



Newsletter

AIChE[®]

Kulik Winner of 2023 CoMSEF Impact Award



Professor Heather J. Kulik from the Department of Chemical Engineering at the Massachusetts Institute of Technology (MIT) is the winner of the 2023 CoMSEF Impact Award. She is cited **“for pioneering methods bridging accelerated first-principles and multi-scale simulations with data-driven machine learning to guide the design of transition metal-based catalysts and enzymes.”** Prior to joining the faculty at MIT in 2013, Heather completed postdocs at Lawrence Livermore (2010) and Stanford (2010–2013). She received her PhD from MIT in 2009. Heather will deliver a presentation describing her research during the CoMSEF Plenary Session at the 2023 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.

November 2023

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Lindsey Winner of the 2023 CoMSEF Young Investigator Award



Professor Rebecca K. Lindsey from the Department of Chemical and Engineering at the University of Michigan is the 2023 winner of the CoMSEF Young Investigator Award. She is cited **“for transformative advances in understanding chemistry under extreme conditions, made possible by her pioneering developments in machine learned interatomic model frameworks.”** Prior to joining the faculty at Michigan in 2022, Rebecca led various research teams within the Energetic Materials Center at Lawrence Livermore National Laboratory as a post-doctoral associate and staff research scientist. She received her PhD from the University of Minnesota, Twin Cities in 2016. Prof. Lindsay will deliver a presentation describing her research during the CoMSEF Plenary Session at the 2023 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.

2023 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded after the AIChE Annual Meeting in Orlando. 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.

CoMSEF Elections

The annual CoMSEF election is currently underway and will select two liaison directors who:

- Facilitate programming with other organizations by identifying opportunities for co-sponsorship
- Communicate and advocate CoMSEF activities with other organizations.
- As members of the Executive Committee, aid the other officers in developing and carrying out CoMSEF activities and preparing the CoMSEF newsletter.

CoMSEF Business Meeting in Orlando

CoMSEF will hold its annual General Meeting on Wednesday November 8 from 6:15-7:15 pm in Rock Spring I/II (Lobby Level, Hyatt Regency Orlando). As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend.

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

A Broader View: A Perspective on DEI and the 2023 Annual Meeting

Andrew L. Ferguson

Associate Professor and Vice Dean for Equity, Diversity, and Inclusion, University of Chicago

Vice Chair of CoMSEF

The AIChE Annual Meeting is a fixture for many of us in the CoMSEF community, presenting an opportunity to connect with colleagues, present work, support our trainees, and keep abreast of new developments in the field. For many of us, the choice of Orlando, FL as the venue for the 2023 Annual Meeting means that this year's event may feel somewhat different. The actions of the DeSantis administration in signing a slate of anti-LGBTQ+ legislation [1], curtailing diversity, equity, and inclusion (DEI) activities within the state educational system [2], and promoting anti-intellectual book banning campaigns [3] has made some within our community reticent to attend the meeting in protest of these policies or, in some cases, out of a fear for personal safety.

The current political stance of the state is chilling towards science and inclusivity and runs counter to the DEI principles of AIChE enshrined in the IDEAL framework [4]. In response to these concerns, AIChE released a special statement [5] in May 2023 announcing that although the meeting would go ahead as planned, steps were being taken to engage local community groups in the Orlando area, evaluate potential future venues for compatibility with the precepts of the organization, and noting that the venue was selected back in 2017 and that there are no current plans to return to Florida. Planning and organizing the Annual Meeting is no small feat and the political climate can change markedly over the years of lead time required to secure venues and organize the event. Moving it at short notice may be impracticable, while canceling it, although representing a strong statement of solidarity with the communities impacted by recent policies in the state, may also harm those in our community, in particular our more junior members, who may be reliant on the meeting as a critical event for professional networking, scientific exposure, and career advancement. Some of us have chosen to boycott this year's event, others would like to do so but feel compelled to attend at risk of damaging their career prospects, and some, like myself as the current CoMSEF Vice Chair, feel compelled to attend to fulfill professional duties and obligations to our professional communities.

Although I found the special statement from AIChE less vociferous than I would have liked [5], I have, in general, been very proud of AIChE's strong stance as an equitable and welcoming professional society. I find the IDEAL – Inclusion, Diversity, Equity, Anti-Racism, Learning – framework to be a strong and thoughtful statement of these values to the AIChE community [4], the Code of Conduct for meeting attendees to reflect these values within an environment of tolerance and respect [6], and appreciate the strong representation of DEI communities such as the LGBTQ+ & Allies, Minority Affairs Community (MAC), Women in Chemical Engineering (WIC), and the Disability & Outreach and Inclusion Community (DORIC) [7]. I have been proud to be a long-time affiliate of CoMSEF, which I have always found to be an extremely supportive and welcoming organization with the good fortune to have had leadership over the years with a strong commitment to advancing DEI efforts in tandem with a commitment to computational molecular science and engineering. I personally have been inspired by the commitment, words, and actions of longtime members, laureates, and leaders within CoMSEF including Jim Pfaendtner, Scott Shell, Coray Colina, and Sapna Sarupria. CoMSEF has presented a welcoming environment for junior researchers and has endeavored to offer them promotion and exposure through the “Graduate Student Award in Computational Molecular Science and Engineering” and “Young Investigator Award for Modeling and Simulation”. The “Spotlights in Thermodynamics and Computational Molecular Science” technical session started by Scott Shell and Coray Colina in 2018 seeks to highlight diverse researchers and research directions and promote emerging leaders in the field.

