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Structural, electronic, and mechanical properties of superlattices of interlayer-bonded domains in twisted bilayer graphene ANDRE MUNIZ, Federal University of Rio Grande do Sul, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We present a comprehensive computational analysis of the atomic and electronic structure and mechanical properties of a novel class of carbon nanostructures, formed due to interlayer covalent sp^3 C-C bonding in twisted bilayer graphene as a result of controlled chemical functionalization (hydrogenation or fluorination). Depending on the twist angle and local stacking of layers, these nanostructures are superlattices of diamond-like nanocrystals or caged fullerene-like configurations embedded within the bilayer. According to density functional theory calculations, the electronic behavior of these sp^2/sp^3 hybrid configurations ranges from semi-metallic, characterized by linear dispersion around the K point in the first Brillouin zone, to semi-conducting/insulating with electronic band gaps ranging from a few meV to $\sim$4 eV; this electronic character depends on the symmetry and periodicity of the superlattices and on the type of chemisorbed species. We have also studied the mechanical response of these superlattices to tensile and shear strain based on molecular dynamics simulations; their interlayer shear modulus increases strongly and their Young's modulus and tensile strength and strain decrease moderately compared to those of pristine bilayer graphene.

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