Tight-binding theory of the spin-orbit coupling in graphene structures\textsuperscript{1} SERGEJ KONSCUH, 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 \textit{intrinsic} gap of 1 \textmu eV for the single layer and several meVs for bi- and tri-layer graphene, based on \textit{\sigma-\pi} coupling. Our first-principles calculations give the value of 24 \textmu eV for all these systems, due to the presence of the orbitals of the \textit{d} symmetry in the Bloch states of the \textit{\pi} bands. A realistic multiband tight-binding model is presented to explain the effects the \textit{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 \textit{extrinsic} spin-orbit coupling, due to an applied transverse electric field. In a single layer the \textit{extrinsic} effect is dominated by the \textit{\pi-\sigma} hybridization. In contrast, in the multi-layer structures the \textit{extrinsic} spin-orbit band splittings come from an interplay of the \textit{d}-orbitals, the inter-layer hopping, and the electrostatic potential from the applied field.

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