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examples include “harder than diamond” carbon-nitrides,<sup>[1]</sup> the room-temperature oxide ferromagnets,<sup>[2]</sup> the new Li battery materials,<sup>[3]</sup> Half-Heusler piezoelectrics,<sup>[4]</sup> the honeycomb-structured topological insulators,<sup>[5]</sup> direct bandgap Si-Ge superlattices,<sup>[6]</sup> and Half-Heusler optoelectronic materials.<sup>[7]</sup> 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  $\approx 10\text{--}40$  meV per atom higher in energy (similar to energy difference between graphite and diamond) than the AC + BC phase-separated system,<sup>[8a,8b]</sup> yet such (AC)/(BC) structures can have very long and technologically useful lifetimes.<sup>[8c]</sup> Experimental synthesis techniques based on high-energy reactants<sup>[8d]</sup> have routinely produced metastable, long lived compounds such as  $\text{Na}_3\text{N}$ <sup>[8d]</sup>

## 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





















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  $\approx 1$  eV, whose model photovoltaic efficiencies for  $\lambda = 0.5 \mu\text{m}$  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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