Metal-Graphene Interfaces: A First-Principles Study

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Metal-graphene contact is one of key issues in graphene-based device applications. Recently, theoretical[1] and experimental[2,3] research found that two types of interfaces are formed between metal and graphene. However, detailed atomic scale investigations based on *ab initio* studies are currently missing, and the physical and electronic behaviors of these interfaces are not well understood yet. In this paper, we apply first-principles calculations to twelve metal-graphene interfaces and find that different metal-carbon interactions lead to two types of interfaces: a) For physisorption interfaces (Ag, Al, Cu, Cd, Ir, Pt and Au), Fermi level pinning and Pauli-exclusion-induced energy-levels shift are two primary factors that dictate graphene's doping types and levels. b) For chemisorption interfaces (Ni, Co, Ru, Pd and Ti), the combination of Pauli-exclusion-induced energy-levels shift and hybridized states' repulsive energy-levels leads to an opening of graphene band gap filled with gap states. Extending this finding to practical applications, we show that external electric field can be applied to modulate graphene's energy-levels, thus manually changing its doping or hybridization region.

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