Atomic Hydrogen Absorption into Hydrogen Terminated Armchair Edges of Bilayer Graphene

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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