Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Addressing Chemical Complexity through Molecular Simulations

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In the six decades since its birth, molecular simulation has advanced to such an extent as to offer itself as a microscope into the molecular world to complement and supplement laboratory experiments. Its scope along the length, time and energy dimensions has been considerably improved through technical innovations including coarse-graining, enhanced sampling, quantum chemical and deep learning treatment of intermolecular interactions. This talk will journey through these developments. Case studies on gas and water adsorption by porous frameworks, the development of interatomic potentials for ethylene glycol, and its manifest impact on properties of its aqueous solutions in bulk and at interfaces will be presented. The talk will conclude with recent results from my group on machine learned potentials for aqueous salt solutions to probe their anomalous diffusion.

Wednesday, Nov 22nd 2023

4:00 PM (Tea / Coffee 3.45 PM)

Auditorium, TIFR-H