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Structural and transport properties of hydrogen in ZIF-22

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ZIF-22 which has a structure similar to A zeolites [1, 2] is investigated in this work because of of its high selectivity for hydrogen with respect to other gases [1]. By using Molecular Dynamics simulations with the DL_POLY package, structural and dynamical properties of hydrogen adsorbed in ZIF-22 are examined.

Moreover, the adsorption of hydrogen in ZIF-22 is simulated by Gibbs-ensemble Monte-Carlo simulation studies.

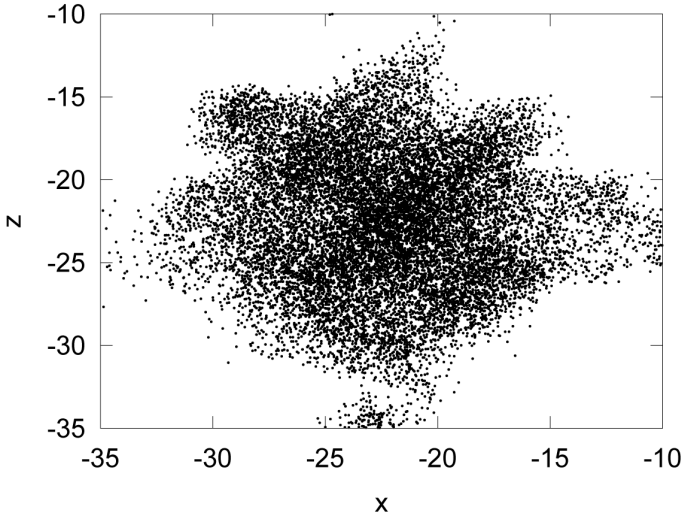

Figure 1: The density plot of hydrogen in one of the cavities of ZIF-22

The small window size turns out to be the most important reason for the high selectivity. The results are compared with experiments [1] and they are discussed by means of spatial density distributions, radial correlation functions and mean square displacements.

References

[1] A. Huang, H. Bux, F. Steinbach, J. Caro: *Molecular-sieve membrane with hydrogen permselectivity: ZIF-22 in LTA topology prepared with 3-aminopropyltriethoxysilane as covalent linker*. Angewandte Chemie International Edition **49**, 4958–4961 (2010)

[2] H. Hayashi, A.P. Côté, H. Furukawa, M. O'Keeffe: *Zeolite A imidazolate frameworks*. Nature Materials **6**, 501–506 (2007)