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Lead-free Halide Perovskites via Functionality-directed Materials Screening[1] LIJUN ZHANG, DONGWEN YANG, JIAN LV, XINGANG ZHAO, Jilin University, China, JI-HUI YANG, Rice University, USA, LIPING YU, Temple University, USA, SU-HUAI WEI, Beijing Computational Science Research Center, China, ALEX ZUNGER, University of Colorado, USA — Hybrid organic-inorganic halide perovskites with the prototype material of $CH_3NH_3PbI_3$ have recently attracted much interest as low-cost and high-performance photovoltaic absorbers but one would like to improve their stability and get rid of toxic Pb. We used photovoltaic-functionality-directed materials screening approach to rationally design via first-principles DFT calculations Pb-free halide perovskites. Screening criteria involve thermodynamic and crystallographic stability, as well as solar band gaps, light carrier effective masses, exciton binding, etc. We considered both single atomic substitutions in AMX_3 normal perovskites (altering chemical constituents of A, M and X individually) as well as double substitution of 2M into B+C in A_2BCX_6 double-perovskites. Chemical trends in phase stabilities and optoelectronic properties are discussed with some promising cases exhibiting solar cell efficiencies comparable to that of $CH_3NH_3PbI_3$.

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