

Abstract Submitted  
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**Finding new ternary transition metal selenides and sulphides<sup>1</sup>**

AWADHESH NARAYAN, ANKITA BHUTANI, JAMES N. ECKSTEIN, DANIEL P. SHOEMAKER, LUCAS K. WAGNER, Univ of Illinois - Urbana — The transition metal oxides exhibit many interesting physical properties, and have been explored in detail over time. Recently, the transition metal chalcogenides including selenium and sulfur have been of interest because of their correlated electron properties, as seen in the iron based superconductors and the layered transition metal dichalcogenides. However, the chalcogenides are much less explored than the oxides, and there is an open question of whether there may be new materials heretofore undiscovered. We perform a systematic combined theoretical and experimental search over ternary phase diagrams that are empty in the Inorganic Crystal Structure Database containing cations, transition metals, and one of selenium or sulfur. In these 27 ternary systems, we use a probabilistic model to reduce the likelihood of false negative predictions, which results in a list of 24 candidate materials. We then conduct a variety of synthesis experiments to check the candidate materials for stability. While the prediction method did obtain compositions that are stable, none of the candidate materials formed in our experiments. We come to the conclusion that these phase diagrams are either truly empty or have unusual structures or synthesis requirements.

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