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Electronic properties of B and Al doped graphane: A hybrid density functional study

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Recently, the two-dimensional (2D) material systems such as graphene, graphane, hexagonal boron nitride and various transition metal dichalconides monolayers have attracted great research interests owing to their peculiar properties. Graphane, a fully hydrogenated graphene, is a wide band gap semiconductor with a large exciton binding energy according to density functional theory (DFT) prediction. Modulating the electronic structure of a semiconductor material is essential for device operations. Doping is recently considered to be a powerful tool to fine tune the band gap of various semiconductor materials. Using the hybrid density functional theory (DFT) approach, we study the electronic properties of a graphane monolayer substitutionally doped with B (B_{CH}) and Al (Al_{CH}) atoms. The density of states (DOS) plot reveals that the band gap of graphane is slightly tuned down due to the B_{CH} doping. Different scenario is observed on the Al_{CH} DOS, where the metallic character has been noted due to the Al dependant spin states crossing the Fermi level. We further examine the response of the Al dependant spin states on the multiple charge states. An addition of the electrons retains the metallic character of Al_{CH}, while the positive charges re-open the band gap, although in a small amount of magnitudes. Our findings suggest the possibility of fine tuning the band gap of graphane through the defect and charge doping.

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