# Ab initio Study of Metal-Graphene Interface

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## Abstract

Graphene has an extended π-electron network similar to organic semiconductors, and metal-graphene contact is critical in graphene-based device applications similar to metal-organic interfaces for organic electronics. We use density functional theory (DFT) calculations to investigate the electronic properties of metal-graphene interfaces. We have considered monolayer, bilayer and trilayer graphenes in contact with Ni metal surface. Ni interaction with graphene depends on contact geometries. Weak interaction maintains graphene's original band structure, but strong interaction shows significant hybridization of Ni d- and C π-orbitals leading to sizable gap opening in graphene. For the bi- and tri-layer graphenes, the second and third layers are not affected by the contact. For realistic metal-graphene interfaces, there is a lattice mismatch leading to weak and strong interactions depending on the local interface geometry, and our work suggests that the metal-graphene interface has complex electronic hybridization patterns of weakly and strongly interacting domains.