Abstract Submitted
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Search of novel photovoltaic absorbers from first-principles spectroscopic screening of hundreds of materials[1] LIPING YU, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado Boulder — Screening for candidate PV absorbers from numerous existing materials would require a good selection criterion. Initial selection criteria generally rest on the intrinsic material properties and abundance, postponing defect and contact issues to after the list of candidates has been narrowed down. The currently available Shockley-Queisser efficiency formula gives a universal efficiency vs band gap curve (no matter whether the gap is direct or indirect) and ignore all radiative recombination loss, and has proven over the years to be insufficient. Here we propose a calculable selection criterion of "spectroscopic limited maximum efficiency (SLME)" which considers the type of band gap (direct allowed, direct forbidden and indirect), the shape of absorption spectra and material-dependent radiative recombination loss by a simple model. First-principles quasiparticle calculations of SLME for ∼300 generalized I-III-VI and ∼500 I-V-VI materials identify over 40 candidates with higher SLME than currently used best thin-film absorbers. Analysis of the electronic structure of the top candidates reveals an interesting mechanism for high absorptivity and shows that some indirect gap materials can even be better than direct gap materials.

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