Tight-binding theory of the spin-orbit coupling in graphene structures\(^1\) SERGEJ KONSCHUH, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg, Germany — Spin-orbit coupling changes qualitatively the electronic band structure of graphene. Most important, the coupling induces spectral gaps at the K(K') points. Earlier theories estimated the *intrinsic* gap of 1 \(\mu\text{eV}\) for the single layer and several meVs for bi- and tri-layer graphene, based on \(\sigma-\pi\) coupling. Our first-principles calculations give the value of 24 \(\mu\text{eV}\) for all these systems, due to the presence of the orbitals of the \(d\) symmetry in the Bloch states of the \(\pi\) bands. A realistic multiband tight-binding model is presented to explain the effects the \(d\) orbitals play in the spin-orbit coupling of graphene and derive an effective single-orbital next-nearest-neighbor hopping model that accounts for the spin-orbit effects. We also study the *extrinsic* spin-orbit coupling, due to an applied transverse electric field. In a single layer the *extrinsic* effect is dominated by the \(\pi-\sigma\) hybridization. In contrast, in the multi-layer structures the *extrinsic* spin-orbit band splittings come from an interplay of the \(d\)-orbitals, the inter-layer hopping, and the electrostatic potential from the applied field.

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