Influence of Interconfigurational Electronic States on Fe, Co, Ni-Silicene Materials Selection for Spintronics

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Abstract

Growth through controlled adsorption of ferromagnetic elements such as Fe, Co and Ni on two-dimensional silicene provides an alternative route for silicon-based spintronics. Plane wave DFT calculations show that Fe, Co and Ni adatoms are strongly chemisorbed via strong sigma bonds, with adsorption energies (1.55 - 2.29 eV) that are two to six times greater compared to adsorption on graphene. All adatoms adsorb more strongly at the hole site than at the atom site, with Ni adsorbing strongest. Of the dimer configurations investigated, the hole – hole, b-atom – hole, vertically stacked at hole, vertically stacked at b-atom and bridge sites were found to be stable. The Co and Ni dimers are most stable when adsorbed in the hole-hole configuration while the Fe dimer is most stable when adsorbed in the atom-hole configuration. Metal-to-silicene and interconfigurational s-to-d electron transfer processes underpin the trends observed in adsorption energies and magnetic moments for both adatoms and dimers. Adsorption of these metals induces a small band gap at the Dirac Cone. In particular Co adatom adsorption at the hole site induces the largest spin-polarized band gaps of 0.70 eV (spin-up) and 0.28 eV (spin-down) making it a potential material candidate for spintronics applications.

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