

Adsorption and storage of hydrogen in porous and layered materials

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Hydrogen adsorption on porous materials is a promising technology for hydrogen storage. Pure carbon materials do not reach the technological targets, but experimental work has shown that doping the porous carbons with palladium nanoparticles enhances the storage capacity of those materials [1]. We have investigated the role of the Pd dopant on the adsorption and storage mechanisms. Density functional calculations indicate that H₂ molecules adsorb on the Pd clusters following two channels: molecular adsorption and dissociative chemisorption [2]. The competition between those two channels on Pd clusters, free and anchored on a vacancy in graphene, has been studied, and the effects of the carbon substrate have been identified. The hypothesis normally used to justify the enhancement of the storage capacity is that the hydrogen molecules dissociate on the Pd particles and then the hydrogen atoms spill over the carbon substrate. To test this hypothesis we have performed ab initio molecular dynamics simulations of the deposition of molecular hydrogen on Pd clusters supported on graphene [3]. The results of the simulations cast doubts on the validity of the spillover mechanism for explaining the enhancement of hydrogen storage in Pd-doped porous carbons.

Layered inorganic materials, like nanotubes and fullerene-like nanoparticles of WS₂ are also investigated as media for hydrogen storage [4]. Using hydrogen activated by radiofrequency plasma increased the efficiency of its absorption on the nanoparticles as compared to hydrogenation by high pressure molecular unactivated hydrogen. The chemical configuration of the absorbed hydrogen is of primary importance, as it affects its absorption stability and possibility of release. Micro-Raman spectroscopy was applied to elucidate the chemical bonding of hydrogen and to distinguish between chemi- and physisorption. A model based on density functional theory was used to simulate the adsorption of hydrogen on the WS₂ nanoparticles, demonstrating good agreement between theory and experiment [5].

References

- [1] C. I. Contescu et al., Carbon **49**, 4050 (2011).
- [2] A. Granja, J. A. Alonso, I. Cabria and M. J. López, RSC Advances **5**, 47945 (2015).
- [3] M. Blanco-Rey, J. I. Juaristi, M. Alducin, M. J. López and J. A. Alonso (submitted for publication).
- [4] A. Laikhtman et al., Int. J. Hydrogen Energy, **39**, 9837 (2014).
- [5] A. Laikhtman, G. Makrinich, M. Sezen, M. M. Yildizhan, J. I. Martinez, D. Dinescu, M. Prodana, M. Enachescu, J. A. Alonso and A. Zak (submitted for publication).