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Neutron scattering investigations of hydrogen storage in porous materials

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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 successful synthesis and design of new materials dictate however the necessity of systematic studies of the storage processes and fundamental understanding of molecular processes involved. We have explored the microscopic mechanism of hydrogen storage in pores of sub-nanometer size in 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. The ability of neutrons to probe both microscopic structure and dynamics combined with high sensitivity to hydrogen makes neutron scattering a powerful tool in the exploration of the confined hydrogen behavior. Our results show that confinement leads to strong variation of molecular mobility as a function of pore size and can be reduced or enhanced compared to those in the bulk solid at the same temperatures. Secondly, hydrogen storage can be improved by smart tuning of the guest-host and guest-guest interactions. In CAU-1 metallic organic framework we have observed a formation of the hydrogen bonds between hydrogen and linkers and strong guest-guest correlations leading to the shrinking of the host framework structure and rearrangements of confined molecules. In extreme cases the contraction of the framework can lead to the expulsion of the gas from the pore. The moderate deformation however promotes the formation additional occupational positions and increase of hydrogen intake.

Biography

Margarita Russina has completed her PhD from Technical University Berlin and postdoctoral studies from Los Alamos National Laboratory (USA). She is the leader of Neutron Time-Of-Flight Spectroscopy group at Helmholtz Centre Berlin Material and Energy Research. She has published more than 60 papers in reputed journals.

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