

Adsorption of molecular hydrogen on nanostructured surfaces

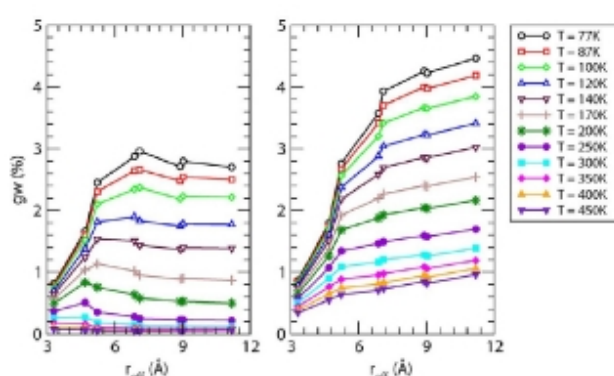
Aliezer Martínez-Mesa^{1,2}, Gotthard Seifert¹

¹) *Institut für Physikalische Chemie und Elektrochemie, Technische Universität Dresden, Germany*

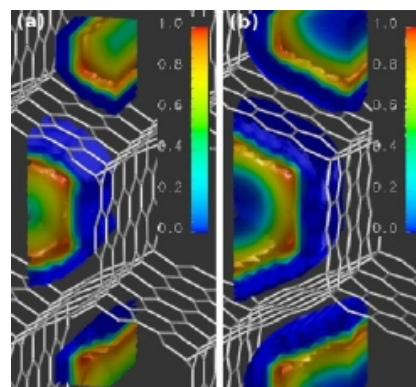
Aliezer.Martinez@chemie.tu-dresden.de, Gotthard.Seifert@chemie.tu-dresden.de

²) *Departamento de Física Teórica, Universidad de la Habana, Cuba*
aliezer@fisica.uh.cu

We investigate the effect of the structural characteristics of idealized nanoporous environments on the adsorption of molecular hydrogen. The adsorption properties of the target nanostructures (graphene and ZnO sheets, carbon foams [1,2], metal-organic frameworks) are evaluated in a broad range of thermodynamic conditions. The study is carried out within the density functional theory for quantum fluids at finite temperature (QLDFT) [3], which allows to account for the many-body and quantum delocalization effects in a single theoretical framework. The exchange-correlation (excess) functional is derived from the empirical equation of state of the homogeneous system. We focus on the evaluation of hydrogen storage capacities of the substrates and on the emergence of quantum effects triggered by the confinement imposed by the host structure. The relation between the microscopic structure of the hydrogen fluid and the calculated adsorption properties is also addressed.



Gravimetric storage capacities of carbon foams at $p=5$ bar (left panel) and $p=100$ bar (right panel).



Spatial distribution of H_2 molecules inside the unit cell of (3,3) armchair (left panel) and (4,4) armchair (right panel) carbon foams.

References:

- [1] A. Martínez-Mesa et al., *J. Chem. Phys.* **135**, 214701 (2011)
- [2] A. Martínez-Mesa et al., *J. Phys. Chem. C* **116**, 19543 (2012)
- [3] S. Patchkovskii, T. Heine, *Phys. Rev. E* **80**, 031603 (2009)