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Iron-Chalcogenide Based Solar Absorbers[1] ROBERT KYKYNESHI, VORRANUTCH JIERATUM, EMMELINE ALTSCHUL, Department of Chemistry, Oregon State University, Corvallis, OR, RAM RAVICHANDRAN, BRIAN PELATT, School of EECS, Oregon State University, Corvallis, OR, LIPING YU, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO , JOHN WAGER, School of EECS, Oregon State University, Corvallis, OR, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR, CENTER FOR INVERSE DESIGN, EFRC COLLABORATION — Earth abundant, nontoxic solar absorbers are greatly desirable to reduce solar cell production cost. FeS_2 pyrite, with a band gap of $\sim$0.9 eV, is well known for outstanding absorption properties, yet significant photoconversion has never been achieved. Our computational and experimental study recognizes the failure mechanism of iron pyrite as an instability with respect to other Fe_xS ($0.5<x\leq1$) metallic compositions. A set of design rules emerges for the realization of high absorption transition metal-chalcogenide absorbers. Fe_2MS_4 (M=Si,Ge) are proposed as viable candidates, and merit for solar absorber application discussed.

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