Soft Porous Crystals: Extraordinary Responses to Stimulation

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Recent years have seen a large increase of the research effort focused on framework materials, including the nowadays-ubiquitous metal–organic frameworks, but also dense coordination polymers, covalent organic frameworks, and molecular frameworks. A large number of these frameworks flexible, or stimuli-responsive, i.e. their structure can undergo changes of large amplitude in response to physical or chemical stimulation.

Our group has put together a "toolbox" of theoretical approaches to shed light into these materials' properties, and in particular to understand their behaviour under mechanical constraints and temperature changes, the interplay between the phenomena of adsorption, deformation and reactivity of these materials, and their optical properties. By means of molecular simulation at varying scale, we can now probe, rationalize and predict the behaviour of stimuli-responsive materials, producing a coherent description of Soft Porous Crystals from the unit cell scale all the way to the behaviour of the whole crystal.

Key references:

▪ *"Liquid metal-organic frameworks", R. Gaillac, P. Pullumbi, K. A. Beyer, K. W. Chapman, D. A. Keen, T. D. Bennett and F.-X. Coudert, Nature Mater., 2017, 16, 1149–1154.*
▪ *"Interplay between defects, disorder and flexibility in metal-organic frameworks", T. D. Bennett, A. K. Cheetham, A. H. Fuchs and F.-X. Coudert, Nature Chem., 2017, 9 (1), 11–16.*
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