Iron Chalcogenide Photovoltaic Absorbers

The Center for Inverse Design has identified the iron-based ternary chalcogenide materials Fe_2SiS_4 and Fe_2GeS_4 as promising new photovoltaic materials, which circumvent the problems historically encountered with iron sulfide FeS_2 (iron pyrite). There is intense interest in earth-abundant materials, including iron-bearing systems, for the widespread development of photovoltaic (PV) technologies to sustainably meet growing energy needs. The inverse design methodology was used to develop and implement design rules to identify new Fe-containing PV materials. These rules have led us to consider the the ternary compounds Fe_2SiS_4 and Fe_2GeS_4. An integrated computational and experimental study of FeS_2 reveals that coexistence of off-stoichiometric secondary phases is an important factor limiting performance as a thin-film solar absorber. Band structure calculations followed by spectroscopy on the ternary materials Fe_2SiS_4 and Fe_2GeS_4 reveal a nearly optimal 1.5 eV direct bandgap with exceptionally strong absorption. Theory also shows that these materials are very stable with respect to decomposition into competing phases, and the Fermi level in these materials is not pinned by defects. These ternaries provide a new entry point for development of thin-film absorbers and high-efficiency photovoltaics.

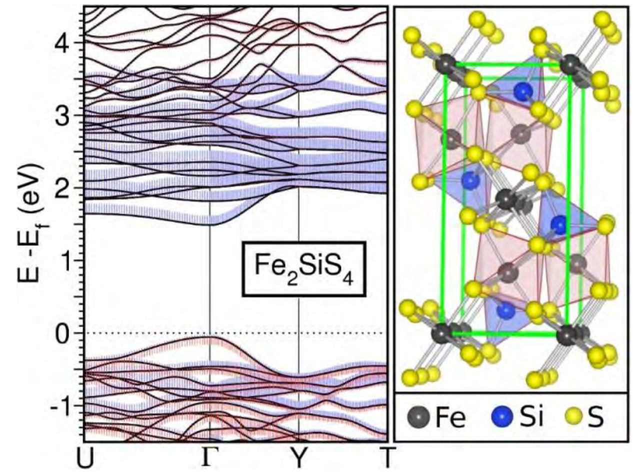

Figure: The calculated band structure and the crystal structure of the proposed Fe_2SiS_4 iron chalcogenide PV absorber

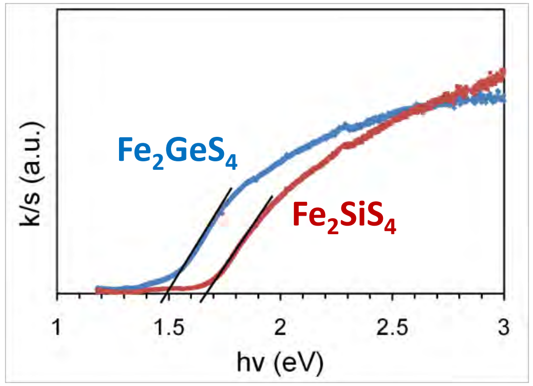

Figure: Diffuse reflectance data showing that the band gap of Fe_2SiS_4 and Fe_2GeS_4 is close to the theoretical optimum of 1.5 eV

Reference: L. Yu, S. Lany, R. Kykyneshi, V Jieratum, R. Ravichandran, B. Pelatt, E. Altschul, H.A.S. Platt, J.F. Wager, D.A. Keszler, A. Zunger Advanced Energy Materials, *doi: 10.1002/aenm.201100351*