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First-principles investigation of graphene-metal interfaces[1] ANDREW ROSS, Saint Anselm College, LYUDMYLA ADAMSKA, YOU LIN, IVAN OLEYNIK, University of South Florida — Epitaxial growth of graphene on Ni(111) substrates is one promising method of large-scale, high-quality graphene wafer production, due to the small lattice mismatch between these two materials. We present results of first-principles density functional theory (DFT) investigation of thestructural, electronic, and magnetic properties of graphene/Ni(111) interfaces relevant to experimental studies of graphene growth on nickel substrates. DFT calculations were performed to identify the favored interface geometries and binding sites for different interface configurations. Additional adlayers of Ni and Cu were either adsorbed on top of the graphene/metal interface, or placed between the graphene and substrate to model processes of metal intercalation. It was also found that the interaction between graphene/Ni(111) and the top Cu adlayer is much weaker compared to that for Ni adlayer. The atomic, electronic, and magnetic properties of these interfaces, including induced magnetic moments in graphene/Ni(111) and Cu,Ni/graphene/Ni(111) systems are also discussed.

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