Atomic relaxation effects in twisted bilayers: insights from large-scale first-principles calculations

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The electronic and structural properties of twisted bilayer graphene down to the first magic angle are discussed and reviewed in the framework of large-scale first-principles calculations. We show that the flat bands, arising around the Fermi level at the first magic angle, are intimately connected to the relaxation pattern. The latter involves both in-plane and out-of-plane atomic displacements, whose magnitude increases upon decreasing the twist angle. Interestingly, the in-plane relaxation shows a vortex-like pattern, with the direction of the displacements that is opposite in the two layers. On the other hand, in-plane relaxation involves a complex "buckled" pattern, with enhanced oscillations at small twist angles. The strength of the interlayer hybridization is responsible for both the flat band bandwidth and the energy gaps separating those flat bands from the bands lying at higher or lower energy. A comparison with computationally less expensive models (tight binding and continuum model) is also discussed. The results shed light on the importance of an accurate inclusion of the interlayer van der Waals interaction to catch the subtle details of the electronic structure in twisted two-dimensional materials [1–4].

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