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Effect of inter-site Coulomb correlation on Band gap of Graphene-on-Substrates

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Abstract. The pristine graphene has zero band gap at Dirac points. However small band gaps have been observed, when graphene is placed on substrates such as silicon carbide (SiC), silicon dioxide (SiO_2) and Gold (Au) on Ruthenium. In order to study the effect of inter-site Coulomb correlation as well as on-site Coulomb correlation on these gaps, we propose here a tight binding model taking into account of electrons hoppings upto third nearest- neighbor hoppings in honeycomb lattice of graphene in presence of on-site and inter-site Coulomb interactions on both sites. Here Coulomb interactions are treated within a mean-field approximation and the difference in electron occupation numbers is computed numerically and self- consistently. Then the effect of Coulomb interaction on the band gap of the graphene is investigated by varying the on-site and inter-site Coulomb interaction Potentials. Finally Results are discussed with respect to experimental observations.

Keywords. Graphene, Coulomb potential , Occupation number

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[Full Paper]