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

June 2023

In This Issue

Pfaendtner Winner of 2022 CoMSEF Impact Award

Professor Jim Pfaendtner from the Department of Chemical Engineering at the University of Washington is the winner of the 2022 CoMSEF Impact Award. He is cited "***for contributions to methods and applications in the field of molecular simulation of interfacial phenomena of biomolecules.***" Before joining the faculty at Washington, Jim completed his B.S. in chemical engineering from Georgia Institute of Technology and obtained a Ph.D. in chemical engineering from Northwestern University in 2007 under the direction of Linda Broadbelt. He also completed postdoctoral research with Greg Voth and Michele Parrinello from 2007-2009. Jim has recently been named the Louis Martin-Vega Dean of the College of Engineering at North Carolina State University with an appointment that becomes effective August 1. Jim delivered a presentation describing his research during the CoMSEF Plenary Session at the 2022 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.

Statt Winner of the 2022 CoMSEF Young Investigator Award

Professor Antonia Statt from the Department of Materials Science & Engineering at the University Illinois Urbana-Champaign is the 2022 winner of the CoMSEF Young Investigator Award. She is cited "***for the development and application of innovative computational method and models to understand polymer thin films, colloid-polymer systems, and disordered proteins***." Statt joined the faculty at Illinois in 2019. Before that she was a postdoctoral fellow at the Princeton Center for Complex Materials where she worked in the lab of Prof. Athanassios Z. Panagiotopoulos. She obtained her PhD in the lab of Prof. Kurt Binder in Physics at the University of Mainz in Germany. Statt delivered a presentation describing her research during the CoMSEF Plenary Session at the 2022 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.

Nandy and Jones win 2022 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 AIChE Annual Meeting: Aditya Nandy (MIT, Advisor: Heather Kulik) and Mike Jones (U. Chicago, Advisor: Andy Ferguson). 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.

Research Highlight: From Movies to Materials – Computational Recommendations of Nanoporous Materials

Reid C. Van Lehn, Department of Chemical and Biological Engineering, University of Wisconsin-Madison

A common challenge in materials design is identifying materials that satisfy constraints on multiple properties simultaneously when information for some of these properties is missing. For example, large numbers of unique nanoporous materials (NPMs), such as metal-organic or covalent organic frameworks, can be synthesized for applications in gas storage, separations, or sensing. For these applications, materials design requires knowledge of gas adsorption properties; however, it is likely that adsorption properties are only available for a fraction of all relevant NPM-gas combinations and obtaining a complete set of adsorption properties using experiments or simulations is prohibitively time-consuming.

To address this challenge, a recent article published in *Chemistry of Materials* by Sturlson, Raza, McConachie, Siderius, Zern, and Simon, entitled "Recommendation System to Predict Missing Adsorption Properties of Nanoporous Materials," describes a computational method to simultaneously predict multiple adsorption properties for NPMs. In analogy to the recommendation system used by Netflix to suggest movies based on user ratings, the authors' approach fills in missing entries of an NPM-property matrix that has rows representing NPM materials ("movies"), columns representing adsorption properties ("users"), and entries representing numerical values of these properties ("ratings"). Each entry of the full NPM-property matrix is approximated as the sum of an NPM-specific bias and the dot product of two low-dimensional vectors, one for the NPM and one for the property. Entries in all such vectors define latent space representations of the NPMs and properties, respectively, and are learned based on known entries of the full NPM-property matrix then used to predict values for unknown entries.

