Satyendra Nath Bose National Centre for Basic Sciences

Azadi Ka Amrit Mahotsav

Visitor, Associates and Students' Programme (VASP) presents Webinar Series on

Statistical Mechanics

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07:00 PM (IST)

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TITLE

Elucidating the mechanisms of synthesis of zeolites using molecular simulations

ABSTRACT

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 and machine learning to elucidate at which stage zeolitic order emerges from the synthesis mixture, the roles of nucleation and growth in the selection of zeolite polymorphs, and what is the smallest size of nanozeolite that can be synthesized.

SPEAKER

Professor Valeria Molinero, *The University of Utah*

Prof. Valeria Molinero is Distinguished Professor; Jack and Peg Simons Endowed Professor of Theoretical Chemistry; and Director of the Henry Eyring Center for Theoretical Chemistry at the University of Utah, USA. Her group uses a combination of computer simulations and statistical mechanics, and develops novel models to investigate the interplay between microscopic structure, dynamics and phase transformations in disordered materials. She has made significant contributions towards understanding of structure and anomalies of liquid water and its solutions, mechanisms of ice crystallization in bulk and confined water, nucleation and growth of clathrate hydrates, and development of coarse-grained models among many others. She has been elected as member of the American Academy of Arts & Sciences (2021) and the National Academy of Sciences, USA (2022).