Theoretical Study of the Adsorption and Separation of Gases in Metal-Organic Frameworks

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We perform grand-canonical Monte Carlo simulations to study the adsorption properties of mixtures containing H_2 and CO_2 in MOFs.
We use a simple model of the MOFs that permit us change the interaction parameters and size in the simulation.

The energy of the most attractive site of adsorption in a IRMOF-1 is -29.6 meV and -323 meV for H_2 and CO_2 respectively. The wide range in energies suggest that the MOFs may be use for gas separation by adsorption.

Schematic view of the JGMOF (simple model of a MOF). The parameters of the metallic centers (in purple) and number of linkers (green, yellow) are set to assess the adsorption properties of hypothetical materials.