

Abstract Submitted  
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**Fe<sub>2</sub>MCh<sub>4</sub> (M=Si,Ge, Ch=S,Se): optical, electrical properties and defects** ROBERT KOKENYESI<sup>1</sup>, Department of Chemistry, Oregon State University, Corvallis, OR, LIPING YU, STEPHAN LANY, National Renewable Energy Lab, Golden, CO, ALEX ZUNGER, University of Colorado at Boulder, Boulder, CO, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR, CENTER FOR INVERSE DESIGN, EFRC COLLABORATION — Fe<sub>2</sub>MCh<sub>4</sub> (M=Si,Ge, Ch=S,Se) are proposed as solar absorber materials, as a single phase, stable alternative to FeS<sub>2</sub> pyrite. Native defects have high formation energy in the band gap and no Fermi level pinning is predicted by DFT. External defect calculations, including B,Al,Ga,In, N, P, As, Sb, Bi, O, Se, predict substantial effect on the bulk electronic properties.

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