

Electronic structure and correlations in twisted multilayer graphene and related layered materials

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In the past decade the field of twisted multilayer graphene and other layered materials, like the transition-metal dichalcogenide family, has blossomed to the point of being referred with its own term, "twistronics" [1]. New arrangements, including twisted n -layers ($n=3,4,\dots$), mixed layers, and multilayers of regular few-layer structures, are being studied experimentally and they are revealing ever richer behavior. We review theoretical investigations of some representative systems [2], starting with the iconic twisted bilayer graphene near the magic angle. Our work is based on first-principles tight-binding hamiltonians and includes atomic relaxation through the configuration space approach. A recent focus has been on deriving realistic representations of single-particle states for few-band hamiltonians and how those can be employed in studying many-body physics related to Mott insulator behavior, superconductivity and other manifestations of correlated electronic states [3].

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[3] D. Bennett, D. T. Larson, L. Sharma, S. Carr, and E. Kaxiras, Phys. Rev. B 109, 155422 (2024)