

Abstract Submitted
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Tight-binding theory of the spin-orbit coupling in graphene structures¹ SERGEJ KONSCHUH, MARTIN GMTIRA, 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 μeV for the single layer and several meVs for bi- and tri-layer graphene, based on σ - π coupling. Our first-principles calculations give the value of 24 μeV for all these systems, due to the presence of the orbitals of the d symmetry in the Bloch states of the π 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 π - σ 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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Sergej Konschuh
University of Regensburg, Germany

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