Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Hydrogen adsorption around a hydrogen atom anchored in a graphene vacancy** GERARDO VAZQUEZ, FERNANDO MAGANA, Instituto de Fisica, UNAM, EDUARDO RANGEL, Instituto de Investigacion en Materiales, UNAM — In this work, we study the adsorption of hydrogen molecules around a hydrogen atom anchored in a graphene vacancy. We used density functional theory and molecular dynamics. To study the adsorption of hydrogen molecules on the system we used three hydrogen molecules around each hydrogen atom It was found that raising the temperature of the system up to 900 K the hydrogen molecules remained linked to the system of graphene doped with hydrogen. The results show that doping graphene with atomic hydrogen can be useful to store hydrogen molecules in the system.

Fernando Magana
Instituto de Fisica, UNAM

Date submitted: 14 Dec 2011 Electronic form version 1.4