We can, of course, do more and I believe that it is the duty of those in leadership positions to maintain a commitment to advancing both the scientific and DEI mission of CoMSEF and AIChE. A small-but-vocal minority of our colleagues disagree with this perspective and have positioned DEI efforts as somehow incompatible with meritocratic and objective scientific inquiry [8]. These views, however, are largely based on the faulty logic of a universal objective conception of merit, a denial of the complicity of the scientific enterprise in historical discrimination of particular groups and its duty to repair these past hurts, and a narrow conception of the role of scientific inquiry within a pluralistic and modern society. As I recently argued in an Op Ed written with colleagues at UChicago [9], DEI efforts are completely compatible with rigorous scientific inquiry and a failure to advance these efforts hurts both the “missing scientists” selected out by a biased system and the scientific enterprise at large by failing to recruit and promote the top talent. Policies to recruit, retain, and promote top talent from groups who have suffered historic discrimination is not somehow patronizing, discriminatory, bigoted, or ideological, but rather completely in line with best practices to identify and support the best and the brightest within the context of their own unique circumstances and, to the degree possible, correcting for inherent biases in the system. Indeed, the National Academies of Sciences, Engineering, and Medicine recently published “Advancing Antiracism, Diversity, Equity, and Inclusion in STEMM Organizations: Beyond Broadening Participation” [10] as a thoroughly researched report offering actionable precepts and “evidence-based action to remedy unfair systems, structures, and institutions that advantage some and disadvantage others on the basis of race and ethnicity ... and impede the full talent pool of our nation from pursuing and advancing in STEMM careers.”

The opinions articulated herein are my own, but I believe that they reflect the overwhelming consensus of the scientific community that DEI efforts are completely compatible with rigorous scientific inquiry and, in fact, an essential tool in realizing the full potential of the top talent within our respective disciplines. As we prepare for the 2023 Annual Meeting where some of our colleagues have chosen to be absent, this provides an opportunity to reflect upon and recommit to our values as a community and how we choose to act upon and stand for these beliefs within our own professional and scientific endeavors.

1. <https://www.hrc.org/press-releases/gov-desantis-signs-slate-of-extreme-anti-lgbtq-bills-enacting-a-record-shattering-number-of-discriminatory-measures-into-law>
2. <https://www.npr.org/2023/05/15/1176210007/florida-ron-desantis-dei-ban-diversity>
3. <https://apnews.com/article/ron-desantis-2024-book-bans-libraries-republicans-9f3c944117e58bb5a3e4c9fef0d3b0e0>
4. <https://www.aiche.org/equity-diversity-inclusion/statement>
5. <https://www.aiche.org/annual/special-message>
6. <https://www.aiche.org/resources/conferences/code-conduct>
7. <https://www.aiche.org/community#panels-pane-card-list-card-list>
8. <https://dx.doi.org/10.35995/jci03010001>
9. <https://chicagomaroon.com/39973/viewpoints/op-ed/in-defense-of-dei-in-science/>
10. <http://nap.nationalacademies.org/26803>

Research Highlight: Alleviating Separation Anxiety with Polymer Membranes

Janani Sampath, Chemical Engineering, University of Florida

Separations are at the core of many chemical industries, amounting to 15% of the total energy consumption in the United States.¹ These include purification of crude oil, extraction of rare earth elements, and seawater desalination. Studies show that integrating current methods of industrial separation, such as distillation, with membrane separations, can reduce the energy used by a factor of 2-3. Polymers are attractive membrane materials as they are tunable, scalable, cost efficient and mechanically robust. Despite their many benefits, state-of-the-art polymers are not utilized on a commercial scale due to phenomena like plasticization and aging, which reduces membrane efficiency over time.²

With the advent of high free volume polymers, such as polymers of intrinsic microporosity and thermally rearranged polymers, there has been an uptick in interdisciplinary membrane research, with collaborations cutting across different fields like polymer chemistry, polymer physics, computational science, and separations engineering. This is evidenced in several recent publications; two of which are highlighted below.^{3,4}

In a study published in 2020, Barnett et al. used machine learning on ~700 experimentally available data of polymer gas-pairs. They were able to predict the gas separation performance of over 10,000 untested polymers and synthesized the 2 most promising candidates predicted by model, which they found exceeded the performance of current state of the art membranes.⁵ Recently, Bruno et al. used triazole click chemistry to synthesize a new family of polymers named DUCKY which can be used to extract and purify crude oil.⁶ To understand the separation mechanism in these polymers, molecular dynamics simulations was used. They found that these polymers are moderately dynamic, with transient interconnections between micropores contributing to their high separation efficiencies.

