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Searching for new solar absorber materials for energy applications within the Fe2(IV)VI4 family using electronic structure theory[1] LIPING YU, STEPHAN LANY, ALEX ZUNGER, NREL, Golden, CO — Not all direct gap semiconductors have sufficiently strong absorption at threshold. New semiconducting absorbers, free of expensive, toxic or rare elements are examined to maximize the absorption intensity at E_g+delta for small delta and the band gap E_g in solar range. We search for the "design principles" that control the absorption intensity in the space of chemical composition of Fe_2-(IV)-$(VI)_4$ (where IV=Si,Ge,Sn,Ti and VI=S,Se,Te) as well as structural and configuration degrees of freedom (e.g. crystal distortion). We use the tools of electronic structure theory to identify the chemical and structural motifs that enhance absorption. We investigate the chemical trends for the different elemental compositions within this compound family, focusing on the band gap, effective mass, absorption spectra as well as the interplay between magnetic structure and the optical properties.

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Liping Yu
NREL, Golden, CO

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