Abstract Submitted
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GW band gap of Filled Tetrahedral Structuctures: absorbers and topological insulators ?[1] JULIEN VIDAL, XIUWEN ZHANG, JUN-WEI LUO, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401, USA — Filled Tetrahedral Structures (FTS) such as LiZnP are derived from the binary zincblende material such as GaP by splitting a cation such as Ga into two lower-valent cations Li+Zn, placing one on the original cation site and the other on one of the empty interstitial sites. Generalizing this process, it is possible to generate a few hundred of ABX compounds. Their electronic structure has been previously calculated by bandgap-underestimating DFT assuming a zincblende-derived crystal structure. We use instead GW to establish (i) which ABX materials are potentially suitable as absorbers in solar cells and (ii) which of the ABX materials previously proposed as topological insulators based on DFT may not be so in a better approximation such as GW.

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