Multidisciplinary teams are necessary, owing to the interplay of different microscopic interactions that dictate emergent macroscopic functions in polymer membranes, as well as the vast chemical design space that is now available. And while success stories are encouraging, there are several challenges that need to be overcome, that call for tighter integration between experimental and computational groups.⁷ But this opens the door to new opportunities, and the convergence of different fields makes this an exciting time for separations research!

1 Sholl, D. *et al. Nature* 532, 435 (2016)

2 Koros, W. J. *et al. Nat. Mater.* 16, 289–297 (2017)

3 McDermott, A. G. *et al. J. Mater. Chem. A* 2, 11742–11752 (2014)

4 Kupgan, G. *et al. Chem. Rev.* 118, 5488 (2018)

5 Barnett, J. W. *et al. Sci. Adv.* 6, 1–8 (2020)

6 Bruno, N. C. *et al. Nat. Mater.* (2023)

7 Kumar, M. *et al. Proc. Natl. Acad. Sci.* 118, (2021)

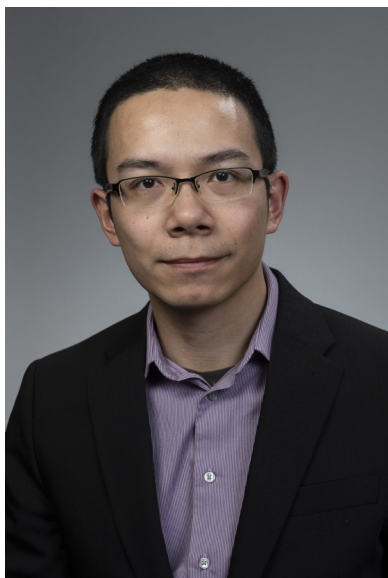
Where are They Now?

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.

Peng Bai

2013 Grad Student Award winner (U. Minnesota, Advisors: J. Ilja Siepmann and Michael Tsapatsis)

Poster Title: [Molecular Simulation Studies of Adsorption and Diffusion of Complex Molecules in Zeolites](#)



Peng Bai received his PhD from the University of Minnesota and continued there with a postdoc in the group of Matthew Neurock, where he learned about computational catalysis and electrochemistry. In 2018, he joined the Department of Chemical Engineering at UMass Amherst as an Assistant Professor. His group's research focuses on the development of molecular simulation, first-principles, and data science methods, with applications to the catalytic upcycling of plastics, separation with nanoporous materials, and ion conduction in solid-state batteries. Away from research, he likes to play VR, 3D printing, and other over-priced toys (LEGO Mindstorms Robots) with his two daughters. He volunteers to mod 3D printers with his experimental colleagues, getting dangerously close to the dark side.

Upcoming Conferences of Interest to CoMSEF Members

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/>

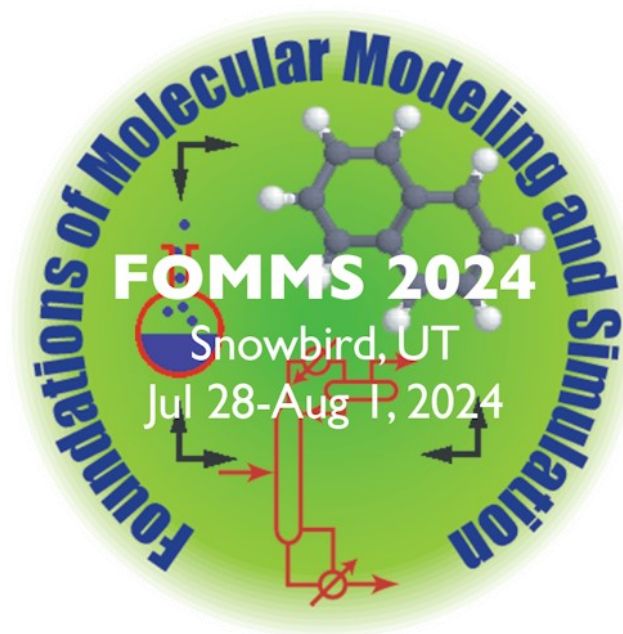
FOMMS 2024

The Foundations of Molecular Modeling and Simulation (FOMMS) meeting will be held July 28-August 1, 2024 in Snowbird, UT. FOMMS 2024 will be the ninth triennial FOMMS conference showcasing new developments and applications of computational quantum chemistry, statistical mechanics, molecular simulation and theory, and continuum and engineering process simulation.

- Erik Santiso (NC State University)
- Paulette Clancy (Johns Hopkins University)
- Jianwen Jiang (National University of Singapore)
- Olexandr Isayev (Carnegie Mellon)
- Sukrit Mukhopadhyay (Dow Chemical)
- Mark Tuckerman (New York University)
- Thijs Vlugt (TU Delft)
- Julia Deshemuchadse (Cornell University)
- Shaama Sharada (University of Southern California)
- Pratyush Tiwary (University of Maryland)
- Rachel Getman (Ohio State University)
- Birgit Strodel (University Düsseldorf)
- Jeetain Mittal (Texas A&M University)
- Tamar Schlick (New York University)
- Tiffany Walsh (Deakin University)
- Nathan Baker (Microsoft)

More information may be found at the conference website

<https://fomms.cache.org/>



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!