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Predicting the Properties of Materials and Biomolecules with Computer Modeling

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Predicting the Properties of Materials and Biomolecules with Computer Modeling

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Abstract

The advance of theoretical chemistry methods and the increase in computing power have resulted in the frequent use of computer in chemistry, material science, and biology. Zeolitic imidazole frameworks (ZIFs) are a subclass of MOFs which are materials that are made by coordinating transition metal ions to organic ligands to form porous network structures. We have performed Gibbs ensemble Monte Carlo simulations to study the equilibrium selectivity for an equimolar mixture of CO2 /CH4 in ZIF-93 at 298K and for pressures up to 80 bar. The results of the simulations revealed the role of pressure in the separation performance of ZIF-93 and the preferential adsorption sites of CO2 and CH4. We also present our initial work for Molecular Dynamics simulations of human Inosine Triphosphatase (ITPA) with a P32T mutation complexed with the ITP substrate in explicit aqueous solution. ITPA is an enzyme that is responsible for maintaining a proper level of nonstandard nucleotides in cells. This studies will improve our understanding of gas separation of porous materials and the mechanism of ITPA substrate Binding.

Introduction

- The burning of natural gas for power generation produces less of the greenhouse gas (GHG), CO_2, per unit energy than the burning of many other fossil fuels, including coal and gasoline.
- Metal− organic framework (MOF) materials, including zeolitic imidazolate frameworks (ZIFs), have been actively investigated for membrane-based gas separation applications.
- ZIFs are composed of tetrahedrally coordinated metal centers such as Zn and Co linked by functionalized imidazole groups.
- ZIF materials display a rich variety of chemistries and structural topologies depending on the type of metal atom and organic linker.
- Here, we present Gibbs ensemble Monte Carlo simulations of an equimolar mixture of CO_2 /CH_4 to study the effect of pressure in the separation performance of ZIF-93.
- The human ITPA enzyme is a 194-amino acid homodimer of which each chain has a central beta sheet with two terminal globular lobes that have alpha/beta structural characteristics and a central cation, presumably Mg2+.
- The computational studies of ITPA P32T variant can supplement the existing experiments and moreover give new insight into the effect of mutations on the structural and dynamics of the enzyme.

Simulation Methods

- The initial structures of the ZIFs were constructed using the atomic coordinates obtained from X-ray diffraction data [1].
- The Monte Carlo for Complex Chemical Systems (MCCCS) Towhee program [2] was used to perform the Gibbs ensemble Monte Carlo simulations.
- We model the methane molecule using the Transferable Potentials for Phase Equilibria United Atom (TraPPE-UA) force field [3].
- The Optimized Potentials for Liquid Simulations All Atom (OPLS-AA) force field [4] was used to model the ZIF-93.
- The Protein Data Bank file 2J4E of the crystal structure of the human ITPA in complex with ITP was used to construct the initial coordinates[1].
- The CHARMM program [2] was used to mutate the residue at the position 32 and generate the topology of the substrate ITP.

Results

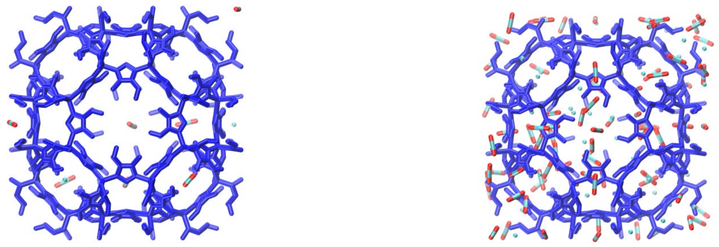

Figure 1: ZIF-93 50/50 mixture of CH_4/CO_2 at 1 bar (left) and 80 bars (right).

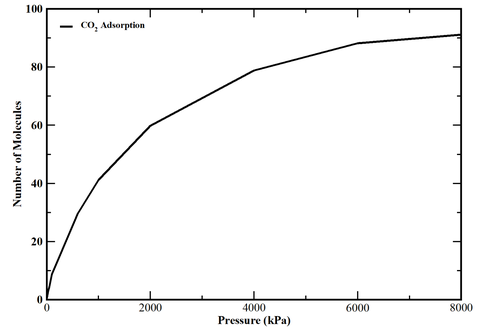

Figure 2: Number of CO_2 molecules absorbed at various pressures

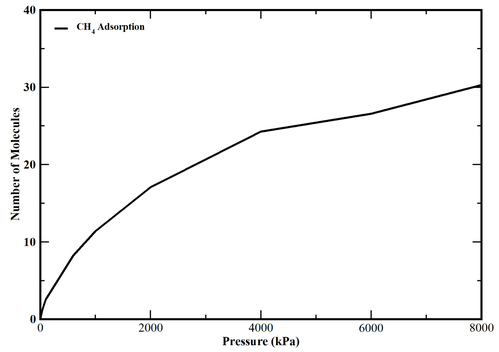

Figure 3: Number of CH_4 molecules absorbed at various pressures

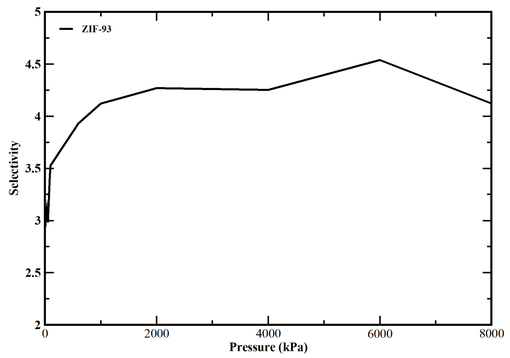

Figure 4: Selectivity of CO_2 over CH4 for various pressures

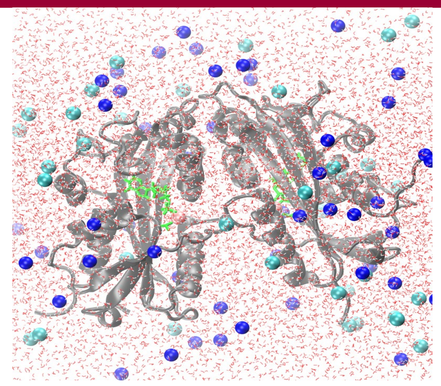

Figure 5. The human ITPA with ITP bound in water box..

Conclusions

- We have examined computationally the selectivity of CO_2 /CH4 in ZIF-93 at 298K.
- We found that that CH_4 adsorption in ZIF-93 is smaller than the corresponding CO_2 adsorption at each pressure.
- Our high-pressure simulations show that the saturation pressure for CO_2 and CH_4 in the ZIFs studied is not yet reached at the maximum pressure considered, 8000.00 kPa.
- Our results show that the average adsorption selectivity of CO_2 from CH_4 is ~ 4 in ZIF-93.
- We have built the the human ITPA in complex with ITP solvated in a box of 15741 water molecules, 59 sodium ions, and 49 chloride ions.

Acknowledgements

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