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Formation of superlattice structures by interlayer bonding in twisted bilayer graphene ANDRE MUNIZ, Universidade Federal do Rio Grande do Sul, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We present a computational analysis of carbon nanostructure formation from twisted bilayer graphene, upon creation of interlayer covalent C-C bonds. The analysis is based on a combination of first-principles density functional theory calculations and classical molecular-dynamics simulations. We demonstrate that the resulting configurations constitute a novel class of stable structures and that their features are determined by the relative angle of rotation between the two graphene planes of the bilayer. For small angles of rotation (near 0 degrees), interlayer covalent bonding generates superlattices of diamond-like nanocrystals embedded within the graphene layers; for rotation angles near 30 degrees, superlattices of caged fullerene-like configurations are generated. We calculate the electronic band structure of these superlattices and show that their band gap can be controlled through selective hydrogenation and creation of interlayer bonds. We also show that the linear dispersion around the K point in the first Brillouin zone (Dirac cones), characteristic of single-layer and non-bonded twisted bilayer graphene, is preserved for some of these structures in spite of the introduction of sp3 bonds due to hydrogenation and interlayer C-C bonding.

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