Abstract Submitted
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Search for highly absorbing thin-film photovoltaic absorbers in the system Cu-V-VI from first principles calculations[1] LIPING YU, University of Colorado at Boulder/National Renewable Energy Laboratory, ROBERT S. KOKENYESI, DOUGLAS A. KESZLER, Oregon State University, ALEX ZUNGER, University of Colorado at Boulder — To enable high-efficiency solar conversion, thin-film absorbers need to have strong absorption of photons across the solar spectrum. While the $CuInSe_2$-like materials have strong absorption, their measured rise in absorption near the band gap necessitates the use of rather thick films. This thickness, coupled with the relatively low abundance of In, potentially limits the scalability of this technology to the terawatt scale. Here we screen and assess absorption properties of ∼40 earth-abundant Cu-V-VI (V = P,As,Sb,Bi) materials, based on the recently proposed selection metric of "Spectroscopic Limited Maximum Efficiency" (SLME) [PRL. 108, 068701 (2012)]. This metric depends explicitly on calculated absorption spectra and accounts for different types of optical transitions near the absorption threshold. According to the SLME values calculated from 1st-principles quasiparticle GW theory, we propose five Cu-V-VI candidate thin-film absorber materials that have optical absorption stronger than $CuInSe_2$, which can be ascribed to the enhancement of the density of states near the conduction band maximum. The finding leads to refined design principles in support of the continuing quest for optimal absorber materials.

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Liping Yu
University of Colorado at Boulder/National Renewable Energy Laboratory

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