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Density Functional Studies of Metal-Graphene Interfaces[1] PINAR BOZKURT, University of South Florida, STEPHEN CANNON, Hastings College, ROMAIN PERRIOT, YOU LIN, MATTHIAS BATZILL, IVAN OLEYNIK, Universith of South Florida, MATERIALS SIMULATION LABORATORY TEAM, NANOPHYSICS AND SURFACE SCIENCE LABORATORY TEAM — Graphene, one-atom-thick layer of carbon has attracted great interest due to unusual physical properties and promising applications. One of the major ways to synthesize graphene is its growth on metal substrates. In addition, the metal/graphene interfaces play important role in establishing electrical contacts to graphene-based electronic devices. Therefore, the understanding of the atomic and electronic structure of metal/graphene interfaces is of key interest for graphene scientific community. In this talk we present results of density functional theory studies of Ni/graphene and copper/graphene interfaces. The strength of metal/graphene interactions was quantified by calculating the work of separation for different adsorption geometries. The electronic structure of the metal/graphene interfaces were compared to those of pure graphene by performing band structure calculations. Connection between the theory and experiment will be discussed as well.

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