The authors demonstrate their approach by predicting numerical values of 16 simulated adsorption properties (related to the uptake of CH_4, H_2O, O_2, and other gases) for 572 experimentally reported porous covalent organic frameworks (COFs), thereby defining an NPM-property matrix with 9,152 entries. The authors randomly remove entries from this matrix to enable model training (on the remaining entries) and testing (on the removed entries). High prediction accuracy was obtained when training with up to 60% of the entries removed; in particular, COFs were ranked accurately for 15 out of 16 of the simulated adsorption properties. Further analysis of the low-dimensional COF and property latent space representations demonstrated that COFs could be grouped by adsorption performance to recommend high-performing materials or guide experimental data collection. Notably, this approach does not require the calculation of hand-crafted COF chemical or structural features, although the authors suggest the addition of such features (in analogy to annotating movies with information on genre or actors) as an opportunity for future exploration. The proposed method is an exciting example of how computational modeling can rapidly identify candidate materials to inform experimental investigation and could be broadly useful for materials systems beyond NPMs. Toward this end, the Julia code used in this work is publicly available to encourage adoption by the community.

A Broader View: Building community through personal stories

Eric Jankowski, Associate Professor, Materials Science & Engineering Department, Boise State University

I'm hunched over a table, blowing eraser shards off my paper, frantically trying to fix an integration-by-parts on a final exam when Professor Gulari swipes my water. He clunks down a heavy-sounding glass bottle in its place. "Maybe this will help you think better?", he mutters, walking out of the classroom with my Michigan-branded nalgene.

It does not help me think better. I have already gotten in trouble as an undergraduate for recycling beer cans in the AIChE office, so there are sirens blaring and red strobes flashing in my mind. I'm a first year graduate student and nothing matters more to me than showing the department that they hadn't made a mistake in admitting me. I'd been rejected everywhere else I applied. I have to make it here. Therefore, instead of integrating by parts, I'm thinking about how this bottle of cognac is alcohol on campus, the same two ingredients that caused so much trouble last year. I'm terrified. My fingers sweat as I visualize getting an email from Sharon, my advisor, with the subject "My Office. Now." I'm even more worried that she will realize she can just Reply-All to an email chain with the same subject from last year.

I need to complete this test, but I can't. I can't stop freaking out about how my time in grad school is up. Am I going to get ejected for having cognac in class? Or Am I going to be ejected because I'm spending this whole test worrying about having cognac in class and I fail the exam? Either way, time's up for Jankowski. Professor Gulari returns to silently swipe my test. My nalgene is not returned. Professor Ziff enters to deliver the fluids exam. He sizes up the bottle and notices "Cognac?"

I panic, pleading: "Professor Gulari proposed a joke-telling contest because we were falling asleep each morning and I think this was the prize he'd promised to the winner and I only won because nobody else told a joke and I would never bring cognac to class, it was Gulari! And I think he stole my nalgene, and please don't expel me!". The email from Sharon comes hours later. As I trudge up the stairwell of GG Brown to my demise, Professor Kotov trots down the other way, singing "Jaaaankowskiiiii! I heard about youuuu!" I'm dead meat. So dead.

Sharon is not happy. She has just come from a faculty meeting where Ziff asked Gulari about the cognac. Apparently, some faculty are shocked and upset that he'd give alcohol to a student during an exam. Apparently, Gulari feels cornered, like he needs to explain why he had done so. Apparently, Gulari repeats the joke that I had inadvisably shared months ago. Telling the joke in the faculty meeting does not help him. Nor me.

There are lots of emails. And meetings that go on. For weeks. They go on long enough that I begin to get less frightened about being kicked out of the program, and increasingly confused about why I haven't. I'm certain I would've fired me if I was in the department's position. It begins to dawn on me that at the very least, Sharon has my back. It dawns on me that it is not uniformly the case that the faculty want me gone. That couldn't possibly be true if we're still having meetings. The cognac that once represented despair and failure is slowly transforming. It's aging into something more like inspiration. I'm inspired when Ziff accepts an invitation to a football tailgate and we try the cognac together: It tastes like faculty believing in me.

