Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Adsorption of molecular hydrogen on Pd(Pt) decorated graphene[1] NARAYAN ADHIKARI, ASIM KHANIYA, SARAN LAMICHHANE, NURAPATI PANTHA, Central Department of Physics, Tribhuvan University, Kathmandu — We have performed the first-principles based Density Functional Theory (DFT) calculations to study the stability, geometrical structures, and electronic properties of a Pd(Pt) atom adsorbed graphene to investigate the possibility of using Pd(Pt) decorated graphene as energy storage materials with reference to pristine graphene. The London dispersion forces have been incorporated by the DFT-D2 levels of calculations implemented in Quantum Espresso packages. Our findings show that Pd and Pt both adsorb on graphene at Bridge site. The electronic structures of Pd(Pt) adsorbed graphene possesses band gap opening due to breaking of the symmetry of graphene. Further we have studied the adsorption of moelcular hydrogen ((H 2) n , n = 1-7) on the Pd(Pt)-graphene system. The adatom Pd(Pt) enhances the binding energy per hydrogen molecule in Pd(Pt)-graphene system in comparison to that in the pristine graphene. The binding energy per hydrogen molecule of the adatom-graphene system decreases as the number of H 2 molecules increases and finally it saturates to 0.15 eV (0.16 eV) per hydrogen molecule for Pd-graphene (Pt-graphene) systems respectively.

[1]ICTP-NET 56/TWAS

Narayan Prasad Adhikari
Central Department of Physics, Tribhuvan University, Kathmandu

Date submitted: 12 Nov 2014 Electronic form version 1.4