Abstract Submitted
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Design Principles and Coupling Mechanisms in the 2D Quantum-Well Topological Insulator HgTe/CdTe[1] JUN-WEI LUO, ALEX ZUNGER, National Renewable Energy Lab, SOLID STATE THEORY TEAM — We present atomistic band structure calculations revealing a different mechanism than recently surmised via $\mathbf{k} \cdot \mathbf{p}$ calculations about the evolution of the topological state (TS) in HgTe/CdTe. We show that *2D interface* (not *1D edge*) TS are possible. We find that the transitions from a topological insulator at critical HgTe thickness of $n = 23$ ML (62.5 Å) to a normal insulator at smaller n is due to the crossing between two interface localized states: one derived from the S-like Γ_{6c} and one derived from the P-like Γ_{8v} light-hole, not because of the crossing of an interface state and an extended QW state. These atomistic calculations suggest that a 2D TS can exist in a 2D system, even without truncating its symmetry to 1D, thus explaining the otherwise surprising similarity between the 2D dispersion curves of the TS in HgTe/CdTe with those of the TS in 3D bulk materials such as Bi_2Se_3. Ref: J.W. Luo and A. Zunger, Phys. Rev. Lett. **105**, 176805 (2010).

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