Crystals with extraordinary behavior under 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, and there is growing evidence that large-scale flexibility, the presence of defects and long-range disorder are not the exception in metal-organic frameworks, but the rule.[1]

Our group has put together a "toolbox" of theoretical approaches to shed light into these materials' properties, and in particular to understand their behavior under mechanical constraints and temperature changes, the interplay between the phenomena of adsorption,[2] 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 behavior of stimuli-responsive materials, producing a coherent description of Soft Porous Crystals from the unit cell scale all the way to the behavior of the whole crystal. This is particularly important in understanding the links between flexibility, defects[3] and disorder, [4] all of which arise from the large dimensionality of these complex supramolecular assemblies.

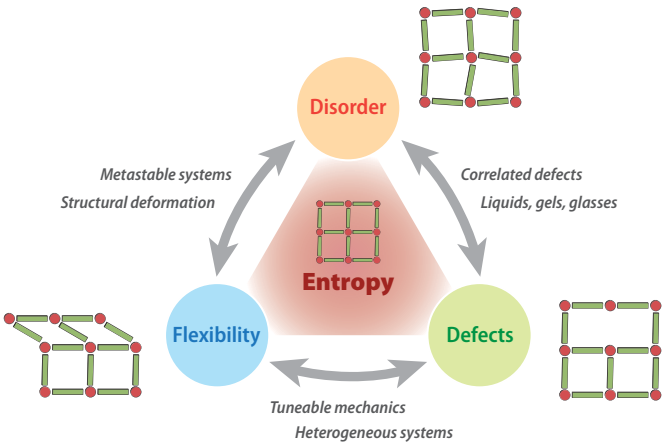

Figure 1. Interplay between flexibility, defects and disorder in soft porous crystals.

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3. "Encoding Complexity within Supramolecular Analogues of Frustrated Magnets", A. B. Cairns, M. J. Cliffe, J. A. M. Paddison, D. Daisenberger, M. G. Tucker, F.-X. Coudert and A. L. Goodwin, *Nature Chem.*, **2016**, 8, 442–447

4. "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.