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Theory Meets Experiments on Gas Adsorption in Porous Materials: Thermodynamics, Dynamics, Kinetics and Beyond

Gas adsorption in porous materials such as metal organic framework solids has been at the forefront of the many applications of such materials. While the adsorption process itself is straightforward to understand as a first order phase transition, experimental observations of the phenomenon in a host of novel hybrid materials have shown rather interesting behavior – such as, anomalous temperature dependence, discontinuities/steps, hysteresis, gate opening etc. The interpretation of all these non-standard behaviour demands a detailed description of intermolecular interactions at the appropriate experimental conditions. The lecture will give the audience an introduction to gas adsorption, a broad overview of metal organic framework solids and examples from our research exploring such exotic phenomena involving carbon dioxide adsorption.

References:

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3. N. Dwarkanath, S. Palchowdhury and S. Balasubramanian, Unraveling the sorption mechanism of CO₂ in a molecular crystal without intrinsic porosity, *J. Phys. Chem. B*, 123, 7471 (2019).
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Balasubramanian Sundaram is a Professor in the Chemistry and Physics of Materials Unit at Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore. His research interests include gas adsorption in porous materials, supramolecular polymerization and self-assembly, enzyme structure, dynamics and function, room temperature ionic liquids and electrolyte solutions. He employs an array of advanced computational tools to pursue these interests.