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

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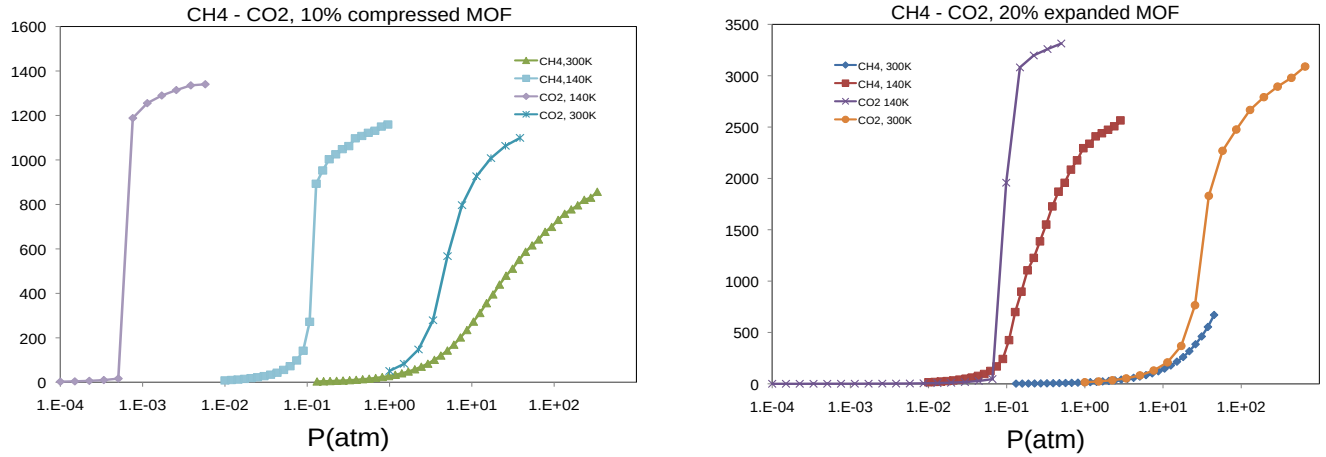
We performed grand-canonical Monte Carlo simulations to study the adsorption properties of mixtures containing CH_4 and CO_2 in MOFs.
We use a simple model of the MOFs that permit us change the interaction parameters and size in the simulation.

- The selectivity of CO_2 is enhanced by compressing the unit cell of the MOF by only 10% or by inserting dipoles at the corners of the MOF.
- The adsorpion properties are sensitive to the detailed charge distribution of the MOF, only if it contains dipolar components.



Compared adsorption of CO_2 and CH_4 in a compressed (left panel) and expanded MOF (right panel). Large gaps between the isotherms indicate high selectivity for CO_2