Diffusion Constant Simulator

a tool to calculate the self diffusion constant of a gas molecule through a metal organic framework

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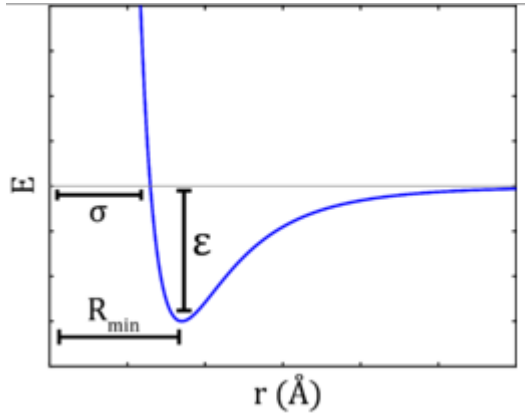
This tool employs the use of RASPA for its backend simulation. RASPA is a molecular simulation software for performing adsorption and diffusion calculations in nanoporous materials. It implements the state-of-art algorithms for Molecular Dynamics and Monte Carlo for various ensembles. In this simulation,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

- Every simulation is performed at room temperature (298 K) with production, equilibration and initialization cycles of 30000, 5000 and 5000 respectively.
  - Initialization cycles (monte carlo) set the configuration for the start of equilibration.
  - Equilibration cycles (molecular dynamics) warm-up the simulation.
  - Production cycles (molecular dynamics) are for the data collection.

- Transferrable Potential for Phase Equilibria (TraPPE) forcefield is used to define the molecular interactions for argon, nitrogen, hydrogen and carbon dioxide while the united atom model of the forcefield (TraPPE-UA) is used to define the molecular interaction for methane.

Mol.	Definition	Ref
CH4	TraPPE-UA	*J. Phys. Chem. B*, 1998, 102, 2569-2577
Ar	TraPPE	*J. Am. Chem. Soc.*,1992, 114, 10024-10035
H2	TraPPE	Vapor-Liquid Equilibria of Mixtures Containing Alkanes, Carbon Dioxide, and Nitrogen; AIChE J., 2001, 47, 1676-1682
N2	TraPPE	
CO2	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

- For the MOFs, forcefields parameterized by the developers of RASPA were used.

Exceptional Negative Thermal Expansion in Isoreticular Metal–Organic Frameworks, Angew. Chem. Int. Ed. 2007, 46, 4496 –4499, DOI: 10.1002/anie.200700218

MOF	Flexibility	Forcefield
IRMOF-1	Rigid	Dubbledam2007FlexibleIRMOF-1
IRMOF-16	Rigid	Dubbledam2007FlexibleIRMOF-16

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

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

Computing the diffusion constant

Einstein's equation of diffusion is used to calculate the self diffusivity

MSD = 6 D t + C

Where;

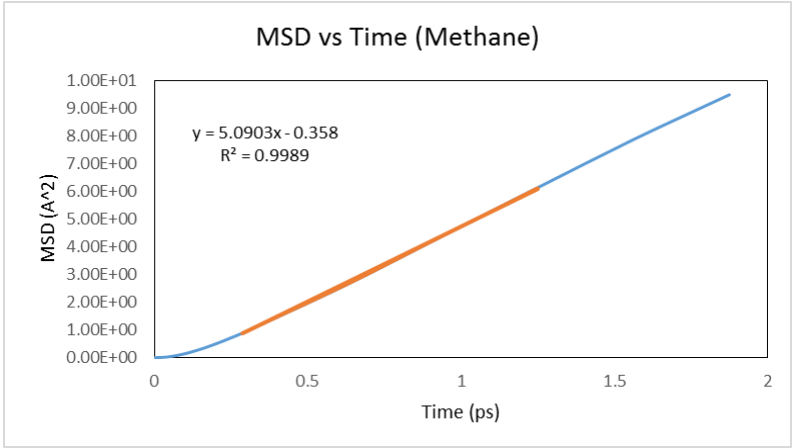
MSD = mean square displacement

msd = $\frac{1}{N}\sum_{j=1}^{n}([r_j(t) - rj(0)]^2)$

D = diffusion constant

t = time

C = constant



The diffusion constant is obtained from the $\frac{slope}{6}$ of the mean square displacement against time graph.

The initial and final few points were omitted and the center points fitted to a straight line.

Its unit is in squared angstrom per picosecond (A^2/ps).

In the graph above, the slope is 5.0903 and diffusivity is $\frac{5.0903}{6}$ = 0.848 A^2/ps