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First-principles study of temperature effects in topological insulator phase diagrams[1] GABRIEL ANTONIUS, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Recent studies have identified several tunable three-dimensional topological insulators. Upon varying experimental parameters such as pressure or doping, these materials exhibit a transition between a trivial and a topological insulating phase. We present a first-principles study of temperature effects in the family of alloyed $BiTlS_2$ / $BiTlSe_2$ topological phase transition materials. Through the electron-phonon coupling, the electronic bands being renormalized at finite temperature allow for a topological phase transition at some critical temperature. We find a temperature-doping phase diagram having a confined topological phase region, with the topological phase suppressed at high temperature. We also discuss the converse scenario in which phonons might favour the topological phase, as previously anticipated.

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Gabriel Antonius
University of California at Berkeley and Lawrence Berkeley National Lab

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