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Atomic reconstruction at van der Waals interface between two-dimensional materials

Crystal interfaces at the boundary between two materials have been essential in engineering material properties in modern materials physics. The interface in two-dimensional (2-D) van der Waals (vdW) heterostructures differs from classical heterogeneous interfaces since it can create high-quality interface structure without any limitation on lattice commensurability between the two layers. Indeed, adjusting stacking angle or lattice mismatch between the layers has proved a fruitful way to tune the electronic properties by producing additional quasiperiodic structure described by a Moiré pattern. However, the interplay between vdW interaction energy and elastic energy at the interface can cause atomic reconstruction, leading into intriguing structures which have not yet been clearly understood. In order to understand the atomic reconstruction mechanism and details of the resulting structures, we choose the simplest form of vdW interface: two layers of graphene with controlled twist angle. Here we show that the atomic-scale reconstruction at the vdW interface can be manipulated to form arrays of commensurate domain structures. A combination of transmission electron microscopy (TEM) with finite element method (FEM) simulation reveals the reconstruction mechanism: periodic rotational modulation of the lattice following the Moiré periodicity forms the local commensurate configurations. More interestingly, a systematic study on a series of different twist angles shows how the commensurability of those domains is modified by tuning the twist angle, revealing a gradual transition from commensurate to incommensurate configuration. We note that the commensurate domain structures in bilayer graphene are topologically nontrivial, providing a network of one-dimensional (1-D) topological channels along their boundaries. The signature of transport behavior through the network of 1-D channels can also be observed in the presence of transverse electric field. Reconstructed vdW interface structures and their correlation with transport properties indicates the importance of understanding the intriguing behavior of atomic reconstruction at the vdW interface for engineering 2-D heterostructures in various applications.