Force fields for porous coordination polymers - a tricky business

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Porous coordination polymers (also known as metal-organic frameworks) are a new and exciting class of porous materials because of their tunability and flexibility. For the theoretical modeling on the other hand, these advantages are a challenge. Because of the mere size of the systems and the need to sample configurational space, a treatment by *ab initio* MD methods is computationally demanding and impossible for routine calculations. Force field models need to be sufficiently accurate to get the proper balance between entropic and energetic contributions. For the organic linker part such parameterizations exist, but for the coordination environments a sufficiently accurate molecular mechanics parameterization is not straight forward. Over the years our group has developed MOF-FF for this purpose, which is a first-principles parameterized force field [1]. In the presentation I will discuss the peculiarities of the force field and the evolutionary strategy parameterization approach. Recently we have developed a hierarchical automated parameter assignment (HAPA) scheme, which retrieves parameters automatically from our MOF+ website (https://www.mofplus.org). I will show how this can be used to investigate the thermal opening of specific MOFs, which undergo a phase transformation from a closed to an open pore structure by increasing the temperature (Figure 1). In addition, also the current limits of such force field models will be discussed for selected application problems.
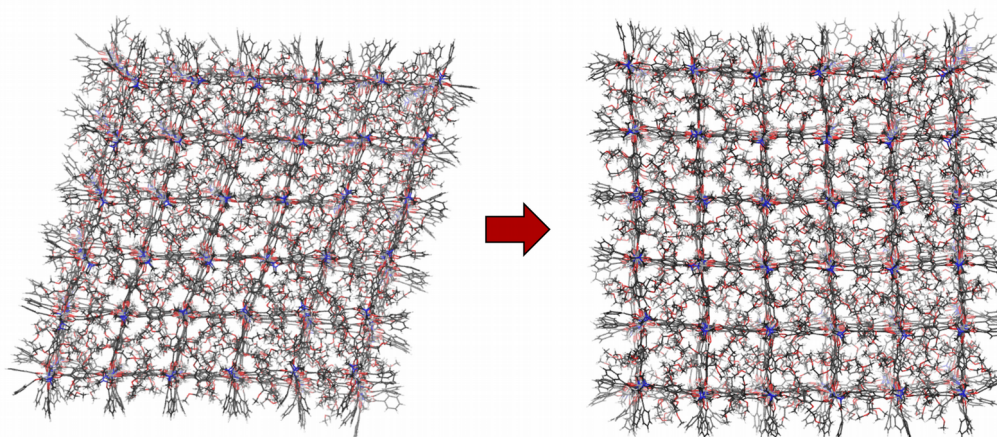

Figure 1: Opening of a 6x6x6 BME-fu-MOF nanoparticle (Cu(BME-bdc)$_2$(dabco), BME-bdc: 2,5-bismethoxyethoxy-benzenedicarboxylate) by heating from 300K to 500K.

[1] a) M. Tafipolsky, R. Schmid, *J. Phys. Chem. B* **2009**, *113*, 1341-1352. b) S. Bureekaew, S. Amirjalayer, M. Tafipolsky, C. Spickermann, T. K. Roy, R. Schmid, *Phys. Stat. Sol. B* **2013**, *250*, 1128-1141. c) J. P. Dürholt, G. Fraux, F.-X. Coudert, R. Schmid *J. Chem. Theory Comput.* **2019**, *just accepted* **DOI:** *10.1021/acs.jctc.8b01041*.