

Abstract Submitted  
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**Energetic of formation of molecular hydrogen on graphene using Eley-Rideal (ER) and Langmuir-Hinshelwood mechanisms** MAJID KARIMI, Indiana University of PA, SEAN MORGAN, IUP, JUSTIN PETUCCI, University of Denver, CARL LEBLOND, Indiana University of PA, RAZI HASSAN, Alabama A&M University, GIANFRANCO VIDALI, Syracuse University — The second generation AIREBO potential for hydrocarbons is modified to accurately reproduce features of the chemical interactions and reaction of H atoms on graphene surface. The adapted potential reproduces many features of the adsorption potential of hydrogen on graphene in close agreement with the corresponding data from DFT. The modified potential is employed to study formation of H<sub>2</sub> on graphene using ER and LH processes. This study will be carried out using classical molecular dynamics (LAMMPS) and nudged elastic band (NEB) for the calculation of barriers. Partition of the internal energy of the nascent H<sub>2</sub> molecule into translational, vibrational, rotational, and graphene phonons will be studied and compared with the first-principles data.

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