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Adsorption, desorption, and diffusion of atomic hydrogen on graphene MAJID KARIMI[1], JUSTIN PETUCCI[2], CARL LEBLOND[3], GIANFRANCO VIDALI[4], None — Using a modified AIREBO bond-order potential for hydrocarbons, adsorption potential, desorption potential, and diffusion barriers of atomic hydrogen on graphene are obtained and compared with the corresponding results from the first-principles. The formation of molecular hydrogen through Eley-Rideal and Hot-Atom mechanisms is investigated. The massively parallel molecular dynamics code lammps and nudged elastic band NEB method are employed to do these calculations

[1]Physics Department, Indiana University of PA
[2]Physics Department, Denver University
[3]Chemistry Department, Indiana University of PA
[4]Physics Department, Syracuse University

Majid Karimi
None

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