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Probing the binding mechanism of toxic gases in Hofmann-clathrates: a combined neutron scattering and DFT study

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We report a joint experimental and computational characterization of the adsorption process of toxic gases, such as CO, CO2 and SO21 in Hofmann-type clathrates with formula {Fe(pz)[MII(CN)4]} (M = metal, pz = pyrazine). These metal-organic frameworks have a 2D layered structure where Fe centers are connected through cyanide ligands to an open-metal site MII, typically Pd, Pt or Ni, offering a binding site with a potentially strong affinity for the gas molecules with potential application for gas capture and sensing.
Neutron characterization techniques combined with density functional theory (DFT) calculations have allowed us to understand the binding mechanism at the open-metal site. The high hydrogen content in these samples makes neutron techniques well suited for this study. The changes in the inelastic neutron scattering (INS) spectra upon gas adsorption, interpreted upon comparison with the normal modes of vibrations from DFT calculations, provide us with a clear signature of the binding mechanism between the MOF and the gas molecules. Our work shows that the adsorption process can be fully characterized by using neutron techniques by combining information of the binding configuration, as characterized by neutron diffraction, and the spectral changes specific of each molecule measured by INS.

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