Abstract Submitted
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Sorting stable from unstable hypothetical compounds and determining the electronic structure of interesting candidates : The case of Half-Heusler Filled Tetrahedral ABX structures[1] XIUWEN ZHANG, Colorado School of Mines, Golden, CO 80401, LIPING YU, ANDRIY ZAKUTAYEV, DAVID GINLEY, National Renewable Energy Lab., Golden, CO 80401, ALEX ZUNGER, University of Colorado, Boulder, CO 80305 — Electronic structure theory has recently been used to propose hypothetical compounds, seeking new useful functional materials. In some cases, such hypothetical compounds in presumed crystal structures may be significantly higher in energy than (i) their lowest-energy structures or, than (ii) a combination of their constituents. We use the first-principles thermodynamics to sort (i) the lowest-energy structure and (ii) the thermodynamic stability with respect to disproportionation of the 488 unreported ABX octet compounds. We find that as many as 235 of the 488 are unstable with respect to decomposition, whereas other 235 of the unreported compounds are predicted to be thermodynamically stable. (18 materials are too close to call). The electronic structures of these predicted stable compounds are evaluated based on GW approximation for electron's self-energy. To support the theoretical predictions of new materials, thin film samples of AgYGe were synthesized using combinatorial Pulsed Laser Deposition. AgYSi-type ground state crystal structure and Y-rich composition stability range of AgYGe agree well with theory.

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