change of words and refrain from such generalizations could easily have avoided such an outcome. Lack of cultural competency has significant repercussions to inclusiveness.

It is in these everyday (simple) activities that we build an inclusive or non-inclusive environment. In a recent survey of 6313 graduate students, 21% reported experiencing bullying [5]. In a survey of international graduate students in the US, 63.1% and 58.9% students reported facing cultural and social barriers, respectively [6]. It is clear that these issues need to be addressed if we are to build an inclusive and thriving community of engineers and scientists. When we can create a more inclusive environment, we are all rewarded with better productivity and progress. [7,8] Here are some of my thoughts on what we can do as faculty and peers to make the academic/professional environment more conducive to cultural diversity.

Empower with sharing knowledge: Educate the students about their rights and your expectations. Educate yourself about different cultures: Being in a completely new and unfamiliar system, most students are unaware of their rights. Educate them – inform them of the policies and clearly discuss your expectations with them. In doing so encourage a balanced life approach. Separately, be aware that cultural influences often permeate professional and scholarly interactions and questioning authority figures (such as teachers) is discouraged in many cultures. As a result, students raised in such societies are not accustomed to freely interacting with the faculty and often shy away from full-throated arguments and discussions. Encourage your students to speak up – provide them with a nurturing atmosphere where they can begin to have honest discussions with you. If graduate student organizations are available at the departmental or the university level, participate in them. You can take steps like creating a peer mentoring program that pairs incoming graduate students with senior students as their mentors, who can help them adapt to the new system. International student offices (ISO) play an important role in assimilating international students when they arrive on campus. Domestic graduate students can also volunteer their time with the office so that they get to meet and mingle with international students.

Sense of belonging: Having a sense of belonging increases productivity. [7,8] One of the effective ways of creating a sense of belonging for the international students is to be welcoming of their culture. Exhibiting curiosity and willingness to learn about different cultures would also encourage your students to become cognizant and accepting of the cultural disparities. For example, you can encourage your students to share pictures from their hometown, and some interesting facts about their hometown or country before group meeting presentations.

Create opportunities that promote intermingling of students. This is important because frequently students tend to phase separate based on cultural background and language. Many students often bond based on overlapping interests and extracurricular activities. In the stressful environment of graduate school, many students fail to find opportunities to pursue their interests and interact with their peers outside of work. Promote practices where students provide comments on each other's manuscripts and presentations. Facilitate peer project pairs or groups where the pair (or group) works together on various aspects of their project. This could be as simple as researching a specific topic and giving joint presentations/ presenting together.

Communication: For any strategy focused on encouraging inclusiveness, communication is key. Cultural differences in communication are bound to lead to tensions on occasion. Make your students aware of this and encourage them to be tolerant and receptive of the differences. Encourage a culture of curiosity and tolerance by fostering open and honest

communication so that they can begin to unravel the nuances involved in developing cultural competency. Facilitate such communication through social gatherings like ice cream outings, mixers or celebrations of various important cultural holidays/ festivals.

Unseen and unappreciated challenges for simple things in life: There are several invisible struggles that international students (and faculty) go through during their stay. For example, many times the students do not visit home for long periods due to the financial (and time) investments involved. In some cases, this goes well beyond financial issues, as for many nationalities, including Iranians — and more recently the Chinese—, student visas are either single-entry, or they have a limited (1-2 year) period of validity. This not only prevents students from traveling home to see family, but also puts major obstacles to attending overseas conferences and workshops. Other travel bans (e.g. Muslim ban) exacerbates this situation, as the students' families are also not able to come to the US to see them, and that creates a lot of stress and anxiety among the affected international students.[9] Such long stints away from home can have subtle psychological effects on the students' wellbeing. Encourage your students to take time off and visit friends or family within the US if they cannot travel home.

Supporting the students' career navigation: The typical trajectory of an incoming international graduate student is to arrive in the US to pursue a higher degree on an F1 visa. These visas can bring their own set of issues that many advisors may or may not be aware of. Educate yourself – ask your students about their experience with visas. Upon graduation the students exercise their Optional Training Program (OPT) extension as work authorization to pursue their careers in the US and pursue the H1B visa for long term employment. These visa processes are expensive, tedious and temporary. This leads to emotional and financial burden. In addition, these visas have term limitations (usually the students have to find a job within 3 months of receiving the OPT card). As a result, the students have to find jobs within short period of time after graduation, while simultaneously, several jobs are unavailable to international students due to lack of visa sponsorships (or positions are only open to citizens and permanent residents) or governmental contractual obligations. For example, studies show that international students are far less likely to join startups compared to domestic students. This disparity is partially explained by differences in the visa sponsorship between established corporates vs startups [10]. These factors put many international students in a disadvantage and makes it more difficult to obtain jobs upon graduation.

Faculty should provide career guidance to students early in their studies and train their students in networking skills. Professional networking is equally challenging for international students due to cultural barriers. We need to work with them to identify and address the challenges they face during networking and proactively help them build their network. When we attend conferences etc we should strive to help students connect and network with potential employers.

