Helical dislocations in 2D materials and the connection to transport in topological insulators

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Layered two-dimensional materials host a variety of crystalline defects, including dislocations either in-plane or out-of-plane with respect to the 2D layered structure. Recently, twisted multilayer 2D material structures have been of interest due to the presence of flat bands and other emergent properties associated with moiré superlattices.[1] Periodic regions of crystalline commensurability making up these superlattices are now understood to be separated by interlayer dislocations, with Burgers vectors and line directions in the plane of the 2D material, and having either edge or screw character.[2] Using density functional theory and quantum Monte Carlo-fitted total energy tight-binding calculations, we show that out-of-plane relaxation of the structures makes possible unique helical dislocations in bilayer graphene, and that the presence of these helical dislocation lines coincides precisely with the so-called magic-angle condition at which unconventional superconductivity is observed.[3] We then illustrate a different dislocation structure, with line direction oriented out-of-plane, but which also has a helical structure. Such a screw dislocation, which adopts a double-helix dislocation core configuration in bilayer structures, is expected to create conditions for exotic transport properties in certain classes of layered topological insulator materials. We present initial results demonstrating this possibility in BiTe and BiSe compounds. In these examples, we present relaxed dislocation core structures computed using first-principles methods, and show that the observed configurations match both experimental observations and the theoretical conditions that are expected to lead to quantum conduction in these otherwise topologically insulating materials.

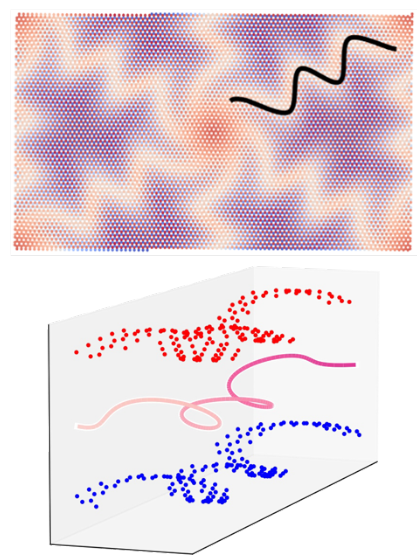

Figure 1: (top) plan view of bilayer graphene moiré superlattice, with local energy shown in color. (bottom) expanded 3D view of atom positions in upper and lower layers along black line from upper image. The center of the helical dislocation core is shown between the layers.

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[2] Pochet, P., B. C. McGuigan, J. Coraux, and H. T. Johnson, Toward moiré engineering in 2D materials via dislocation theory, Applied Materials Today **9**, 240-250 (2017).
[3] Rakib, T., P. Pochet, E. Ertekin, and H. T. Johnson, Helical dislocation in twisted bilayer graphene, Extreme Mechanics Letters, **63**, 102053 (2023).

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