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Twistronics: Manipulating the Electronic Properties of Two-dimensional Layered Structures through their Twist Angle[1] STEPHEN CARR, Harvard University, DANIEL MASSATT, University of Minnesota, SHIANG FANG, Harvard University, PAUL CAZEAUX, MITCHELL LUSKIN, University of Minnesota, EFTHIMIOS KAXIRAS, Harvard University — We have introduced a new method for parameter-free computation of electronic properties in incommensurate layered 2D materials with controllable errors. Although here we have only studied bilayer materials, the method is general and extends to any number of layers and of arbitrary heterostructure composition. Viewing the problem on the space of configurations, Ω, allows us to fully characterize the properties of incommensurate (aperiodic) systems. The method allows for the inclusion of external fields and other sources of disorder, such as strain or defects. We present results of applying the method to twisted bilayer graphene and a representative of the TMDC family of semiconductors. The method is accurate enough to correctly calculate quantization of Hall conductivity in tBLG in the presence of magnetic fields, and reproduces the correct Chern number for the $N = 0$ Landau Level. It also predicts that bilayer TMDC's have a twist-dependent band-gap. The method is a promising candidate for the targeted design of electronic properties in layered heterostructures.

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