Self-Consistent Electronic Modeling of Gated Narrow-Gap Topological Insulators

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Even small electrostatic potentials can dramatically influence the band structure of narrow-gap semiconductors. A quantitative understanding often necessitates a self-consistent Hartree approach. The valence and conduction band states strongly hybridize and/or cross in these systems. This results in failure of the standard effective-mass theory, which relies on a clear distinction between electrons and holes and assumes a flat charge carrier distribution at the charge neutrality point. We show that the alternative full-band envelope-function approach [1], which we have implemented into the open-source band structure software package kdotpy [2], gives numerically stable and quantitatively accurate results where the conventional method fails. We find excellent agreement in modelling the experimental subband density evolution with top-gate voltage in thick (26 nm – 107 nm), topologically inverted HgTe quantum wells [3]. We expect our openly available implementation to greatly benefit the investigation of narrow-, broken-, and inverted-gap materials.

Figures

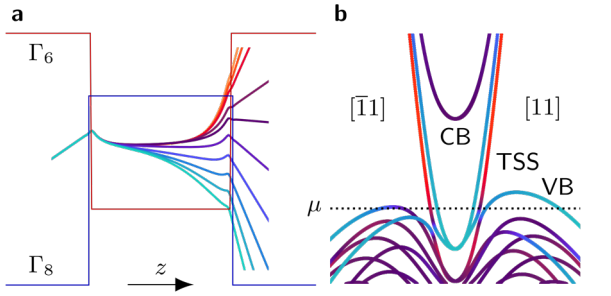

Figure 1: Self-consistent $\boldsymbol{k \cdot p}$ calculation results for an electrostatically gated 45 nm thick HgTe/(Hg,Cd)Te quantum well (3D topological insulator). (a) Band edge diagram and Hartree potentials along the growth direction z at different gate voltages. (b) In-plane energy dispersion with prominent Rashba-Bychkov-type splitting of the top and bottom topological surface states (TSS). VB and CB are the bulk valence and conduction band, respectively. μ gives the position of the chemical potential. Adapted from [3].

References

[1] Andlauer and Vogl, Phys. Rev. B, 80 (2009) 035304
[2] Beugeling et al., SciPost Phys. Codebases (2025) 47
[3] Hofer et al., arXiv:2510.18778 (2025)