diffusion-fundamentals.org

The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Molecular dynamics investigation of the transport of hydrogen in ZIF-7

Pooneh Pilvar[1*], **Siegfried Fritzsche**[1], **Jürgen Caro**[2], **Wolfhard Janke**[1]

[1]Universität Leipzig, Institute for Theoretical Physics,
Leipzig, Germany
[2]Leibniz University Hannover, Institute of Physical Chemistry and Electrochemistry,
Hannover, Germany
[*]p.pilvar@gmail.com

The importance of hydrogen-based clean energy systems due to the global climate change, air pollution and energy security has lead to several studies of hydrogen production, separation and storage in industry and science [1, 2].

In the current study, we have investigated the diffusion of hydrogen within a novel Zeolitic imidazolate framework (ZIF-7, Figure 1a). ZIFs are a subfamily of porous metal-organic frameworks (MOFs) [3, 4]. For investigating diffusion behavior of hydrogen in this lattice, we have applied Molecular Dynamics (MD) simulations. At the studied temperatures in a series of MD simulations performed with a rigid lattice, no diffusion of any gas was observed in ZIF-7. The same behavior has been reported by A. Battisti et al. [5]. Applying the flexibility to the framework, the measured diffusion coefficient for hydrogen was about 2.7×10^{-9} m^2 s^{-1} while nearly no diffusion was observed for any other studied gas in ZIF-7. These results clearly elucidate the molecular sieving behavior of this material for hydrogen reported by Caro et al. and represent it as a promising membrane in this domain which is due to its very small pore structure and window size (0.3 nm) that is close to the kinetic size of the hydrogen molecule [1].

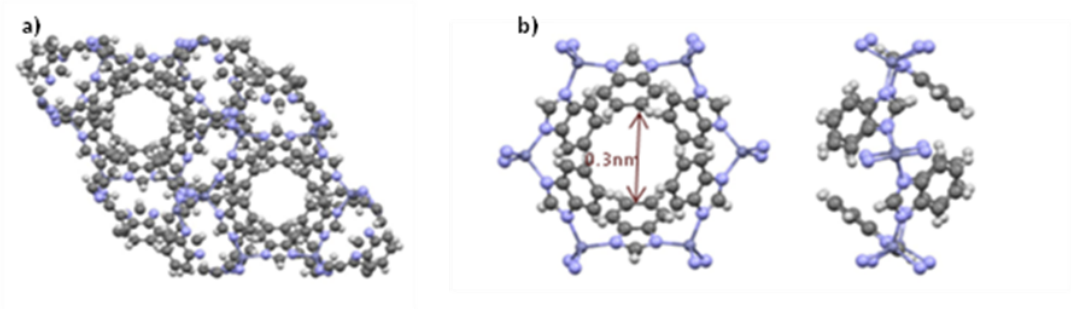

Figure 1: ZIF-7 unit cell (a). The main six-member window of ZIF-7 (b); Top view (left), side view (right).

References

[1] Y. Li, F. Liang, H. Bux, W. Yang, J. Caro: *Zeolitic imdazolate framework ZIF-7 based molecular sieve membrane for hydrogen separation*. Journal of Membrane Science **354**, 48–54 (2010)

[2] B. Assfour, S. Leoni, G. Seifert: *Hydrogen adsorption sites in zeolite imidazolate frameworks ZIF-8 and ZIF-11*. Journal of Physical Chemistry C 2010 **114**, 13381–13384 (2010)

[3] S.L. James: *Metal-organic frameworks*. Chemical Society Review **32**, 276–288 (2003)

[4] A.W. Thornton, D. Dubbeldam, M.S. Liu, B.P. Ladewig, A.J. Hill, M.R. Hill: *Feasibility of zeolitic imidazolate framework membranes for clean energy application*. Energy & Environmental Science **5**, 7637–7616 (2012)

[5] A. Battisti, S. Taioli, G. Garberoglio: *Zeolitic imidazolate frameworks for separation of binary mixtures of CO_2, CH_4, N_2 and H_2: A computer simulation investigation*. Microporous and Mesoporous Materials **143**, 46–53 (2011)