

# Understanding adsorption in Zr-organic frameworks: A computational study

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Metal-organic frameworks (MOFs) represent a class of porous materials that have emerged as an important new class of crystalline materials over the last decade. These compounds are assembled from organic molecules as linkers and metal clusters as joints resulting in robust frameworks. Depending on the choice of the linker molecule, pore sizes can be engineered for a wide range of applications like gas storage, catalysis or in biomedicine. PIZOFs (porous interpenetrated Zr-organic frameworks) are a class of two-fold interpenetrated Zr-MOFs, the internal voids can be tailored in a wide range by changing the substituents of the central phenylene ring of the organic linker molecules (PIZOF structure with an accessible pore highlighted by sphere (a) Rod-like PIZOF-linker with side chains R<sup>1</sup> and R<sup>2</sup> (b), Fig. 1).[1]

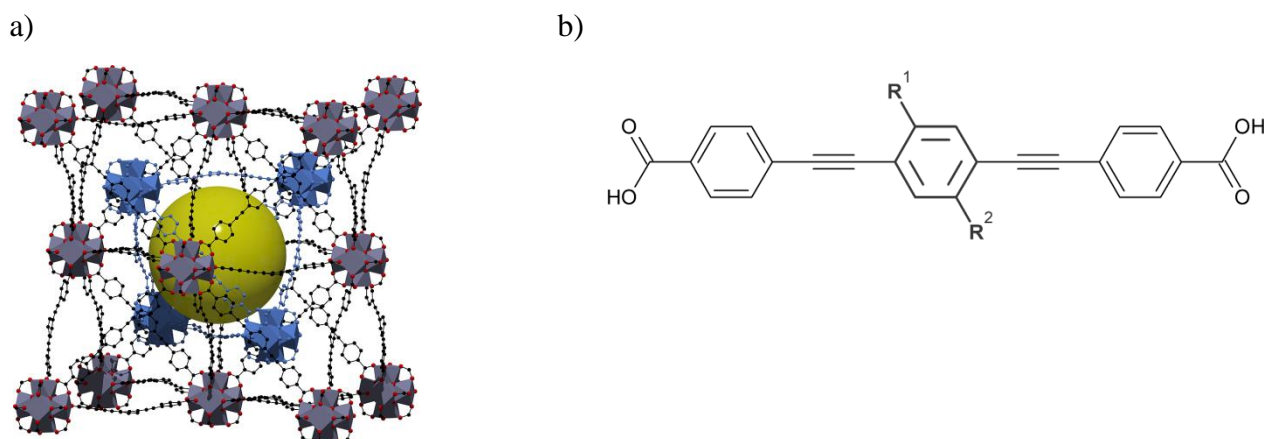


Figure 1

Grand Canonical Monte Carlo (GCMC) simulations were performed on different PIZOFs and other Zr-MOF compounds [2] to investigate the adsorption of various adsorptives (Argon, Nitrogen, Carbon dioxide, Methane). However, it turned out, that the choice of the partial charges is crucial for the simulation results. In this work, we present DFT calculations on clusters cleaved from the unit cell of each MOF structure. The electrostatic potential charges obtained with MERZ-SINGH-KOLLMAN (MK) scheme were used to determine the atomic charges. We present a molecular model that predicts the shape of the isotherms mostly in good agreement with experimental data and helps to explain the adsorption mechanisms that are responsible for this behavior.

[1] A. Schaate, P. Roy, T. Preuße, S. J. Lohmeier, A. Godt, P. Behrens, *Chem. Eur. J.*, **2011**, *17*, 9320-9325.

[2] G. Wißmann, A. Schaate, S. Lilienthal, I. Bremer, A. M. Schneider, P. Behrens, *Micropor Mesopor Mat.*, **2012**, *152*, 64-70.