Creating an inclusive environment with cultural competence does not require massive resources and can be achieved through small changes. These human gestures can go a long way in making a productive diverse environment where everybody benefits and is well taken care of [11,12]. I hope these suggestions motivate you to begin (and continue) on this journey of creating an environment where diversity can thrive and make giant scientific and cultural leaps. I want to end by thanking the CoMSEF community for giving me this opportunity, and for continually striving to create an inclusive and welcoming environment for all to thrive and succeed.

Acknowledgements: I want to thank Apoorv Balwani (recent PhD of our department) and Vasu Venkateshwaran (W. L. Gore and Associates) for comments on the first draft of this article. Amir Haji-Akbari (Yale), Sumit Sharma (U. Ohio), Neeraj Rai (MSU) and Jindal Shah (OSU) provided feedback on the later drafts. I want to thank Jindal and Neeraj for motivating me to write this article and Jim Pfaendtner (UW) for giving me this platform. Opinions expressed here are my own and not representative of Clemson University or the Chemical Engineering dept at Clemson.

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Research Highlight: New and Improved: How CoRE MOF 2019 is Advancing Computational Modeling of Metal-Organic Frameworks

Heather Kulik, Associate Professor of Chemical Engineering, MIT

The unique materials chemistry of porous metal-organic frameworks (MOF) has attracted intense, sustained interest for possible applications in gas storage and separation as well as selective catalysis and even quantum computing. Each MOF forms a periodic structure that can be broken down into its substituent linkers and secondary building units or metal nodes in addition to any functional groups. Early on, computational modeling has led the way in identifying new candidate MOF structures for relevant applications. However, to bridge the gap between what the experimentalist can make in the lab and what a computational modeler can imagine on a computer, it is essential to know and work with materials that reflect those that have already been synthesized. First introduced in 2014 by Chung, Snurr, Sholl, Siepmann and coworkers[1], the Computationally Ready, Experimental MOF (CoRE MOF) database provided an important first step toward that goal. The CoRE MOF database consists of structures deposited into the Cambridge Structural Database (CSD)[2] that have been prepared for computational modeling. The authors have since refined[3] their approach in the past year to expand the original set of 5,109 3D MOFs to a larger set of 14,142 3D MOFs along with several key advances. The new CoRE MOF database[3] has an improved procedure for identifying and removing free solvent molecules, recovering disordered structures, and mapping between literature references and CSD structural files. While experimentalists will often deposit fairly similar structures in different works that will all enter into the CoRE MOF database, the authors estimate[3] the database likely contains nearly 80% unique structures or around 11,000-12,000 of the total set.

This significant CoRE MOF database advance is already being exploited to accelerate innovation in computational modeling. These include new attempts at high-throughput screening of MOFs for C-H activation[4] or in building machine learning models to predict properties related to gas separations and storage such as surface area[5] and adsorption isotherms[6]. Given that the CoRE MOF resource provides a mapping between the structures and the literature associated with them in an easy to use resource, one can easily imagine continued applications that bring computational chemists and data scientists ever closer toward understanding and working directly with data from hundreds of experimental efforts, for example through using natural language processing[7] to learn more about properties of computationally-ready MOFs. Other researchers have recognized the immense possibilities and demand for new MOF structures, and new tools are also being developed in conjunction with the CSD itself to allow for expansion and analysis of experimental structures[8]. A caveat should be raised that working only with CoRE-MOF or other data sets of experimental structures may lead us as computational modelers to inherit the biases that scientists are beginning to uncover from analysis of experimental synthesis efforts[9]. Nevertheless, CoRE MOF 2019 represents an excellent starting point to bridge between what the experimentalist and computational modeler can imagine, allowing the two to speak (more of) the same language in advancing the design and discovery of materials.

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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.

Sumeet Pandey
2010 Grad Student Award winner (University of Massachusetts Amherst, Advisor: Dimitrios Maroudas)
Poster Title: Thermodynamic and Electronic Properties of Ternary Compound Semiconductor Quantum Dots

S. C. Pandey received a Ph.D. degree in Chemical Engineering from University of Massachusetts-Amherst (Amherst, Massachusetts USA). He joined Micron Technology, Inc. (Boise, Idaho USA) in 2011 as an engineer in the Emerging Memory Group developing fundamental understanding of materials and device physics of new memory cells for ReRAM, CBRAM, PCRAM, STT-RAM, FeRAM. He has led projects on DRAM cell development and predictive modeling of materials (HM, cell, WL) and NAND processes (DE, CVD/ALD, PVD, WP, ALE, etc.). He is currently Senior Member of Technical Staff, leading the advanced materials, process, chemistry, and structure modeling activities for Memory Technology Development. His technical interest is in synergistically combining *ab initio*, first-principles, atomistic, computational materials, plasma, feature-scale, multi-scale, and multi-physics (DFT, MD, MC/kMC, PI, PF, CFD, FEA, FD, FV, etc.) approaches with targeted experiments, characterization, statistical and ML/DL/AI techniques to enable accelerated and differentiated memory technology development at reduced cost. Dr. Pandey holds over 44 patents, 6 innovation awards, COMSEF GS and MRX EI awards, and has published more than 25 papers in refereed journals. He has presented at 30 technical conferences and delivered 6 invited talks/tutorials. He is SRC liaison and a member and reviewer for over 12 external journals from various professional societies.

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 17-22, 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. 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!