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**Graphene/Ni Nanocomposite Materials from First Principles**
DALAL K. KANAN, CHRIS A. MARIANETTI, Columbia University — Nanocomposite materials made by alternating layers of graphene and nickel offer exciting new possibilities for light-weight, high-strength materials. To better understand these systems, we used density functional theory with dispersion to first study graphene adsorbed onto Ni(111). The results indicate strong binding at the interface and a substantial perturbation of the graphene electronic structure, consistent with previous work. We mapped out the potential energy for sliding graphene on Ni(111) along the C-C bond and find a maximum binding energy that is substantially stronger than the interlayer binding in graphite. Ni $3d$ to graphene $\pi^*$ charge transfer causes the strong chemisorption; although occupation of graphene's antibonding states likely affects the C-C bond strength. Next, we studied the bulk composite material with varying Ni layer thickness. Charge density analysis shows graphene sandwiched between Ni layers accepts charge from both layers, which should enhance the binding. The computed elastic coefficients will be presented.

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