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Andrew Masuda

Career distinction awarded for pioneering advances in multiscale modeling

A chemical engineer is being recognized for his achievements in changing the way scientists approach complex molecular systems through multiscale modeling.

UC Santa Barbara chemical engineering professor M. Scott Shell has been elected a Fellow of the American Institute of Chemical Engineers (AIChE), the world's leading organization for chemical engineering professionals. This honor highlights his pioneering work in multiscale modeling and innovative computational techniques. Shell's relative entropy approach, which has advanced large-scale molecular simulations, exemplifies his continued efforts to push the boundaries of engineering and science.

AIChE, with nearly 60,000 members across 110 countries, grants the title of Fellow through election by its board of directors. This highest membership grade acknowledges those with significant professional accomplishments and contributions to the field.

"I am remarkably fortunate to have grown up professionally in the chemical engineering community, where I have been continuously inspired by talented mentors, collaborators, colleagues and students," said Shell, vice chair of UCSB's Chemical Engineering Department and the John Myers Founder's Chair of Chemical

Engineering. “This distinction carries significant personal weight because it comes from an organization of experts with whom I’ve closely worked throughout my career.”

Shell leads the Shell Lab, which develops molecular-simulation, multiscale-modeling and statistical-thermodynamic approaches to address challenges in biophysics and soft materials. His research group pioneered the relative entropy coarse-graining approach, enabling large-scale simulations of complex molecular systems. This method transforms small-scale atomic simulations into accurate coarse-grained models that can be simulated at much larger scales, advancing a new class of coarse-graining algorithms used across a variety of scientific problems.

Shell’s expertise extends to numerous interdisciplinary projects at UCSB, from water-filtration membranes and bio-derived technologies to plastic waste recycling and neurodegenerative diseases like Alzheimer’s.

His publications have been influential to his discipline, including the article, “Systematic coarse-graining of potential energy landscapes and dynamics in liquid,” (2012) — one of the seminal papers from the journal of Chemical Physics’ history selected for its 80th anniversary collection.

The Shell Lab has continued to push the boundaries of what molecular modeling can do, using the relative-entropy approach to understand and accurately simulate a wide range of phenomena. Most recently, his group pioneered computational techniques for the inverse design of soft materials, such as chemically patterned surfaces to program solute-to-surface interactions in aqueous solutions.

An elected Fellow of the American Association for the Advancement of Science, Shell previously received an Early CAREER Award from the National Science Foundation, a Sloan Research Fellowship, the Impact Award by the Computational Molecular Science and Engineering Forum of the AIChE, as well as the Outstanding Graduate Mentor Award and Distinguished Teaching Award from UCSB’s Academic Senate.

Shell, who joined UCSB’s faculty in 2007, has published nearly 100 articles, delivered more than 120 invited talks at major meetings and institutions around the world, and written the textbook, “Thermodynamics and Statistical Mechanics: An Integrated Approach,” which has been adopted by more than 130 departments worldwide.

Shell has played an active role in AIChE since 2007, having sat on the programming committee and served as a session chair during the annual meeting. Over the years, he also launched three new session series at the annual meeting to benefit the thermodynamics community.

Shell has been highly committed to the issues of diversity, equity and inclusion, leading efforts at UCSB to support students from diverse backgrounds and to engage the community in creating an inclusive and equitable environment.

AIChE will recognize Shell and other newly elected Fellows during its 2025 national conference.

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About UC Santa Barbara

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