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Electronic States of the Moiré superlattice (I)

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Two-dimensional (2D) van der Waals (vdW) heterostructures have attracted great attention in the past five years. By stacking different 2D materials to bond via the vdW force, these artificial heterostructures provide new material phase space for exploration. In this work we focus on one aspect of the 2D vdW material: the Moiré pattern. In visual arts, Moiré pattern is an optical perception of a new pattern formed on top of two similar stacking patterns. In 2D vdW materials, Moiré pattern can be a physical superlattice which brings about novel electronic properties. Using our recently developed solver of the Kohn-Sham density functional theory that can handle very large systems –as large as more than ten thousand atoms, we have calculated electronic properties of the Moiré superlattices. We show multiple and topologically protected helical valley currents to be easily achievable by certain Moiré patterns formed on the 2D vdW heterostructure of graphene on boron-nitride.

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