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# Neutron scattering insight at hydrogen storage in sub-nanopores

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Safe and effective hydrogen storage is widely recognized as a key technology for hydrogen economy in the 21st century, with porous materials being one of the highly potential storage media. The hydrogen storage in such materials is often realized by means of weak Van der Waals interactions between the stored molecule and the pore surface. However, in addition to the surface, interactions between guest and matrix can be expected to be sensitively influenced by structure of the confining host and, in particular, the dimension of the confinement cages. We have explored the microscopic mechanism of hydrogen storage in pores of sub-nanometer size in a broad range of materials, namely ice-based clathrates, recently synthesized CAU-1 metallic organic framework and porous carbide derived carbon (CDC) with help of neutron scattering techniques. Our observations reveal the large quantitative and qualitative impact of details of the confinement structure on the functionally decisive dynamic behavior of the stored molecules.

Thus, in clathrate hydrates we have found that by varying the size of the pore the diffusive mobility of confined hydrogen can be modified in both directions, i.e. reduced or enhanced compared to those in the bulk solid at the same temperatures [1],[2]. In the small cages with a diameter of 0.8 nm the confinement reduces diffusive mobility by orders of magnitude. The observed localization of the hydrogen around the center of the cage provides for the improved functional properties such as gas degassing temperature and the gas loading pressure. In contrast, in large cages with a mean diameter of 0.9 nm hydrogen molecules displays diffusive jump motion between different equilibrium sites inside the cages, observed at temperatures where bulk solid $H_2$ exhibits no visible mobility. Strong slow-down of diffusion was also observed in CDC with the pore size of 0.8 nm. The experimentally determined self-diffusion coefficient in TiC-CDC with cylinder like pores [3] is about $2.35 \pm 0.7$ Å$^2$/ps at 100 K [4], which is only the third of the diffusion coefficient measured at surface of nanohorns at 25K [5]. In CAU-1 metallic organic framework the sub-nanometer size of the pores promotes the formation of the hydrogen bonds between hydrogen and linkers and the onset of guest-guest correlations [6]. Consequent shrinking of the host framework structure changes in the electronic potential surface inside the pores, leading to the formation additional occupational positions and increased hydrogen intake.

[1] E. Pefoute, E. Kemner, J. C. Soetens, A. Desmedt, M. Russina, J. of Phys. Chem. C, 116, 16823 (2012); [2] M. Russina, E. Kemner, F. Mezei, submitted; [3]. H. Kürig, M., Russina et al, Carbon 100 (2016) 617-624; [4] and submitted, [5] F. Fernandez-Alonso et al, PRL 98, 215503 (2007), [6] M. Schlegel et al, submitted

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