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Study of Hydrogen Adsorption in Titanium, Nickel and Pd Cluster Supported on Graphene Monovacancies CARLOS MANUEL RAMOS CASTILLO, ROMEO DE COSS GMEZ, Department of Applied Physics Centro de Investigacion y Estudios Avanzados del Instituto Politecnico Nacional, Mexico, JOSE ULISES REVELES, Department of Applied Physics Virginia Commonwealth University , VA USA — A detailed description of the atomic structure and the energetics of H₂ adsorption on Ti₄, Ni₄, and Pd₄ clusters on graphene monovacancies is presented. The large binding energy of that clusters on vacancies is a result of strong hybridization between the unsaturated carbon. We found that the binding energy of a single H₂ is strongly dependent on the specific cluster. In particular, the H₂ bond cleavage is favored by titanium clusters. On the other hand, the Ni and Pd clusters favours the formation of Kubas complexes. The analysis of the adsorption energies and H₂ average bond lengths suggests that supported Ti₄ cluster is a potential hydrogen storage candidate, being able to hold up to 6 molecules covalently with moderate average binding energy within the optimal range for an efficient cyclic adsorption/desorption process at room temperature and moderate pressures. These results give physical insights about how the interaction between graphene monovacancies and metal clusters can be used to enhanced the hydrogen uptake, towards of design of new graphene-based material for hydrogen storage.

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