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Effect of Defects on Doping, Magnetism, and Reactivity in Hexagonal Boron Nitride / Graphene Layered Systems ALEJANDRO SUAREZ, NRC Research Associate at U.S. Naval Research Laboratory, Washington, DC , THOMAS L. REINECKE, U.S. Naval Research Laboratory, Washington, DC — Boron nitride is a promising substrate for graphene devices due to its ultra-flat and insulating characteristics. However, the interactions between defects within a hexagonal boron nitride (h-BN) substrate and a graphene layer are not yet well understood. Using ab-initio methods, we calculate the ground state energies of h-BN/ graphene bilayer systems with a number of defects including vacancies, substitutions, and interstitials. Lattice distortion, charging, and magnetism due to defects are reported and compared with literature on boron nitride bilayers. We also model the adsorption of hydrogen and fluorine atop the various defect configurations. Differences in adsorption energy, bonding geometry, and density of states of such adsorbates help elucidate which defects may be desirable for controlling graphene reactivity.

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