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Tailoring the Energy Gap of Hexagonal Boron Nitride Sheets Embedded with Carbon Domains of Different Shapes and Sizes[1] CHERNO KAH, MING YU, CHAKRAM JAYANTHI, University of Louisville — We present in this work the structure, stability and electronic properties of hexagonal boron nitride sheets embedded with carbon domains of different shapes and sizes with the goal of understanding their roles in tuning the energy gaps of h-BN/C composite sheets compared to pristine $h-$BN sheets. We have considered triangular, hexagonal, circular, and rectangular carbon domains embedded in h-BN sheets and calculated their formation and cohesive energies using a semi-empirical method [Phys. Rev. B 74, 155408 (2006)] developed at the University of Louisville. Irrespective of the shape of the domain, we find the formation energy per atom to decrease in a power law fashion as the carbon domain size increases. The energy gap behaviors of h-BN/C composite sheets exhibit interesting size- and shape-dependence and will be understood in terms of competing bond lengths, broken symmetry, and mid-gap states in the density of states.

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