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Electronic structure of bilayer graphene out of Bernal stacking

MARCELO KURODA, U. of Illinois and IBM T. J. Watson Research Center, RAZVAN NISTOR, GLENN MARTYNA, IBM T. J. Watson Research Center — The electronic properties of bilayer graphene have thus far been studied in the Bernal (AB) stacking, in which the A-carbon of one sheet lies on top of the B-carbon of the other. However, other configurations have been observed experimentally. In this work, we study the electronic properties of bilayer graphene using the density functional theory for the case when the two graphene layers are not aligned. We compare our results as a function of the angle between the two graphene lattices. We find that in contrast to the Bernal stacking, which exhibits parabolic band dispersion at the K-point, arbitrary alignments of the lattices recover the linear band dispersion of graphene, and the system behaves as two independent layers. In addition, the rotated graphene bilayers show weak energy dependence under translations.

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