[illegible]

1. Introduction

The quest for physically interesting and potentially technologically useful functional materials has recently propelled numerous proposals of hypothetical materials with exciting properties promised by first-principles calculations. Some examples include "harder than diamond" carbon-nitrides,[1] the room-temperature oxide ferromagnets,[2] the new Li battery materials,[3] Half-Heusler piezoelectrics,[4] the honeycomb-structured topological insulators,[5] direct bandgap Si-Ge superlattices,[6] and Half-Heusler optoelectronic materials.[7] Some of these hypothetical materials are metastable, but metastability is not a concern if the hypothetical structure is both locally stable and is protected from fast decay into the lowest-energy structure by practically insurmountable activation barriers. For example, semiconductor superlattices and quantum-wells (AC)/(BC) made of the binary constituent semiconductors AC and BC may be ≈10–40 meV per atom higher in energy (similar to energy difference between graphite and diamond) than the AC + BC phase-separated system,[8a,8b] yet such (AC)/(BC) structures can have very long and technologically useful lifetimes.[8c] Experimental synthesis techniques based on high-energy reactants[8d] have routinely produced metastable, long lived compounds such as Na_3N[8d]

predicted stable compounds in their lowest-energy structures based on GW approximation for electron's self-energy. Remarkably, we find that a few ABX compounds made of three metals with bandgaps of ≈1 eV, whose model photovoltaic efficiencies for t_x = 0.5 μm thin-film solar cell are higher than 15%.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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