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Bonding and charge transfer induced by metal adatom adsorption on graphene XIAOJIE LIU, C.Z. WANG, M. HUPALO, Y.X. YAO, M.C. TRINGIDES, Ames Laboratory - USDOE, Iowa State University, WEN-CAI LU, Institute of Theoretical Chemistry, Jilin University, Changchun, China, K.M. HO, Ames Laboratory - USDOE, Iowa State University — Structures and adsorption energies of alkali, simple, transition as well as rare earth metal adatoms on graphene were studied systematically by first-principles calculations. Bonding character and charge transfer between the metal adatoms and the graphene were also analyzed using the quasi-atomic minimal basis set orbitals (QUAMBOs) approach. We showed that the interaction between the alkali metal adatoms and graphene can be characterized as ionic with minimal effects on the lattice and electronic states of the graphene layer. On the other hand, transition metal adsorption exhibits strong covalent bonding and induces large distortion in the lattice and electronic states of the graphene. For trivalent simple metal adatom adsorption, mixed covalent and ionic bonding is observed. Interaction of rare earth adatoms with graphene can be either ionic or covalent depending on the specific elements. Charge redistributions upon the metal adsorptions also induce significant electric dipole moments and changes in the magnetic moments of the adatoms. These results are confirmed by STM studies of the nucleated island density in epitaxial growth experiments.

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