Topological Properties of Atomically Modified Graphene Systems

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Finding an effective and controllable way to create a sizable energy gap in graphene-based systems has been a challenging topic of intensive research. We propose that the hybrid of boron nitride and graphene (h-BNC) at low BN doping serves as an ideal platform for band-gap engineering and valleytronic applications. We report a systematic first-principles study of the atomic configurations and band gap opening for energetically favorable BN domains embedded in graphene. The calculations find a linear dependence of the band gap on the BN concentration at low doping, arising from an induced effective on-site energy difference at the two C sublattices as they are substituted by B and N dopants alternately. The significant and tunable band gap of a few hundred meVs, with preserved topological properties of graphene and feasible sample preparation in the laboratory, presents great opportunities to realize valley physics applications in graphene systems at room temperature.

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