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Tuning topological phases in the XMnSb$_2$ system via chemical substitution from first principles[1] SINEAD M. GRIFFIN, JEFFREY B. NEATON, Department of Physics, UC Berkeley Molecular Foundry, LBNL — New Dirac materials are sought for their interesting fundamental physics and for their potential technological applications. Protected symmetries offer a route to potential zero mass Dirac and Weyl fermions, and can lead unique transport properties and spectroscopic signatures. In this work, we use first-principles calculations to study the XMnSb$_2$ family of materials and show how varying X changes the nature of bulk protected topological features in their electronic structure. We further discuss new design rules for predicting new topological materials suggested by our calculations.

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