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The size and shape dependence of graphene domain on the band gap of h-BN CHERNO B. KAH, SALIYA KIRIGEEHANAGE, LYLE SMITH, MING YU, CHAKRAM JAYANTHI, SHIYU WU, University of Louisville — This talk will report the structure and electronic characteristics of graphene domains embedded in a hexagonal boron-nitride sheet (h-BN) with the goal of band gap tuning in mind. Different shapes (triangular, circular, rectangular, and irregular structures) and sizes of graphene domains will be studied. The structural stability of these hybrid materials will be studied using a new generation of the semi-empirical Hamiltonian (SCED-LCAO) developed recently [arXiv:1408.4931]. It is found that the lattice mismatch between graphene domains and the h-BN generates large strain, leading to a reduction or a symmetry breaking of the hexagonal lattice of h-BN. The extent of the strain depends on the shape and the size of the domain, as well as on the distribution of B atoms around the graphene domains. This effect also creates impurity states in the band gap of h-BN and changes the band gap. The interplay between the shape and size of graphene domains, the local strain around the domains and the nature of the impurity states on the band gap of h-BN will be discussed.

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