

Seminar

Study of impact of structural dynamics on adsorption and diffusion properties of MOFs

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This study explores diffusion selectivity and host–guest interactions in metal–organic frameworks (MOFs). The first study investigates pore surface modulation with aliphatic functionalities to enable shape-selective kinetic diffusion in Cu-based pillared-layered MOFs. Three molecular pairs were examined: hexane isomers (2,2-dimethylbutane and 2,3-dimethylbutane), benzene and cyclohexane, and styrene and ethylbenzene. Systems such as hexane isomers as well as styrene and ethylbenzene exhibit selectivity, whereas benzene and cyclohexane show minimal differences. In $\text{Cu}_2(\text{bicyclo})_2(\text{DABCO})$ MOFs, such modulation also influences linker rotational dynamics, enhancing selectivity for hexane isomers.

The second study explores host-guest interactions through torsional energy profiles of biphenyl dicarboxylic acid (bpdc) and methyl-substituted bpdc linkers of UiO-67 MOF. Molecular dynamics simulations using GROMACS and LAMMPS were employed to study CO_2 and CH_4 diffusion in UiO-67 and methyl-substituted UiO-67 MOFs. Analysis of dihedral angle distributions shows repopulation of higher-energy states in the presence of CO_2 , without significant structural changes. This suggests limitations of the Universal Force Field (UFF) in capturing MOF–guest interactions. The study highlights the need for more accurate approaches such as ab initio molecular dynamics or machine learning potentials for providing insight into the relationship between structural modifications and gas diffusion in MOFs.

Wednesday, Mar 25th 2026

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Trishul Hall, TIFRH