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Density functional investigation of epitaxial silicene on semiconducting substrates G.P. DAS, A. BHATTACHARYA, S. BHATTACHARYA, Indian Association for the Cultivation of Science, Kolkata-700032, India — In spite of the uniqueness of carbon to form pristine fullerene, nanotube and graphene, there have been attempts to replicate these nanostructures with silicon. Most recently, the free-standing quasi-2D honeycomb structure of silicene 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 already been reported [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 0.5 - 0.7 eV/atom and their behavior can be metallic, semi-metallic or even magnetic, depending on the choice of substrates. The silicene overlayer undergoes n-/p-type doping on MT/NMT semiconductor surface, depending upon the direction of the charge transfer. [1] P. Vogt, et al, Phys. Rev. Lett. **108** (2012) 155501. [2] A. Fleurence et al, Phys. Rev. Lett. **108** (2012) 245501 [3] A. Bhattacharya et al,, to be published.

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