MM 33: SYM Hydrogen in Materials: New Developments I

Time: Thursday 10:15–11:25 Location: H 1058

Invited Talk MM 33.1 Thu 10:15 H 1058

Hydrogen Physisorption in MOFs — •Barbara Panella[1,2] and Michael Hirscher[2] — [1]Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, Hönggerberg, Zürich, Switzerland — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Metal-organic frameworks (MOFs) are due to their extremely high porosity and defined structure very attractive materials for hydrogen storage at cryogenic temperatures (77 K). The storage capacity of molecular hydrogen in MOFs is higher than for any other porous material and further improvements are expected if the framework structure of novel MOFs will be optimized. This optimization can involve different routes like increasing the specific surface area, tuning the size of the pores and introducing metal centers which might strongly polarize the molecule. This presentation will give an overview on the most important results obtained in the last years on hydrogen storage in MOFs focusing on the correlation between structure and hydrogen adsorption properties. Additionally, a comparison between MOFs and other classes of porous materials for hydrogen physisorption will be presented. Finally several experimental techniques will be shown which allow to investigate the interaction between hydrogen and metal-organic frameworks.

MM 33.2 Thu 10:45 H 1058

Isosteric heat of adsorption for hydrogen in microporous materials — •Barbara Schmitz[1,2] and Michael Hirscher[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Universität Bonn, Germany

The adsorption of hydrogen in activated carbon and metal organic frameworks is measured with an automated Sieverts apparatus. The pressure dependent hydrogen uptake is investigated at several temperatures above 77K and pressures up to 20bar. The total uptake is correlated to the specific surface area. From the adsorption isotherms the isosteric heat of adsorption is evaluated within a wide range of surface coverage between 0.2 and 0.8. The results are related to the structure of the different materials.

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MM 33.3 Thu 11:05 H 1058

Hydrogen storage in nanoporous materials — •Sergei Yurchenko[1], Lyuben Zhechkov[1], Thomas Heine[1], Aliezer Martinez[1], Gotthard Seifert[1], and Serguei Patchkovskii[2] — [1]Institut für Physikalische Chemie und Elektrochemie, TU Dresden, D-01069 Dresden, Germany — [2]Steacie Institute for Molecular Sciences, NRC Canada, 100 Sussex Drive, Ottawa, Ontario, K1A 0R6 Canada

In this study we investigate the effect of the structural characteristics of the nanoporous environment on the hydrogen abundance in the material. For this purpose we evaluate the hydrogen adsorption in well-defined hypothetical systems as well as in realistic environment, which have been studied in experiment before. We calculate storage capacity of the adsorbed hydrogen gas at different conditions, varying the gas temperature and pressure.

For our simulations we employ the quantized liquid density functional theory (QLDFT), developed recently as an extension of the density functional theory of liquids to quantized liquids at finite temperatures. We introduce a reference fluid of non-interacting featureless hydrogen molecules obeying Boltzmann statistics in connection with the rigorous Kohn-Sham formulation. Following the liquid DFT this functional is extracted from thermodynamical experimental data for uniform hydrogen fluids. Thus the method allows us to take into account directly the interaction between the hydrogen molecules, which usually is a large source of errors for systems with highly inhomogeneous guest density.