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Iron chalcogenide photovoltaic absorbers – problems and opportunities ROBERT KOKENYESI[1], VORRANUTCH JIERATUM, EMMELINE ALTSCHUL, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR, RAM RAVICHANDRAN, BRIAN PELATT, JOHN WAGER, School of EECS, Oregon State University, Corvallis, OR, LIPING YU, STEPHAN LANY, National Renewable Energy Laboratory, Golden, CO, ALEX ZUNGER, University of Colorado at Boulder, Boulder, CO, CENTER FOR INVERSE DESIGN, EFRC COLLABORATION — Realizing new, efficient solar absorbers containing earth-abundant materials represents a critical element for expanding the reach of photovoltaic (PV) technologies, meeting growing energy needs. The use of Fe in PV was proposed more than 25 years ago in the form of FeS_2 pyrite. We report a concerted and integrated theoretical and experimental study that provides new insight into the problem of FeS_2. Computational results on FeS_2 reveal high formation energies for bulk point defects and small formation energies for S vacances near the surface. These findings are consistent with the formation of metallic S-deficient binary Fe-S phases at low temperatures that affect the electrical and optical properties of thin films. We have used this new understanding to propose and implement design rules for identifying new Fe-containing materials—Fe_2SiS_4 and Fe_2GeS_4– that may circumvent the limitations of pyrite. These ternary materials are *p*-type with direct allowed optical band gaps near 1.5 eV.

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