Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Physisorption, Diffusion, Adsorption/Desorption of Molecular Hydrogen on Graphene MAJID KARIMI, Indiana University of PA, JUSTIN PETUCCI, Indiana Univesity of PA, GIANFRANCO VIDALI, Syracuse University — The interaction of a H2 molecule with a graphene surface is studied using AIREBO bond -order potential. Adsorption potential, desorption potential, and diffusion barriers of H2 on graphene are obtained and compared with the corresponding results from the first-principles. The massively parallel molecular dynamics codes (lammps) and nudged elastic band (NEB) method are employed to do these calculations.

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Date submitted: 12 Nov 2012 Electronic form version 1.4