Physisorption, Diffusion, Adsorption/Desorption of Molecular Hydrogen on Graphene MAJID KARIMI, Indiana University of PA, JUSTIN PETUCCI, Indiana University 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.