

## Title: Low dimensional physics in Metal-Organic Frameworks: a DFT-study of the breathing MIL-47

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### Abstract:

Metal-organic frameworks (MOFs) are a relatively young class of materials showing properties akin to both solids and molecular systems. They consist of inorganic metal clusters connected through organic molecules, giving rise to porous, highly tunable frameworks. Their porous nature and chemical tunability makes them versatile materials of interest for industrial, chemically oriented processes, such as catalysis, gas separation and gas storage.[1] Their framework nature, on the other hand, provides new opportunities to investigate low dimensional physics and the associated exotic phenomena.[2]

In this work, we focus on breathing MIL-47 MOFs, which can reversibly switch between a large-pore (LP) and narrow-pore (NP) configuration under the influence of guest molecules, temperature or pressure.[3,4] These MOFs consist of transition-metal (TM) oxide chains linked by benzenedicarboxylate (BDC) linkers. We investigate the stability, both electronic and mechanic, of this MOF with respect to the spin configuration of the TM-chains. An anti-ferromagnetic groundstate is found, with a very weak interchain coupling, making the chains quasi-1D systems.[3] More interestingly, the spin configuration of the single chains has a strong influence on the mechanical properties of this MOF, varying its bulk modulus by 25% between the ferromagnetic and anti-ferromagnetic configurations. Although the spin configuration are extremely difficult (or impossible) to directly measure in experiments for these MOFs, we will show how they can be related to experimental results, and that excellent agreement can be obtained.[2,4]

[1] Shyam Biswas, Danny E. P. Vanpoucke, *et al.*, **J. Phys. Chem. C** **117(44)**, 22784-22796 (2013), doi: [10.1021/jp406835n](https://doi.org/10.1021/jp406835n)

[2] Danny E. P. Vanpoucke, Jan W. Jaeken, *et al.*, **Beilstein J. Nanotechnol.** **5**, 1738-1748 (2014), doi: [10.3762/bjnano.5.184](https://doi.org/10.3762/bjnano.5.184)

[3] Karin Barthelet, Jérôme Marrot, J., *et al.*, **Angew. Chem., Int. Ed.** **41**, 281–284 (2002). doi:10.1002/1521-3773(20020118)41:2<281::AID-ANIE281>3.0.CO;2-Y

[4] Pascal G. Yot, Quintain Ma, *et al.*, **Chem. Sci.** **3**, 1100–1104 (2012). doi:10.1039/C2SC00745B