Structural and electronic properties of low-angle twisted bilayer graphene

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Around a specific magic twist angle, twisted bilayer graphene exhibits correlated insulating phases and superconductivity, thus boosting the new field of "twistronics" where strong electron-electron interactions play a dominant role on its electronic properties.
In this work, atomistic calculations using the Green's function techniques are developed to solve the tight-binding Hamiltonian for low-angle multilayer graphene, whose atomic structures have been previously optimized [1].
Below a threshold twist angle θ_c~1.1°, the twisted bilayer graphene superlattice undergoes lattice reconstruction (Figure 1), leading to a periodic Moiré structure which exhibits a slight-corrugation that is found to strongly modify both its electronic structure [2] and its vibrational properties [1,3]. The electron-phonon coupling [4] is also found to be affected by the atomic structure reconstruction at the magic angle.
In twisted multilayer graphene [5], the dependence of the local electronic properties on the twist angle and on the stacking configuration are also investigated in order to fully taking into account atomic reconstruction effects.

References

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Figures

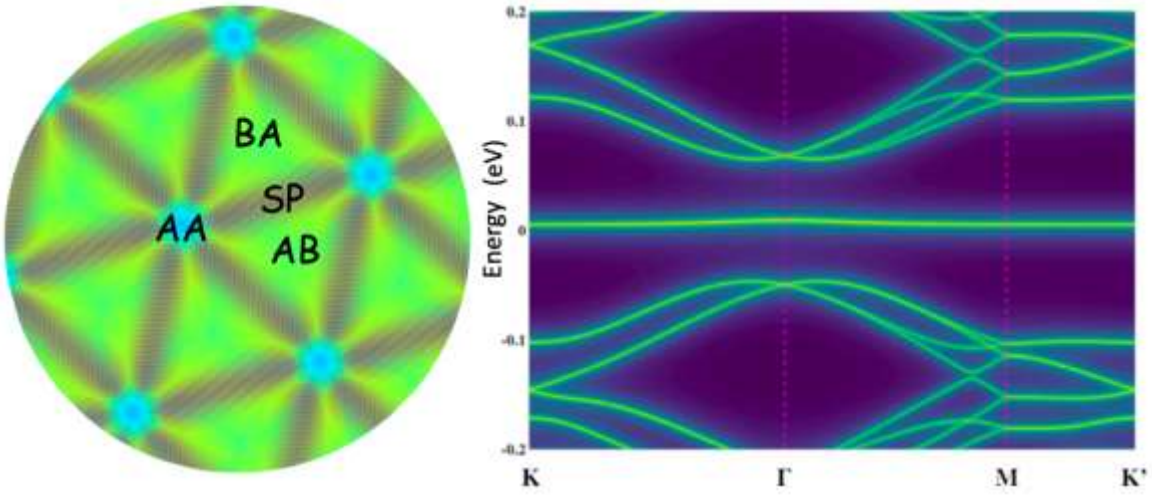

Figure 1: Atomic reconstruction (left) and electronic properties (right) of twisted bilayer graphene at the 1.1° magic angle.