UC San Diego
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Virtual SEMINAR SERIES

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Seminar Presentation: 11:00am – 12:00pm PDT
Zoom Seminar

"Ice nucleation without supercooling: on the search for the most potent ice nucleants"

Valeria Molinero, PhD

Jack and Peg Simons Endowed Professor of Theoretical Chemistry and Distinguished Professor at The University of Utah, and also leads the Henry Eyring Center for Theoretical Chemistry

Abstract: The crystallization of water in clouds plays a key role in weather and climate through its effect on albedo and precipitation. The unassisted, homogeneous nucleation of ice occurs only at temperatures lower than -32°C, which are only achieved in high altitude clouds. Ice formation in lower lying, warmer clouds is promoted by atmospheric aerosols. These aerosols include minerals, organics, and biological molecules. Bacterial proteins are the most potent ice-nucleating agents in the atmosphere and the biosphere, able to nucleate ice at temperatures as high as -1°C. Some organics reach reach comparably high ice nucleation potencies, and have been used for the seeding of clouds to promote precipitation. The molecular mechanisms by which these potent nucleants interact with ice, and the mechanisms by which they promote crystallization have long been debated, but only recently it has been possible to access them through molecular simulations. In this presentation, I will discuss our work to elucidate the mode of binding and nucleation of ice by proteins and organics, how ice nucleation is modulated by the size and interactions of these particles, and our quest to find even stronger ice nucleants that can form ice without supercooling. I will discuss how to achieve the latter through prefreezing of water above the melting temperature, and present an integrated view of ice premelting, ice nucleation, and prefreezing in water. The enticing possibility of accessing the prefreezing regime by small modifications of existing surfaces opens the doors to the design of materials for energy-efficient formation of artificial snow and the induction of precipitation through cloud glaciation.

Biosketch: **Valeria Molinero** is the Jack and Peg Simons Endowed Professor of Theoretical Chemistry and Distinguished Professor at The University of Utah, where she also leads the Henry Eyring Center for Theoretical Chemistry. A physical chemist by passion and training, she performed research in electrochemistry as an undergraduate at the University of Buenos Aires, before turning to computational and theoretical chemistry for her doctoral studies. Upon completion of her Ph.D. at the University of Buenos Aires, she moved to the United States to pursue postdoctoral research at Caltech with Bill Goddard and –later but simultaneously- at Arizona State University with Austen Angell, before starting her independent career at the University of Utah in 2006. Molinero's research focuses on understanding and controlling phase transformation and dynamics in materials, with an emphasis on water. She is past Chair of the Theory Subdivision of ACS and of the Gordon Research Conference on Liquids. Molinero serves in the Board of Managers of AIP Publishing, and in the advisory board of several physical chemistry journals. Molinero's research has been recognized with multiple awards, including the Beckman Young Investigator Award, Camille Dreyfus Teacher Scholar Award, the Cozzarelli Prize of the Proceedings of the National Academy of Sciences, and the election to the American Academy of Arts and Sciences.

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