

Abstract Submitted  
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**The reason FeS<sub>2</sub> is not a good PV absorber**<sup>1</sup> LIPING YU, S. LANY, A. ZUNGER, NREL, H.A.S. PLATT, R. KYKYNESHI, B. PELATT, R. RAVICHANDARIN, D.A. KESZLER, J.F. WAGER, Oregon State University — FeS<sub>2</sub> is representative of an ideal earth-abundant candidate absorber for thin film PV, because of its appropriate band gap, high absorption coefficient and good electron/hole mobility. Yet, despite ~15 years of research, the promise of FeS<sub>2</sub> as an absorber layer has been unrealized, manifesting as a low open circuit voltage which has been attributed to  $E_f$  pinning arising from bulk sulfur vacancies. Our first-principles calculations and experimental thermogravimetric analyses, however, show that S vacancies and other point defects have rather high formation energies. Hence, they are unlikely to form and pin  $E_f$ . We find that the widely observed S deficiency in FeS<sub>2</sub> is accommodated by phase-coexistence of a few Fe<sub>1-x</sub>S compounds, rather than S vacancies. These minority phases are metallic and detrimental for PV. We find select ternary Fe sulfides do not have thermodynamically-mandated phase-coexistence like FeS<sub>2</sub>, yet they retain optimal band gaps and high absorption strengths comparable to FeS<sub>2</sub>. These properties and associated surface-defect calculations will be discussed.

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