BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA
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SEMINARIO

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"Hydrogen adsorption in transition-metal clusters supported on graphene monovacancies: a first-principles study."

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In this talk, a detailed description of the atomic structure and the energetics of H_2 adsorption on Pd_4, Ni_4, and Ti_4 clusters supported on graphene monovacancies is presented. The large binding energy of that clusters on vacancies is a result of strong hybridization between the unsaturated carbon and the metal atoms, and it furthermore indicates that anchoring avoids migration of metal clusters on the graphene surface. We found that the binding energy of a single H_2 is strongly dependent on the specific cluster. In particular, the H_2 bond cleavage is favored by titanium clusters indicating the formation of metal hydrides. On the other hand, the Ni and Pd clusters favours the formation of Kubas complexes. The analysis of the absorption energies and H_2 average bond lengths suggests that supported Ti_4 cluster is a potential hydrogen storage candidate, being able to hold up to six H_2 molecules covalently with moderate average binding energy within the optimal range for an efficient cyclic adsorption/desorption process at room temperature and moderate pressures. Finally, the present theoretical results are discussed in the light of very recent experimental reports on hydrogen adsorption and desorption measurements in titanium-decorated graphene samples. This work was done in collaboration with Carlos Ramos-Castillo (Cinvestav-Mérida, México), José Ulises Reveles (Virginia Commonwealth University, USA) and Rajendra Zope (University of Texas at El Paso, USA).

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