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Electronic Properties of Graphene and Single Wall Carbon Nanotubes in the Presence of Hexagonal BN Islands MOHAMMED ALABBOODI, JAIME BOHORQUEZ, ERIKA PUTZ, HANSIKA SIRIKUMARA, THUSHARI JAYASEKERA, Southern Illinois University, Carbondale, SIUC TEAM — Controlled chemical doping with Boron (B) and Nitrogen (N) is a promising approach for electronic band engineering of carbon-based materials. Based on the first-principles Density Functional Theory (DFT) calculations, we investigated the effect of hexagonal BN islands on the electronic properties of graphene as well as carbon nanotubes. Our results are in agreement with recent experimental observations that hexagonal BN islands in graphene open a sizable electronic band gap in graphene. Our detailed analysis show that, the electronic properties not only depend on the impurity concentration, but also depend on the geometrical pattern of impurity atoms in the honeycomb network of C atoms in graphene. We identified interesting symmetry properties, which controls the band gap of the system. A similar behavior was observed in the effect of hexagonal BN islands on electronic properties of zigzag single wall carbon nanotubes (SWCNT). Using the Density functional Perturbation Theory, we also investigated the vibrational properties of SWCNTs with hexagonal BN islands, which confirm the stability of these systems.

Mohammed Alabboodi
Department of Physics, Southern Illinois University Carbondale

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