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Electronic signatures of stacking domain boundaries in twisted bilayer graphene¹ FERNANDO GARGIULO, BASTIEN GROSSO, GABRIEL AUTÈS, OLEG YAZYEV, EPFL — Experiments on bilayer graphene (BLG) show the coexistence of regions of inequivalent stacking order (AB and BA) separated by domain boundaries, topological defects akin to solitons [1]. The Frenkel-Kontorova model predicts that in-plane atomic displacements result in stacking domain boundaries of few nanometers width. We show how a hexagonal network of stacking domain boundaries naturally arises in twisted BLG in the limit of small twist angle (below ca. 1°). Equilibrium configurations of twisted BLG have been produced by means of classical force-field simulations. Atomic displacements diminish the area of AA stacking regions and extend the AB and BA stacking regions to triangular domains separated by boundaries of 7–8 nm width. Large-scale tight-binding simulations unveil the electronic properties of such twisted BLG models. A charge density depletion is the low-energy signature of stacking domain boundaries with electronic states mostly confined in AB and BA domains. Zero-energy states at the network nodes reach an asymptotic localization for vanishing twist angles. We propose STM experiments for confirming our predictions.

[1] L. Brown et al., Nano Lett. 12, 1609 (2012).

[2] J. S. Alden et al., PNAS 110, 11256(2013).

[3] J. Linang et al., Nano Lett. (2013).

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