Computational study for SF_6 storage and separation in metal-organic frameworks(MOF)

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Sulfur hexafluoride(SF_6) is widely used in dielectric industries as an insulated gas and used as a mixed gas with nigrogen(N_2) due to its high global warming potential. Used in the form of a mixed gas, it is not well separated by cracking and toxic substances are also generated. In this regard, adsorption using porous materials has attention as an effective SF_6 separation method such as Pressure-swing adsorption(PSA) process which is worked on current chemical plants. Generally, MOF, zeolite are used as an adsorbent in PSA. Specifically, Metal-organic frameworks(MOFs) are porous materials consisting of metal ions and organic ligands and are suitable for gas separation by its high surface area, thermal stability and tunability. Selectivity for specific gases in mixed gas separation using adsorbents is one of the critical criteria. This work search the suitable MOF with high SF_6 selectivity for SF_6/N_2 separation by High-throughput computational screening(HTS) based on CoRE MOF database using combination two force field and two SF_6 computational model. HTS structures are classified three criteria; 1)SF_6 model PLD, 2)exception of expensive metal, 3)Henry's coefficient selectivity.