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Transforming common III-V/II-VI insulating building blocks into topological heterostructure via the intrinsic electric polarization¹ ALEX ZUNGER, XIUWEN ZHANG, LEONARDO ABDALLA, QIHANG LIU, University of Colorado, Boulder — Currently known topological insulators (TIs) are limited to narrow gap compounds incorporating heavy elements, thus severely limiting the material pool available for such applications. We show how a heterovalent superlattice made of common semiconductor building blocks can transform its non-TI components into a topological heterostructure. The heterovalent nature of such interfaces sets up, in the absence of interfacial atomic exchange, a natural internal electric field that along with the quantum confinement leads to band inversion, transforming these semiconductors into a topological phase while also forming a giant Rashba spin splitting. We demonstrate this paradigm of designing TIs from ordinary semiconductors via first-principle calculations on III-V/II-VI superlattice InSb/CdTe. We illustrate the relationship between the interfacial stability and the topological transition, finding a “window of opportunity” where both conditions can be optimized. This work illustrates the general principles of co-evaluation of TI functionality with thermodynamic stability as a route of identifying realistic combination of common insulators that could produce topological heterostructures.

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Qihang Liu
University of Colorado, Boulder

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