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Real-structure influence on topological states of HgTe quantum wells: Ab initio studies[1] SEBASTIAN KUEFNER, FRIEDHELM BECHSTEDT, Friedrich-Schiller Universitaet Jena — The electronic properties of HgTe quantum well structures are studied by means of *ab-initio* calculations including spin-orbit interaction and quasiparticle effects. In agreement with earlier $\mathbf{k} \cdot \mathbf{p}$ calculations and experiments we find a topological transition from the trivial insulator into the quantum-spin Hall (QSH) state with increasing QW thickness. The QSH state is characterized by the existence of spin-polarized helical edge states bridging the fundamental gap giving rise to intrinsic spin currents. The occurrence and localization of the edge states are independent of the interface orientation and barrier material. Together with their spin polarization this indicates that they are topologically protected. The nonexistence of inversion symmetry, the atomic geometry, and the real QW barriers do not completely destroy the predictions within toy models but cause significant deviations. The deviations concern the critical thickness, the number and localization of edge states, and the possibility to find QW subbands between edge states.

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