Epitaxial Silicene on Semiconductor Substrates: a Density Functional Study

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In spite of the uniqueness of carbon to form pristine fullerene, nanotube and graphene, there have been attempts to replicate these nanostructures with silicon. The latest in this game is the quasi-2D silicene whose free-standing honeycomb form has been predicted to be stable with linear band dispersion and Dirac cone feature similar to graphene. Epitaxial silicene on Ag(110) and on ZrB_2(0001) substrates have been reported recently [1,2]. We have carried out first principles density functional investigation of the structural and electronic properties of silicene monolayer on various wurzite structured III-V and II-VI semiconducting substrates, with metal terminated (MT) as well as non-metal terminated (NMT) top surface [3]. The binding energies of silicene on MT semiconductors are in the range ~0.56±0.12 eV/atom and their behavior can be metallic, semi-metallic or even magnetic, depending on the choice of substrates. The silicene overlayer undergoes n-type (p-type) doping on MT (NMT) semiconductor surface, depending upon the direction of the charge transfer.

References

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