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ab initio based tight-binding investigation of quantum spin Hall effect in InAs/GaSb quantum wells QUANSHENG WU, ALEXEY SOLUYANOV, MATTHIAS TROYER, ETH Zurich — Quantum spin Hall state is a topologically non-trivial quantum state, which can be used for designing various quantum devices including those potentially useful for quantum computing. Type-II InAs/GaSb semiconductor quantum well was predicted to realize this state of matter. In this work, we systematically investigate topological properties of this system using symmetrized Wannier-based tight-binding models. The model parameters are derived from first-principles hybrid functional calculations, which capture the right band gap and effective masses of both InAs and GaSb. By varying the thickness of InAs and GaSb layers, three possible phases are obtained: normal insulator, quantum spin Hall insulator, and semimetal, allowing us to optimize the growth conditions for the quantum spin Hall phase realization. Most importantly, we identify optimal growth directions, showing that a significant increase of the topological gap can be obtained by growing the quantum well in the [111]-direction. Phase diagrams are obtained for different layer thicknesses and growth directions. Effects of strain and applied electric fields are also discussed.

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