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First-principles Studies of Metal Adsorption on Graphene[1]
KEVIN T. CHAN, Department of Physics, University of California, Berkeley, J. B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, MARVIN L. COHEN, Department of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Quantitative first-principles theory can aid in understanding many experimental phenomena involving metal adsorption on graphene and carbon nanotubes, including adatom mass transport, modification of electronic, mechanical, and magnetic properties, and adhesion and efficacy of electrical contacts. In this work, the binding energy and geometry, charge transfer, work function, and electronic structure of adatom-graphene systems are calculated using first-principles density functional theory for a variety of metal elements. Trends in these calculated data are analyzed, and their implications for graphene-based devices are discussed.

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