**Towards the elucidation of the mechanisms of synthesis of zeolites**

Zeolites are porous silicates that constitute the main solid catalysts used by the chemical industry. These structurally complex solids are synthesized from aqueous solutions through a multi-stage process that involves multiple phase transformations mediated by the chemistry of polymerization of silica. Organic cations, typically tetraalkylammonium ions, are used to direct the synthesis towards specific zeolite polymorphs. Nevertheless, the molecular mechanisms by which the cations and silicates form the zeolites are not well understood. This presentation will discuss our current work using molecular simulations to elucidate at which stage zeolitic order emerges from the synthesis mixture, and the roles of nucleation and growth in the selection of zeolite polymorphs.

**Photo & bio**



Valeria Molinero is the Jack and Peg Simons Endowed Professor of Theoretical Chemistry and Distinguished Professor at The University of Utah, where she leads the Henry Eyring Center for Theoretical Chemistry. A physical chemist by passion and training, Molinero received her undergraduate degree in Chemistry (1994) and a Ph.D. in Physical Chemistry (1999) from the University of Buenos Aires, before moving to the United States to pursue postdoctoral research at Caltech. Molinero joined the faculty at The University of Utah in 2006, where she has developed a computational and theoretical research program on the interplay between structure, phase transformation and dynamics in materials. A large part of her focus has been on investigating the behavior of water, silica and materials for energy. Molinero has been recognized with multiple awards, including the Helmholtz Award from the International Association of the Properties of Water and Steam, the Beckman Young Investigator Award, the Camille Dreyfus Teacher Scholar Award, the Cozzarelli Prize on Physical and Mathematical Sciences of the Proceedings of the National Academy of Sciences, a Doctor Honoris Causa from the University of Buenos Aires, and the Irving Langmuir Award in Chemical Physics. Molinero is an elected member of the Utah Academy of Engineering and Science, the American Academy of Arts and Sciences, and the National Academy of Sciences of the United States.