Molecular-level modeling of metal-organic frameworks: Breathing, adsorption, and proton conduction

Francesco Paesani

Department of Chemistry and Biochemistry
University of California, San Diego

Over the last decade metal-organic frameworks (MOFs) have emerged as a new class of porous materials with great potential for a wide range of applications, including gas storage, catalysis, separation, sensing, and proton conduction. Unlike traditional porous materials, such as zeolites, MOFs are often characterized by unusually flexible frameworks that undergo large structural deformations upon external stimuli such as temperature and pressure changes, and gas adsorption. In this talk, I will describe our current efforts aimed at developing a molecular-level understanding of the physicochemical properties of the MOF materials with a particular focus on the mechanisms that determine the breathing behavior, water adsorption, and proton conduction.