

WP n°:

Title: Advanced molecular simulations to accurately characterize metal-organic frameworks

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Summary (max 200 words):

Metal-organic frameworks (MOFs) are a class of porous crystalline materials which are made up by metal clusters connected by organic linkers. These materials can be synthesized with a large versatility and can be tuned both chemically and structurally [1]. QuickFF [2], an in-house developed code, was recently proposed to derive accurate force fields for MOFs in an automated fashion. It was designed in such a way that more advanced force field energy expressions can easily be introduced for an improved description of e.g. the complex coordination environments often found in MOFs. Ab initio calculations on smaller building units are used as input for QuickFF to generate the force field. A first and useful validation of the force fields is the prediction of the crystallographic unit cell of a test set of materials. Thermal and elastic properties of MOFs are studied in a second step using these first-principles derived force fields. One spectacular property is the structural flexibility observed for some MOFs [3]. Recent studies have shown that a characterization of the anisotropic elastic behavior can predict this flexibility [4]. This work shows that a good agreement with experimental results is possible for the crystallographic unit cell, thermal and elastic properties.

[1] G. Férey, *Chem. Soc. Rev.*, **37**, 191 (2008)

[2] L. Vanduyfhuys *et al.*, *J. Comput. Chem.*, **36**, 1015 (2015)

[3] A. Schneemann *et al.*, *Chem. Soc. Rev.*, **50**, 6062 (2014)

[4] A. U. Ortiz *et al.*, *Phys. Rev. Lett.*, **109**, 195502 (2012)