

## Hydrogen adsorption on palladium clusters deposited on graphene

María J.López<sup>1</sup>, I.Cabria<sup>1</sup>, S. Fraile<sup>2</sup>, and J.A. Alonso<sup>1</sup>

<sup>1</sup> *Departamento de Física Teórica, Atómica y Óptica, University of Valladolid, Spain*

<sup>2</sup> *Departamento de Física Aplicada-LATUV, University of Valladolid, Spain*

maria.lopez@fta.uva.es

The Palladium might enhance hydrogen storage in porous carbons by surface reactions, especially by hydrogen spillover which consists in the dissociation-storage-recombination of hydrogen in the material. To gain some insight on the possible structures formed by palladium on nanoporous carbons, and on the role played by palladium in the storage of hydrogen, we have investigated the adsorption of palladium on a graphene surface and the adsorption and dissociation of molecular hydrogen on the Pd clusters. Density functional calculations show that, even at the earlier stages of Pd deposition on the graphene surface, the Pd atoms have a strong tendency to form clusters [1]. Three-dimensional clusters are more stable than planar clusters and the transition from planar to three-dimensional Pd clusters adsorbed on graphene occurs very early as a function of cluster size, at Pd<sub>4</sub>. This tendency is a consequence of the strong Pd-Pd interaction. We have also investigated the adsorption and the dissociation of molecular hydrogen on the deposited Pd clusters as a function of cluster size. The mechanism for the activation of the hydrogen molecule and its possible subsequent dissociation is discussed. We also discuss the implications for the hydrogen storage capacity of Pd-doped nanoporous carbon materials.

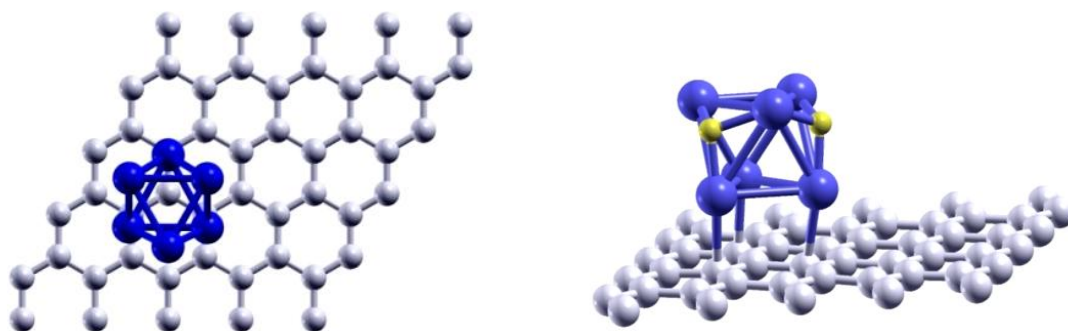


Figure 1: Pd<sub>6</sub> cluster deposited on graphene (left), and H<sub>2</sub> dissociated on the deposited Pd cluster (right).

### References

[1] I. Cabria, M.J. López, and J.A. Alonso, Phys. Rev. B 81, 035403 (2010).