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Water adsorption and proton conduction in metal-organic frameworks: Insights from molecular simulations[1]

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Metal-organic frameworks (MOFs) are a relatively new class of porous materials that hold great potential for a wide range of applications in chemistry, materials science, and nanoengineering. Compared to other porous materials such as zeolites, MOF properties are highly tunable. In particular, it has been shown that both size and shape of the MOF pores can be rationally designed for specific applications. For example, the ability to modify the framework properties with respect to hydrophilicity/hydrophobicity and acidity/basicity can enable the direct control of proton conduction through carrier molecules adsorbed inside the pores. Here, I report on our current efforts aimed at providing a molecular-level characterization of water-mediated proton conduction through the MOF pores. Particular emphasis will be put on correlation between proton conduction and both structural and chemical properties of the frameworks as well as on the dynamical behavior of water confined in the MOF pores.

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