

Diffusion and adsorption of N₂ and C₂H₆ in ZIF-8 MD and MC simulations

**Tadija Chokbunpiam^{1,2,4*}, Rungroi Chanajaree^{2,3}, Oraphan Saengsawang²,
Siegfried Fritzsche⁴, Christian Chmelik⁵, Wolfhard Janke⁴, Jürgen Caro⁶,
Tawun Remsungnen⁷, Supot Hannongbua^{2,3}**

¹Petrochemical Science Program, Chulalongkorn University, Bangkok, Thailand

²Chulalongkorn University, Computational Chemistry Unit Cell (CCUC),
Department of Chemistry, Bangkok, Thailand

³Chulalongkorn University, Metallurgy and Materials Science Research Institute (MMRI),
Bangkok, Thailand

⁴Universität Leipzig, Institute for Theoretical Physics, Leipzig, Germany

⁵Universität Leipzig, Institute for Experimental Physics I, Leipzig, Germany

⁶Leibniz University Hannover, Institute of Physical Chemistry and Electrochemistry,
Hannover, Germany

⁷Khon Kaen University Department of Mathematics, Khon Kaen, Thailand

*dinga303@hotmail.com

Molecular Dynamics (MD) and Gibbs-Ensemble Monte-Carlo (GMC) simulations give insight into the adsorption and diffusion properties of N₂ and C₂H₆ molecules adsorbed in ZIF-8 [1]. The framework flexibility plays an important role in achieving correct transport properties [2]. Particularly, for N₂ a gate opening effect could be observed. The window sizes were determined by the orientation of the imidazolite linkers and a transition from a closed structure at low N₂ loading (approximately 0.5–18.4 N₂/cage), to an open one, at high loading (approximately 20–30 N₂/cage) was found (see Fig. 1). This is in agreement with [3]. The results of MD simulations and of experiments for N₂ and C₂H₆ are compared. The simulation results illustrate that the transition of the orientation of imidazolite linkers of the ZIF-8 framework for both, 4 and 6-membered rings were induced by N₂ guest molecules.

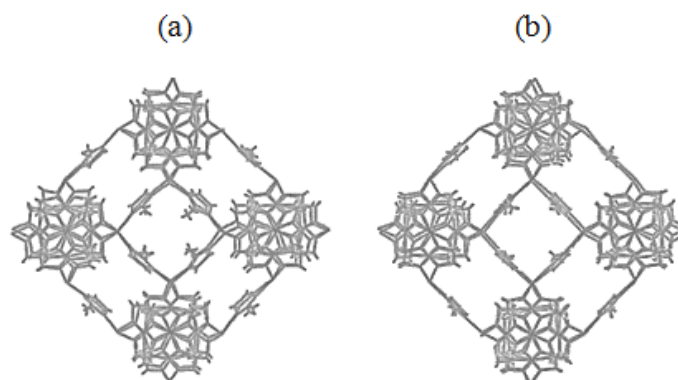


Figure 1: ZIF-8 window structures at (a) low loading and (b) high loading of N₂ guest molecules.

References

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