First Principles Validation of CdTe Properties via Comparison with ARPES towards use as a Tunnel Barrier

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Majorana zero modes, with prospective applications in topological quantum computing, are expected to arise in semiconductor-superconductor devices. Investigating material properties and their interfacing is pivotal to progress in this area, which can be performed via density functional theory (DFT) and angle resolved photoemission spectroscopy (ARPES). Proximity to the superconductor may adversely affect the semiconductor's local properties. A tunnel barrier inserted at the interface could resolve this issue. We assess the wide bandgap semiconductor, CdTe, as a candidate material to mediate the coupling at the interface between α-Sn and InSb. To this end, we use DFT with Hubbard U corrections, whose values are machine-learned via Bayesian optimization (BO). The results of DFT+U(BO) are validated against ARPES experiments for α-Sn and CdTe. We discuss how, for CdTe, the z-unfolding method is used to resolve the contributions of different k_z values in experimental ARPES data. We also implement a 2X2 surface reconstruction to display surface states seen in the ARPES data. This allows for excellent agreement between theory and ARPES, which contains prominent surface effects and k_z broadening due to CdTe's band gap and the ARPES acquisition energy. We then study the band offsets and the penetration depth of metal-induced gap states (MIGS) in bilayer interfaces of InSb/α-Sn, InSb/CdTe, and CdTe/α-Sn, as well as in tri-layer interfaces of InSb/CdTe/α-Sn with increasing thickness of CdTe. We find that 16 atomic layers (3.5 nm) of CdTe can serve as a tunnel barrier, effectively shielding the InSb from MIGS from the α-Sn. This may guide the choice of dimensions of the CdTe barrier to mediate the coupling in semiconductor-superconductor devices in future Majorana zero modes experiments.