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Topological insulators in the quaternary chalcogenide compounds and ternary famatinite compounds Y.J. WANG, H. LIN, Northeastern U. (NU), TANMOY DAS, LANL and NU, M.Z. HASAN, Princeton U., A. BANSIL, NU — We present first-principles calculations to predict several three-dimensional (3D) topological insulators in quaternary chalcogenide compounds of compositions I_2-II-IV-VI_4 and ternary famatinite compounds of compositions I_3-V-VI_4. Among the large number of members of these two families, we give examples of naturally occurring compounds that are mainly Cu-based chalcogenides. We show that these materials are candidates for 3D topological insulators or can be tuned to obtain topologically interesting phases by manipulating the atomic number of the various cations and anions. A band inversion can occur at a single point Γ with large inversion strength, in addition to the opening of a bulk bandgap throughout the Brillouin zone. We discuss how the two investigated families of compounds are related to each other by cross-substitution of cations in the underlying tetragonal structure. Work supported by the US DOE.

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