

Internal Seminar

Computational Studies of Selective Ion Transport in Metal-Organic Frameworks

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Metal-organic frameworks (MOFs) are solid porous materials with several eco-friendly applications, including water harvesting, gas and energy storage, and membrane-based separation.^[1] A post-synthetic modification (PSM) of MOFs opens up opportunities for specific applications such as ion transport and purification.^[2]

All-atom molecular dynamics (MD) simulations of aqueous electrolyte (KCl, NaCl, LiCl) in MOF were carried out to investigate ion-transport mechanisms in post-synthetic modified MOF 808, where in experiment the photoresponsive azobenzene derivatives ((4-phenylazophenyl) acetate) are attached to the five sites of the hexagonal openings of the pore channels of the MOF. It was observed that, at a higher number of azobenzene substitutions (e.g., four and five positions) and under UV irradiation (where azos in the trans configuration convert to cis), K⁺ ions pass, and Li⁺ and Na⁺ ions are restricted (as determined by I-V analyses). Our results from all-atom MD simulations and pore geometry analyses indicate that the cation MSDs are faster in the cis system compared to the trans-system, and the K⁺ ion moves faster than the Na⁺ and Li⁺ ions, which corroborates the experimental results. Furthermore, we uncovered several intricate phenomena, including diversity in ion coordination, ion-dipole interactions, and the slower dynamics of both water molecules and ions in the confined environment of the MOF, and we also identified limitations in the current MOF potential.

References:

[1] R. Freund et al. *Angew. Chem. Int. Ed.* **2021**, 60, 23975.

[2] S. Mandal, S. Natarajan, P. Mani, A. Pankajakshan, *Adv. Funct. Mater.* **2021**, 31, 2006291.

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