Contribution ID: **362** Type: **Poster**

In-situ neutron scattering study of adsorption induced structural deformation in CAU metal organic frameworks –can structural contraction increase hydrogen uptake?

Monday, 17 September 2018 17:45 (15 minutes)

Understanding the molecular mechanism of adsorption in porous materials is important for a broad range of modern technologies staring from energy storage and conduction to heterogeneous catalysis and to the development of the novel drug carriers. Recent theoretical studies hint at adsorption induced structural changes and the onset of stress in porous materials contradicting broadly accepted assumption that the structure of the porous materials does not change during the sorption process. In order to understand the origin of such changes and their impact of the adsorption behavior we have studied hydrogen sorption in CAU-1 and CAU-8 metal organic frameworks. The structures of CAU-1 and CAU-8 consist from 3D pore network and 1D confining channels respectively [2],[3]. Built from aluminum polyhedra with fully coordinated metal ions CAU-1 and CAU-8 provide an environment with similar pore wall interactions for guest molecules. This allow us to systematically follow the intermolecular interactions as a function of the pore geometry.
Using in-situ neutron scattering techniques we observe a substantial structural contraction at the initial stages of adsorption in both materials, which originate from interactions between the hydrogen and organic linkers. In CAU-1 such contraction triggers the rearrangements of confined molecules and, surprisingly, to the formation of new occupational positions, increasing the hydrogen uptake [4]. In 1D channel system CAU-8 the adsorption of hydrogen on the linkers is followed by the formation of the hydrogen chains close to the channel center and, as a result, to the structural relaxation of the host framework. In both systems we see novel structural arrangements of confined hydrogen at nanoscale.
[1]. F.-X. Coudert, A.H. Fuchs, A.V. Neimark, A. V. Dalton Trans. 2016, 45 (10), p. 4136–4140
[2]. F. Hinterholzinger N. Stock et al, Phys. Chem. Chem. Phys., 2010, 12, 4515–4520
[3]. H. Reinsch et al, Inorg. Chem., 2013, 52 (4), pp 1854–1859
[4]. M. C. Schlegel, M. Russina et al, PCCP, 2016, DOI: 10.1039/C6CP05310F

Primary authors: RUSSINA, Margarita (Helmholtz Zentrum Berlin für Materialien und Energie); Dr GRZIMEK, Veronika (Helmholtz Zentrum Berlin); Dr SCHLEGEL, Moritz-Casper (2 BAM Federal Institute for Materials Research and Testing,); Mr SVETOGOROV, Roman (NRC Kurchatov Institute); Dr TÖBBENS, Daniel M. (Helmholtz-Zentrum Berlin für Materialien und Energie); Dr HOFFMANN , Jens-Uwe (Helmholtz Zentrum Berlin); Dr REINSCH, Helge (Christian-Albrecht-Universität zu Kiel,); Prof. STOCK, Norbert (Institute of Inorganic Chemistry, Christian-Albrecht-Universität zu Kiel)

Presenter: RUSSINA, Margarita (Helmholtz Zentrum Berlin für Materialien und Energie)

Session Classification: Poster session 1

Track Classification: P8 Functional materials and materials science