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First Principle study of Electronic Structure of Silicene Doped with Galium

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Abstract : Gallium with three outer electrons commonly are used as dopants of silicon to make it P type and N type semiconductor respectively. Silicene, one-atom-thick silicon layer is one of emerging two dimension materials after the success of graphene. The effects of Gallium doping on electronic structure of silicine are investigated by using first principle calculation based on Density Functional Theory (DFT) calculation and norm conserving pseudopotential method implemented in ABINIT code. Bandstructure of Pristine silicene is similar to that of graphene. Effect of Ga doping on bandstructure of silicene depend on the position of Ga adatom on silicene

Keywords : silicene, effects of Gallium doping, Density Functional Theory (DFT), graphene
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