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Hydrogen storage, adsorption induced deformation and the role of confinement dimensionality in CAU metal organic frameworks

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We have studied mechanism of hydrogen storage in CAU-1 and CAU-8 metal organic frameworks synthesized at Christian-Albrechts-University of Kiel, Germany 1, [2]. The structures of these compounds are built from aluminum polyhedra with fully coordinated metal ions. Using various types of organic linker molecules tunable structures with channels of different geometries, but very similar chemical composition can be formed. Thus, CAU-1 consists of a three-dimensional confinement network with cavities of 10 Å and 5 Å of average cross section, while the structure of CAU-8 contains one-dimensional channels of about 8 Å diameter.
We observed striking differences in hydrogen sorption of these compounds. CAU-1 exhibits a considerable hydrogen uptake reaching about 6 wt. % percentage at 50 K at the pressure of 1 bar which stays stable after several sorption cycles. Hydrogen uptake of CAU-8, in contrast, is substantially lower of only about 2.7 wt.% at 50 K and quickly erodes after few sorption/ desorption cycles. In order to understand the mechanism of such differences on the microscopic level we have conducted an extensive study using in-situ neutron scattering diffraction and spectroscopy [3]. We observe that hydrogen sorption in both compounds is driven by interactions between guest hydrogen molecules and the organic linkers having, however, a very dissimilar impact. In CAU-1, the adsorption of hydrogen on the organic linkers in the initial stages leads to the contraction of the framework structure and as a result to changes in the electronic potential landscape inside the pores. This in turn causes the increase of hydrogen uptake by triggering the rearrangement of the adsorbed molecules and the formation of additional occupied positions. Guest-host interactions in one-dimensional channels in CAU-8 lead high possibly to the partial collapse of one-dimensional channels and to the consequent decrease of hydrogen uptake. One can argue that a three-dimensional porous framework could better resist an adsorption induced mechanical stress [4] as one-dimensional channel structures. Furthermore, smart tuning of adsorption-induced structural deformation of porous materials could be used for further improvement of storage capacities in metal-organic frameworks alongside with other recently reported approaches such as sorption of two hydrogen molecules at a single metal site [5].

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