I wish I learned quickly from this brush with trouble, but it would take years to recognize how my fear had stemmed from my lack of power, how privileged I was to have faculty in my corner, and how incidents like these happen all the time, but without a happy ending. Those power structures persist in our departments today, and I think about that cognac every time we make decisions about whom to support, about whom to punish, about whom to protect.
And I think about Gulari, and whether my nalgene stuck with him the way his cognac stuck with me.
//
As you read this personal, true, story about science, did you find yourself connecting? Maybe you also struggled with trouble, or maybe you had a mentor stand up for you? Whatever your response, the personal stories are an opportunity to engage with audiences in multiplex ways, orthogonal to the unambiguous interpretations we strive for in our papers, posters, and talks. Because personal stories help us understand each other, I think writing and sharing them can play a role in our profession. In the classroom, they offer an opportunity to show vulnerability and build trust. At conferences, they provide a rare forum for catharsis of failures. In our departments, they are a way to understand with whom we work and how they're motivated. Sharing stories is the fundamental mechanism by which communities are created.

For the past five years, I've been working with The Story Collider, a national nonprofit whose mission is to share the humanity behind science through live shows, podcasts, and workshops. We run faculty workshops centered on how to teach story writing in STEM contexts, student workshops focused on drafting personal stories, and live performance shows on stage. Our studies are revealing that student stories about overcoming hardship and choosing engineering are correlated with increased confidence and belonging in the major. Less measurable–but still real–is observing students seizing control over their narratives and the classmates transforming into support networks.

At the workshops we show how personal stories are characterized by (1) believable characters, (2) who experience meaningful events, and (3) who have to deal with the consequences. In my example above cognac trouble happens, but it's really about how I changed from being self-centered to more attuned to the power structures in higher education. The believability of my character is built through vulnerability, and through describing a few scenes in the first-person. Through scene identification activities, analysis of change, and tips for starting and stopping we help tellers craft their first drafts.

Now funded by the NSF (#2142137), this collaboration is expanding, taking the preliminary studies from my thermodynamics classes and testing them across disciplines. We're also developing pedagogical materials to make it easier to try out with students and colleagues. I'm hopeful that someday soon we'll have enough interest for a CoMSEF show, and I'm curious to see the connections, collaborations, and support it might catalyze.

Where are They Now?

Andrew White
2012 Grad Student Award winner (University of Washington, Advisor: Shaoyi Jiang)
Poster Title: Modeling Nonspecific Interactions in Biology

Andrew White received his PhD from University of Washington in 2013 and then did a postdoc at University of Chicago. Andrew is now an associate professor at the University of Rochester department of chemical engineering. His research group develops computational methods to study peptides and proteins. Since winning the CoMSEF graduate student award, Andrew got married, bought a house, adopted a dog, had 2 sons, and of course wrote the famous emoji-chem software that draws molecules with emojis instead of element symbols. In addition to science, Andrew likes eating good food, going on vacation, spending time with family and friends, and running fast. And where is Andrew now? Probably on Twitter.

Upcoming Conferences of Interest to CoMSEF Members

International Congress on Quantum Chemistry
Bratislava, Slovakia
June 26-July 1, 2023
https://icqc2023.org/

9th Annual CCPBioSim Conference: Biomolecular Simulations for a Better World
Leeds, UK
July 10-12, 2023
LINK

Data Analytics and Computational Modeling for Next Generation Molecular Design
West Dover, VT
July 16-21, 2023
LINK

Foundations of Process/product Analytics and Machine learning (FOPAM)
Davis, CA
July 30-August 3, 2023
https://fopam.cache.org/

26th International Conference on Chemical Thermodynamics (ICCT-2023)
Osaka, Japan
July 30-August 4, 2023
https://iupac.org/event/icct-2023/

STATPHYS28
Tokyo, Japan
August 7-11, 2023
https://www.statphys28.org/

ACS Fall Meeting
San Francisco, CA
August 13-17, 2023
LINK

AIChE Annual Meeting
Orlando, FL
November 5-10, 2023
LINK

Supercomputing 23
Denver, CO
November 12-17, 2023
https://sc23.supercomputing.org/

33rd European Symposium on Applied Thermodynamics
Edinburgh, UK
June 9-12, 2024
https://www.esat2024.eng.ed.ac.uk/

