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Theoretical study of topological phase transitions in $(Bi_{1-x}In_x)_2Se_3$ and $(Bi_{1-x}Sb_x)_2Se_3$ JIANPENG LIU, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — We use first-principles calculations to study the phase transition from a topological to a normal insulator with concentration x in $(Bi_{1-x}In_x)_2Se_3$ and $(Bi_{1-x}Sb_x)_2Se_3$ in the Bi_2Se_3 crystal structure. The spin-orbital coupling (SOC) strength is similar in In and Sb, which have similar atomic numbers, so that if the topological transitions in $(Bi_{1-x}In_x)_2Se_3$ and $(Bi_{1-x}Sb_x)_2Se_3$ are purely driven by the decrease of SOC strength, we would expect to see similar critical concentrations x_c in the two systems. However, based on our preliminary calculations, x_c is much lower in $(Bi_{1-x}In_x)_2Se_3$ than in $(Bi_{1-x}Sb_x)_2Se_3$, indicating that different mechanisms control the behavior in the two cases. Specifically, in $(Bi_{1-x}Sb_x)_2Se_3$ we find that the phase transition is mostly dominated by the decrease of SOC. However, for $(Bi_{1-x}In_x)_2Se_3$, the In $5s$ orbitals also play an important role, both in the phase-transition behavior and in determining the indirect bulk band gap. Finally, we discuss the accuracy of the energy-level position of the In $5s$ orbitals in $(Bi_{1-x}In_x)_2Se_3$ as predicted by density-functional theory and more advanced methods.

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