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Assessing and predicting flexibility in MOFs with molecular simulation

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Much attention has recently been focused flexible metal-organic frameworks (MOFs), or Soft Porous Crystals, that behave in a remarkable stimuli-responsive fashion upon guest adsorption, temperature, or mechanical pressure. It was shown that these different stimuli-driven structural transitions can be rationalized by combining an understanding of adsorption thermodynamics and mechanical properties of the host phases. We will show how the combination of a large range of molecular simulation methods can assess the extent of flexibility of known MOF structures, as well as give physical insight into their deformation mechanisms, and predict the occurrence of new phases. In particular, we will demonstrate the breathing nature of recently synthesized MOFs CAU-13 and NOTT-300, that have not been observed experimentally.

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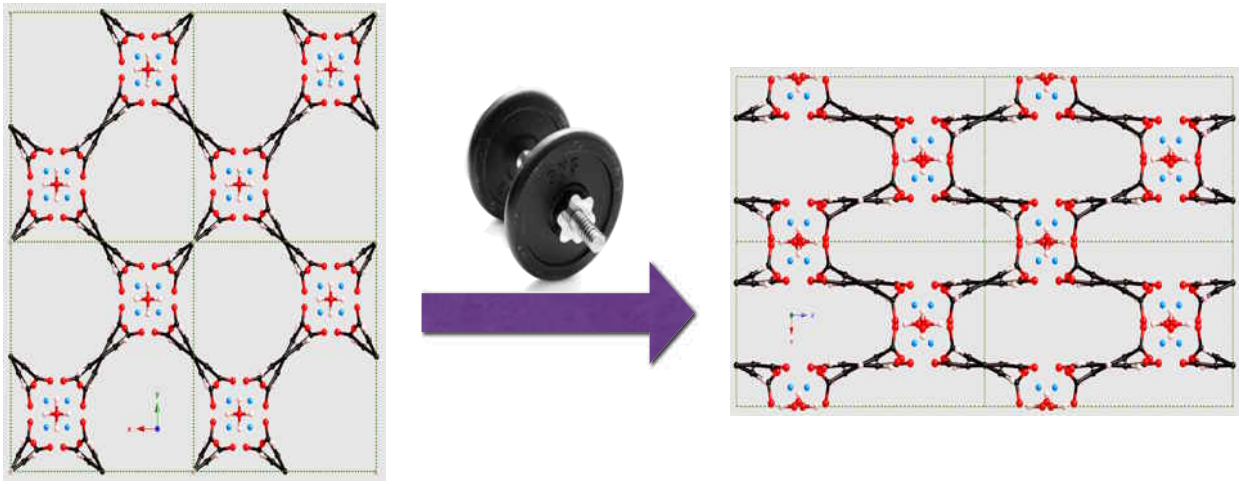

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