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

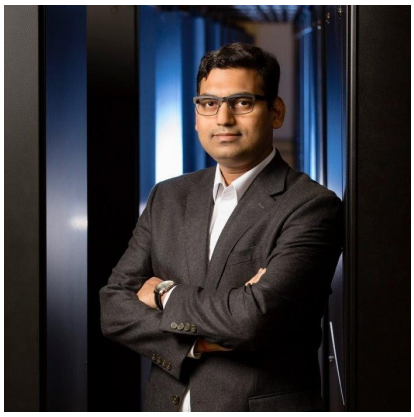
AIChE

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Shukla Winner of 2026 CoMSEF Impact Award



Dr. Diwakar Shukla, the J. W. Westwater Professorial Scholar Professor of Chemical and Biomolecular Engineering at University of Illinois at Urbana-Champaign, is the winner of the 2026 CoMSEF Impact Award. He is cited "***for development of computational molecular science and engineering methods related to biomolecular dynamics and their application to plant biology***." Prior to joining the faculty at UIUC in 2015, Diwakar was a SIMBIOS Distinguished Postdoctoral Fellow with Prof. Vijay Pande at Stanford University (2011-14) and earned a PhD in chemical engineering with Bernhardt Trout at MIT (2007-11). Dr. Shukla also won the CoMSEF Graduate Student Award in 2010 and the Young Investigator Award in 2018. He will deliver a presentation describing his research during the CoMSEF Plenary Session at the 2026 AIChE Annual Meeting. The CoMSEF Impact Award recognizes outstanding research in computational molecular science and engineering, encompassing both methods and applications, and is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

Sampath Winner of the 2026 CoMSEF Young Investigator Award



Dr. Janani Sampath, Assistant Professor of Chemical Engineering at the University of Florida is the 2026 winner of the CoMSEF Young Investigator Award. She is cited "***for advances in molecular simulation linking polymer physics, biomolecular systems, and data-driven design to reveal structure–property relationships and enable predictive modeling of complex soft materials***." Prior to joining the University of Florida faculty in 2021, Janani was a postdoctoral research associate with Jim Pfaendtner and Chris Mundy at UW Seattle and Pacific Northwest National Laboratory (2018-20), and earned a PhD in chemical engineering with Lisa Hall at The Ohio State University (2014-18). Janani will deliver a presentation describing her research during the CoMSEF Plenary Session at the 2026 AIChE Annual Meeting. The CoMSEF Young Investigator Award recognizes outstanding research in computational molecular science and engineering, encompassing both methods and applications, and is given annually to a CoMSEF member who is within 7 years of completion of their highest degree.

Yu Winner of the 2026 CoMSEF Postdoctoral Scholar Award for Modeling and Simulation sponsored by MSDE

Dr. Jiwon Yu, Postdoctoral Fellow at the University of Texas at Austin is the 2026 winner of the CoMSEF Postdoctoral Scholar Award for Modeling and Simulation. She is cited "***for advancing molecular simulations of reactive systems by combining quantum mechanics and machine learning, enabling predictive design of energy and environmental processes***." Prior to commencing her postdoctoral research position, Jiwon earned a PhD in chemical engineering at UT Austin (2020-24) after completing a MS and BS in chemical engineering and materials science at Ewha Womens University. Jiwon will deliver a presentation describing her research during the CoMSEF Plenary Session at the 2026 AIChE Annual Meeting. The CoMSEF Postdoctoral Scholar Award for Modeling and Simulation recognizes outstanding research in computational molecular science and engineering, encompassing both methods and applications, among postdoctoral scholars. The award is sponsored by Molecular Systems Design & Engineering (https://www.rsc.org/journals-books-databases/about-journals/msde/), an interdisciplinary journal reporting cutting-edge molecular engineering research that is jointly owned by the Royal Society of Chemistry (RSC) and the Institution of Chemical Engineers (IChemE).

CoMSEF Business Meeting in Minneapolis

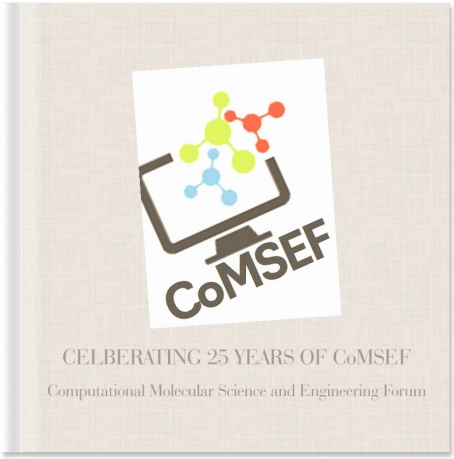
CoMSEF will hold its annual General Meeting on Wednesday November 11 from 6-7 pm in 210 (Room 213AB on Level 2, Minneapolis Convention Center). As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend.

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

CoMSEF's 25th Anniversary Celebration at the 2025 Annual Meeting

We celebrated the 25th anniversary of CoMSEF at last year's AIChE Annual Meeting in Boston with two special events…

First, a session titled "25 Years of CoMSEF: Past, Present, and Future" was organized featuring invited talks addressing aspects of the session theme:



CoMSEF Today -- and Its Origins
Phillip Westmoreland

25 Years of CoMSEF
Sapna Sarupria

Future of CoMSE Methods and Computation - Chemistry
J. Ilja Siepmann

Future of CoMSE Methods and Computation from a Materials Perspective
Sharon Glotzer

Future of CoMSE Methods and Computation from a Bio Perspective
Andrew Ferguson

Future of CoMSE Industrial Applications
Jonathan Moore



Invited speakers: (from left) J. Ilja Siepmann, Sapna Sarupria, Jonathan Moore, Phillip Westmoreland, Sharon Glotzer, and Andrew Ferguson

Sapna Surpria also created a small book with content contributed by various members of CoMSEF that "...captures and celebrates the 25 years of the history of CoMSEF with the narrative of its origin and journey." The book is available for purchase from Shutterfly in hardcover and softcover versions.

