Adsorption Energy Calculator

A tool to calculate the adsorption energy of gas molecules in a MOF.

This tool uses RASPA for its backend simulation. RASPA is a molecular simulation software for performing adsorption and diffusion calculations in nanoporous materials. It implements state-of-art algorithms for Molecular Dynamics and Monte Carlo for various ensembles. In this simulation, we used Monte Carlo algorithm.

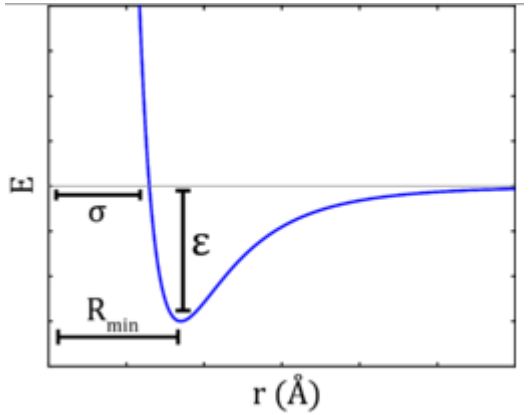
Every simulation is performed with initialization and production cycles of 5000 and 10000 respectively.

- Initialization cycles set the configuration for the start of equilibration.
- The data is collected during production cycles.

Transferrable Potential for Phase Equilibria (TraPPE) forcefield is used to define the molecular interactions for every molecule in this tool.

Molecule	Forcefield	Reference
Methane	TraPPE	J. Phys. Chem. B, 1998, 102, 2569-2577
Ethane	TraPPE	
Hydrogen	TraPPE	*Theor. Chem. Acc.* 2006, 115, 391–397
Nitrogen	TraPPE	
Carbon dioxide	TraPPE	

Lennard-Jones Potential



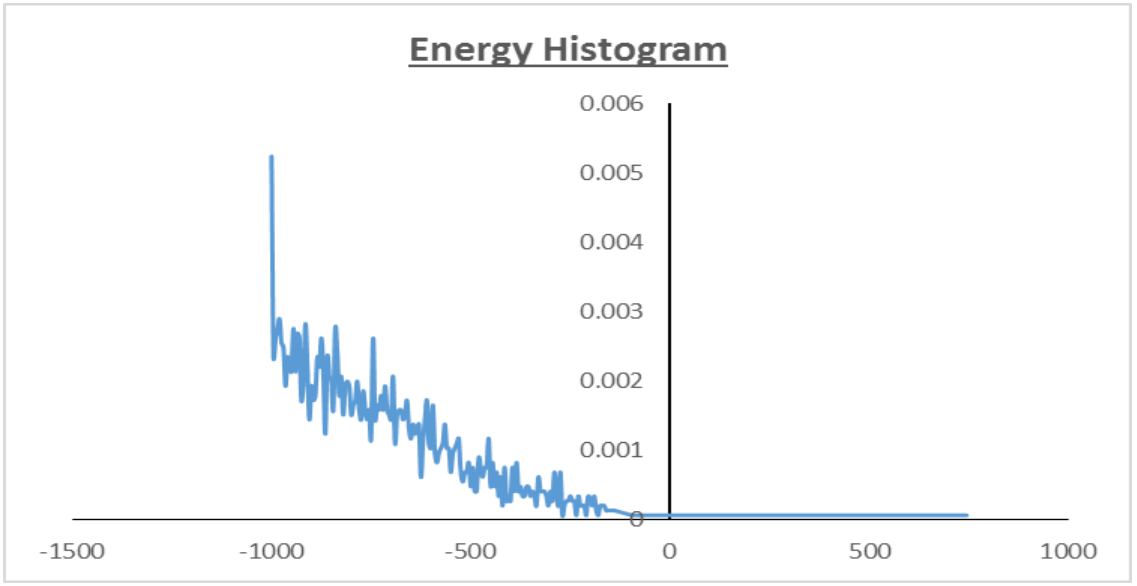
https://upload.wikimedia.org/wikipedia/commons/thumb/f/fe/Schematic_of_the_Lennard-Jones_6-12_Potential.png/255px-Schematic_of_the_Lennard-Jones_6-12_Potential.png

- Lorentz-Berthelot's model was used as the general mixing rule for the Lennard-Jones potentials

$$\sigma_{ab} = \frac{\sigma_a + \sigma_b}{2} \qquad \varepsilon_{ab} = \sqrt{\varepsilon_a \varepsilon_b}$$

Adsorption energy is the energy required to have one molecule of the gas adhere onto the surface of the material which in this case is a metal organic framework. When the energy is given as a negative value, it denotes attraction between the gas molecule and the material surface (adsorption occurs) and a positive value denotes repulsion between molecule and material (no adsorption).

The tool allows the option of selecting the material (MOF), molecule and the temperature and then it outputs the energy histogram of adsorbates as they move around inside the framework, and finally the adsorption energy. RASPA uses a unit convention different from the standard international system of units (SI), length is measured in angstrom and energy is measured in Kelvin. To convert the unit of energy from Kelvin to J/mol, multiply by the gas constant 8.314 J/mol K.



The graph above depicts the energy histogram of CO_2 as it moves around IRMOF-1. The simulation was performed at 300K and the energy of adsorption was calculated to be -1253.055 Kelvin (-10.42 KJ/mol).