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Structural diversity and electronic properties of Cu2SnX3 (X=S,Se): \mathbf{A} first-principles investigation YINGTENG ZHAI, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China, SHIYOU CHEN, Key Laboratory of Polar Materials and Devices (MOE), East China Normal University, Shanghai 200241, China, JIHUI YANG, HONGJUN XIANG, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China, ARON WALSH, Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom, JOONGOO KANG, SUHUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — The ternary semiconductors Cu_2SnX_3 (X=S, Se) are found frequently as secondary phases in synthesized Cu₂ZnSnS₄ and Cu₂ZnSnSe₄ samples, but previous reports on their crystal structures and electronic band gaps are conflicting. Here we report their properties as calculated using a first-principles approach. We find that: (i) the diverse range of crystal structures can all be derived from the zinc-blende structure. (ii) The energy stability of different structures is determined primarily by the local cation coordination around anions, which makes Cu and Sn partially disordered in the cation sublattice. (iii) The direct band gaps of the low energy compounds Cu_2SnS_3 and Cu_2SnSe_3 should be in the range of 0.8-0.9 eV and 0.4 eV respectively.

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