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

Pooneh Pilvar\textsuperscript{1*}, Siegfried Fritzsche\textsuperscript{1}, Jürgen Caro\textsuperscript{2}, Wolfhard Janke\textsuperscript{1}

\textsuperscript{1}Universität Leipzig, Institute for Theoretical Physics, Leipzig, Germany
\textsuperscript{2}Leibniz University Hannover, Institute of Physical Chemistry and Electrochemistry, Hannover, Germany
\textsuperscript{*}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\cite{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)\cite{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.\cite{5}. Applying the flexibility to the framework, the measured diffusion coefficient for hydrogen was about $2.7 \times 10^{-9} \text{m}^2 \text{s}^{-1}$ 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\cite{1}.

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

\textbf{References}

\begin{enumerate}
\item A. Battisti, S. Taioli, G. Garberoglio: Zeolitic imidazolate frameworks for separation of binary mixtures of CO\textsubscript{2}, CH\textsubscript{4}, N\textsubscript{2} and H\textsubscript{2}: A computer simulation investigation. Microporous and Mesoporous Materials \textbf{143}, 46–53 (2011)
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