Abstract Submitted
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**Materials predicted to be topological insulators in hypothetical structures assumed by theorists might be trivial insulators in their stable phases**[1] GIANCARLO TRIMARCHI, Northwestern U., Evanston, IL, XIUWEN ZHANG, ALEX ZUNGER, U. of Colorado, Boulder, CO — The quest for new topological insulators (TIs) has motivated numerous *ab initio* calculations of the topological metric $Z_2$ of candidate compounds in hypothetical crystal structures, or in assumed pressure or doping conditions. However, TI-ness might destabilize certain crystal structures that would be replaced by other structures, which might not be TIs. Here, we discuss such false-positive predictions recurrent in the *ab initio* search for new TIs: (i) Various ABX compounds, predicted to be TIs in the assumed ZrBeSi-type structure that turns out to be unstable, become trivial insulators in their stable structures. (ii) Band-inversion-inducing structure perturbations destabilize the system which is instead trivial at equilibrium: examples of this scenario are the cubic $A^{\mathrm{III}}BiO_3$ perovskites that transform from topological to trivial when they relax to their equilibrium structures. (iii) Doping destabilizes the band-inverted system that relaxes to a trivial atomic configuration (orthorhombic band-inverted $BaBiO_3$ becomes trivial upon electron doping). This shows the need of performing total energy along with $Z_2$ calculations to predict stable TIs.

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