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Band Structures of bilayer graphene with experimentally measured twisting angles HOULONG L. ZHUANG, Department of Materials Science and Engineering, Cornell University, ROBIN W. HAVENER, School of Applied and Engineering Physics, Cornell University, JIWOONG PARK, Department of Chemistry and Chemical Biology, Cornell University, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — Using density functional theory (DFT) and tight binding calculations, we study the band structure of bilayer graphene as a function of twisting angles and compare the results to spectroscopic measurements.To test the accuracy of DFT, we first compare the band structure with DFT and the G_0W_0 approximation for several bilayer graphene systems with special twisting angles.Our DFT results agree with previous DFT calculations for the weak coupling between the two layers and the band structure.Calculations of the quasiparticle dispersion using the G_0W_0 approximation show that DFT underestimates the Fermi velocity of bilayer graphene and the bandgap away from the K point.Scaling of the DFT band structure by an empirical parameter that depends on the twist angle accounts for most of the difference between the DFT and the G_0W_0 approximation. Based on the G_0W_0 calculations, we fit a set of tight-binding parameters for the interlayer coupling Hamiltonian. Using this tight-binding model we study the band structure of bilayer graphene for twist angles that closely match experimental systems and have larger unit cells. The results of these band structure calculations explain the experimentally observed G band resonance in Raman spectroscopy for specific twist angles.

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