Insights Into Gas Storage and Separation in MOFs Using DFT and Molecular Simulations

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Metal-organic frameworks (MOFs) are basically a combination of metal nodes and organic linkers that have been one of the hottest research topics in material research since their versatile structure with high surface area, porosity can be viable candidates for many applications including gas adsorption/separation, catalysis, sensing, drug delivery etc. Due to the large number of metal nodes and organic linkers, it has been shown that a plethora of MOFs can exist. Recently, researchers have built a solvent and disorder-free collection of already-synthesized MOFs called Computation-Ready Experimental (CoRE) MOFs to aid the computational efforts on MOFs. In the first part of this talk, two methane recovery scenarios – recovery from five-component biogas and three-component sour natural gas – using CoRE MOFs will be discussed where atomically detailed simulations are employed. In both scenarios, the top performing materials are identified based on their gas selectivity, regenerability, and working capacity. The relation between these performance metrics and MOF pore characteristics will be described through correlations. In the second part of the talk, a DFT investigation on the separation performance of small gas molecules (CH_4, N_2, CO_2, NH_3, H_2S, SO_2, H_2O) in Zr-based UiO-type MOFs (UiO-66, -67, and -68), will be discussed before and after the incorporation of the metal (Co, Mg, Ni, and Zn) catecholates. The effect of different metals in metal catecholates on gas separation performances will be depicted for two gas separation applications, natural gas purification and toxic gas removal.