

Gas storage carbon meso- and nanoporous materials

Opportunity

There are needs for developing new methods for hydrogen storage using gas adsorption methods. Understanding room temperature phase behavior of thin layers of confined gases in mesoscopic porous materials is still a challenge.

Meso Challenge

Understanding the adsorption of gases and liquids in confined porous materials. New measurement techniques are needed to probe the structure of these materials.

References: N. C. Gallego, L. He, D. Saha, C. I. Contescu, and Y. B. Melnichenko, JACS (2011)

Approach

Develop and apply new in-situ methods for determining the phase diagrams and pore size dependent density of thin, adsorbed H₂ layers confined in pores. Small angle neutron and x-ray scattering combined with the traditional “macroscopic” methods of adsorption measurements (gravimetric, volumetric, helium porosimetry, low-pressure adsorption of N₂ and CO₂ can yield new insights to the complex interactions between the gases and the porous host material. The data of neutron scattering experiments analyzed in a tandem with computer simulations based on the deployment of petascale and future exascale computing systems will enable predictive simulations of realistic device structures from first-principles.

Impact

The studies can be used to guide the development of new carbon adsorbents tailored to approach the DOE target of 4.5 wt % at near-ambient conditions.

