

Origins of Distinct Contact of Pd and Pt Nanolayers on Graphene

Q. J. Wang and J. G. Che

Surface Physics Laboratory, Physics Department,
Fudan University, Shanghai, 200433, China

Abstract

Based on the first principle calculations, we demonstrate the physical reason that accounts for the distinct contacts between Pd and Pt nanolayers on graphene. Pd monolayer favors hybridization and charge transfer between $d_{xz}+d_{yz}$ and d_{z2} orbitals and π states of graphene, which leads to a strong hybridization bond between Pd and graphene. On the contrary, stronger interaction between Pt atoms weakens the bond between Pt monolayer and graphene, prevents the hybridization to occur.