We also marked this special milestone with a happy hour complete with bowling, games, food, and drinks at Kings Dining & Entertainment. It was a great time to connect, celebrate, and share in the fun with the CoMSEF community! A special thank you to the NC State College of Engineering for generously sponsoring this event.

FOMMS 2027 abstract submissions are now open

Abstract submissions are open for FOMMS 2027, taking place July 11-16, 2027, at The Cliff Lodge at Snowbird, Utah! Celebrating the 10th FOMMS Conference and three decades of FOMMS, this year's conference will center on the theme "Molecular Modeling and Simulation: From Property Prediction to Inverse Design."

An outstanding set of confirmed keynote and plenary speakers have been assembled. Visit the FOMMS 2027 website to learn more about the conference and view the confirmed speakers.



Submit Your Abstract

FOMMS 2027 welcomes submissions describing new research in molecular modeling and simulation, including work based on AI and machine learning, electronic structure methods, classical force fields, and theory.

For the first time, abstracts will be reviewed on a rolling basis throughout the submission period. Authors may submit at any time, with submissions grouped into review batches and decisions communicated following the completion of each batch.

This new process provides authors with greater flexibility to plan their attendance and allows additional time for those who may need to complete a visa application. International authors who may require a visa are encouraged to submit early.

The final abstract submission deadline is March 31, 2027, Anywhere on Earth (AoE).

[SUBMIT AN ABSTRACT]
Submission guidelines, the abstract template, topic themes, keywords, and rolling review schedule are available on the FOMMS 2027 website.

Get Your Movies Ready!

FOMMS Movie Night is returning in 2027! Authors of accepted abstracts will be invited to optionally contribute a movie showcasing the visual side of their science.

We welcome beautiful, informative, creative, and memorable visualizations, including competition entries, non-competition simulation movies, impressive visualizations of computational data, movies from the archives, and even simulations that have brought you humor or joy along the way.

As we celebrate 30 years of FOMMS, we especially encourage movies that showcase the evolution of molecular modeling and simulation or trace your own growth and journey as a simulator.

Movie submissions are optional and open to FOMMS participants.
The movie submission deadline is May 1, 2027.

[SUBMIT A MOVIE]
Competition details and movie submission instructions are available on the FOMMS 2027 website.
We look forward to seeing your latest research-and your simulations in motion-at FOMMS 2027!

Conference Alert: Recent Advances in Modeling Rare Events: Methods and Applications (RARE)

RARE 2027 will be held from 15 to 18 March 2027 in Jaipur, India.

RARE meetings are a series of international symposia organized to discuss recent advances in the field of rare event sampling of molecular systems. RARE2027 is the fifth in the series, with very successful symposiums organized in 2014 (RARE2014), 2017 (RARE2017), 2021(online) (RARE2021), and 2025 (RARE2025). The meeting will bring together participants to discuss established and novel methods to sample rare events as well as underlying theoretical principles in detail, and to form collaborations to develop new techniques to tackle this long-standing challenge. The meeting will take place in largely informal settings with relaxed schedules and post-dinner brainstorming/discussion sessions.

Broad topics covered in RARE2027 are:

- New methods for free energy calculations
- New methods for enhanced sampling
- Collective variables
- Transition path sampling and reaction kinetics
- Machine learning tools for rare event sampling
- Advanced applications of rare event sampling techniques

Further details are available on the conference website:

https://sites.google.com/view/rare2027/home

Organizers of RARE 2027: Andrew Ferguson (U Chicago); Nisanth N. Nair (IIT Kanpur); Jagannath Mondal (TIFR Hyderabad); Sapna Sarupria (U Minnesota)

Early-career researchers working on free energy calculations and enhanced sampling (methods & advanced applications) can submit an abstract for the poster session.

Abstract submission deadline: 25 October 2026

Application form: https://forms.gle/HNv1knNFHKn9ZJg87

Abstracts will be reviewed for their relevance to the conference theme, and applicants whose abstracts are selected will be invited to register.

Upcoming Conferences of Interest to CoMSEF Members

AIChE Annual Meeting
Minneapolis, MN
November 8-12, 2026
LINK

Supercomputing 26
Chicago, IL
November 15-20, 2026
https://sc26.supercomputing.org/

MRS Fall Meeting
Boston, MA
November 29-December 4, 2026
LINK

Virtual Winter School on Computational Chemistry
January 25-29, 2027
https://winterschool.cc/

RARE 2027
March 15-18, 2027
Jaipur, India
https://sites.google.com/view/rare2027/

ACS Spring Meeting
New Orleans, LA
March 21-25, 2027
https://www.acs.org/events/spring.html

MRS Spring Meeting
Seattle, WA
April 5-9, 2027
LINK

ESAT 2027
Pont Royal, France
May 9-12, 2027
https://www.esat2027.com/

FOMMS
Snowbird, UT
July 11-16, 2027
https://fomms.cache.org/