MRS Fall Meeting
Boston, MA
November 26-December 1, 2023
LINK

MRS Spring Meeting
Seattle, WA
April 22-26, 2024
LINK

22nd Symposium on Thermophysical Properties
Boulder, CO
June 23-28, 2024
https://thermosymposium.org/

The Role of Theories, Simulation, and Machine Learning in Materials Discovery
Newry, ME
July 21-26, 2024
LINK

Foundations of Molecular Modeling and Simulation (FOMMS)
Snowbird, UT
July 28-August 1, 2024
https://fomms.cache.org/

12th Liquid Matter Conference
Mainz, Germany
September 22-27, 2024
http://lmc2024.com/

13th Triennial Congress of the World Association of Theoretical and Computational Chemists
Oslo, Norway
June 22-27, 2025
https://watoc2025.no/

The 12th Industrial Fluid Properties Simulation Challenge

The 12th Industrial Fluid Properties Simulation Challenge will focus on the topic of reliably predicting physical properties of fluid mixtures. From industrial processes to formulated products, the properties of complex multi-component mixtures are important in many industrial contexts, and the number of possible combinations of ingredients exceeds what is practical to screen by relying only on experimental data (even if high throughput). In terms of physical property models, mixture properties can be challenging to predict without relying on empirical binary interaction parameters or mixing rules. This limits the usefulness of modeling to truly lead new formulation design efforts with ingredient combinations that are lacking in existing experimental data. New machine learning approaches to formulation design are less advanced than those for molecular design and will also be limited by available experimental data. Thus, physics-based and/or hybrid fundamental/empirical modeling approaches for predicting mixture properties that are broadly applicable and reliable and require minimal supporting experimental data are highly desirable. Note that, for example, a public data resource titled "Experimental data sets for viscosity and surface tension of binary mixtures at the temperatures (293.15 to 323.15) K and the pressures (99.325 to 103.325) kPa" has recently been published by NIST: LINK.

Timeline

- As Soon As Possible: communicate your intention to submit predictions from either molecular modeling or other methods by email to admin@fluidproperties.org
- October 23, 2023: Final entries due (email entries to admin@fluidproperties.org)
- November 2023: Champions announced at the AIChE Annual Meeting

Challenge

Predict the viscosity of the following binary mixtures

- 1-decanol and Tributyrin (Propane-1,2,3-triyl tributanoate)
- 1-decanol and 1,2-butanediol

at 25 degrees Celsius and mixture compositions of 10, 33, 50, 67, and 90 weight percent of 1-decanol.

The scoring criteria will include comparison of both

- the predicted and measured viscosity values at the listed compositions
- the predicted and measured viscosity values at the listed compositions relative to the predicted and measured viscosity of 1-decanol

More info about the 12th Challenge is available at http://fluidproperties.org/12th

The Industrial Fluid Properties Simulation Challenge is an open competition with the goals of driving 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.

Foundations of Process/product Analytics and Machine learning

FOPAM 2023

University of California, Davis **July 31-August 3, 2023**

fopam.org

- Preceded by an optional 1-1/2-day workshop (Leo Chiang, Bhushan Gopaluni, Ali Mesbah)
- Opening keynote by Cenk Ündey, VP & Global Head of PTD Data & Digital, Roche/Genentech.
- Morning and evening presentation sessions with panel/audience Q&A:

Zavala (Wisconsin)	Severson (Microsoft)	Findeisen (Darmstadt)
Kevrekidis (JHU)	Ulissi (META / CMU)	Wang (Tsinghua)
Ozkirimli (Roche)	Garcia (Eli Lilliy)	Venkatasubramanian (Columbia)
Hohl (Shell)	Braun (Dow)	Hedengren (BYU)

- Breakfast, lunch, evening hospitality.
- Two afternoon poster sessions plus small-group discussions, unstructured activities.
- On the last evening, conference banquet with brief rapporteur analyses.
- See website for speakers, deadlines, and rates; watch for possible junior-attendee travel awards.

Poster submission / travel award applications by May 15; early registration by ~~June 5,~~ June 19

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!