Presented at the DLSU Research Congress 2014
De La Salle University, Manila, Philippines
March 6-8, 2014

Atomic Hydrogen Absorption into Hydrogen Terminated Armchair Edges of Bilayer Graphene

Michelle Natividad[1]*, Raymund Bolalin[1], Gerardo Janairo[1], Hideaki Kasai[2], Nelson Arboleda Jr[1]
[1]*Physics Department, De La Salle University, 2401 Taft Avenue, Manila, Philippines*
[2]*Department of Applied Physics, Suita Campus, Osaka University, 2-1 Yamadaoka, Suita City, 565-9871 Osaka, Japan*
*michelle.natividad@dlsu.edu.ph

Abstract: Density functional theory (DFT)-based calculations are performed to determine the effects of preadsorbed atomic hydrogen (H) and substrate reconstruction on the absorption of H into bilayer graphene via the armchair edge. The total energy is calculated using the Vienna Ab-initio Simulation Package (VASP) software for various X-,Y- and Z-positions of H with respect to a predetermined reference point. The potential energy along Z (surface normal) is plotted as functions of the X- and Y-lateral positions of H. From these plots, the potential energy surface (PES) is obtained and the reaction path for the absorption of H into bilayer graphene via the armchair edge is determined. Results show that without surface reconstruction, absorption of H into the region between the graphene sheets is hindered by the preadsorbed H atoms since a barrier exists on the surface. By allowing surface reconstruction, this barrier is lowered thus enhancing H absorption into the bilayer.

Key Words: density functional theory; graphene; hydrogen storage; potential energy surface