 ICCES, vol.18, no.1, pp.21-21

# HYDROGEN STORAGE IN CARBON NANOSTRUCTURES AND ORGANIC FRAMEWORKS

**Gotthard Seifert, Aliezer Martinez Mesa, Sergei Yurchenko,Bassem Assfour1, Thomas Heine3, Sergei Patchkovski**

## Summary

In this study structural characteristics of several carbon based nanostructures and organic frameworks as metal organic frameworks (MOF) and covalent organic frameworks (COF) on the hydrogen abundance in the material are investigated with the quantized liquid density functional theory (QLDFT), Molecular Dynamics (MD) and Grand Canonical Monte Carlo (GCMC).

We applied these theories to evaluate the hydrogen storage capacities of nanoporous materials: Compact storage of hydrogen is the key challenge facing adoption of hydrogen as fuel for mobile applications. A promising approach to increase the storage densities is the adsorption of molecular hydrogen in porous environments. We have studied in detail the role of the host structure, the pressure and temperature dependence as well as the importance of quantum effects on the hydrogen storage capacity of a broad range of materials. A critical comparison with available experimental data is also given