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Diffusion investigation for hydrogen guest molecules in an adapted force field for ZIF-11

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The large family of Metal Organic Frameworks, to which ZIF-11 belongs, demands for the possibility to predict properties regarding adsorption and diffusion behavior from their crystal structure.

Therefore, as a first step, it is important to find good parameters to describe some members of the MOF family and to try in a second step to draw conclusions to other materials from the gained experience.

In this work the structure of ZIF-11 was investigated and a force field was found that was able to reproduce experimental adsorption behavior [1]. The force field was based on the AMBER [2] parameters and was adapted to get good agreement with measured properties. Connections between adjacent cavities were identified and a way has been described to deal with uncertainties in the provided X-Ray structures [1].

Afterwards longer simulations runs have been performed to get estimates for the behavior of the diffusion coefficient.

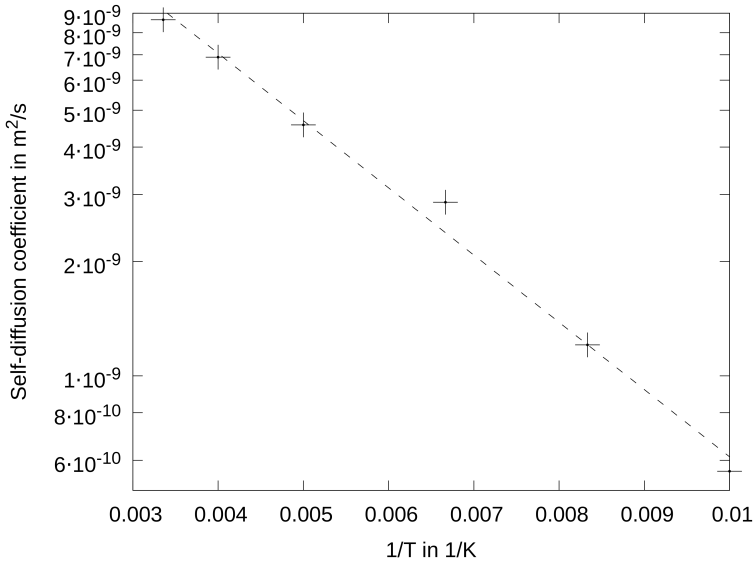

Figure 1: The temperature dependence of the diffusion coefficient for hydrogen in ZIF-11 together with a linear fit

References

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