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The electronic structure of graphene layers on SiO_2 substrate
YONG-JU KANG, JOONGOO KANG, KEE JOO CHANG, Korea Advanced Intitute of Science and Technology — Graphene is a single layer of carbon atoms packed in a honeycomb lattice, and its quasiparticles behave like massless Dirac fermions. Since graphene is usually supported and deposited on dielectric materials such as SiO_2 and SiC, interactions between graphene and substrate atoms can modify the electronic structure of graphene. In this work we study the structural and electronic properties of a few graphene layers on SiO_2 surfaces through first-principles calculations within the local-density-functional approximation. We examine interactions between graphene layers and Si- and O- terminated surfaces of α-quartz and the substrate-induced doping effect. For a single graphene layer, we find that graphene strongly interacts with the O-terminated surface. A charge transfer occurs from the graphene to the surface O atoms, leading to the p-type doping. For a bilayer graphene in AB stacking, the charge transfer mostly occurs for the graphene layer right on the substrate, resulting in an asymmetric distribution of electron charges between two graphene layers and thus a gap opening at the Dirac point.

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