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Band gap engineering iron pyrite for sustainable solar energy conversion ALISON HATT, Lawrence Berkeley National Lab, ALEXANDER SEBENIUS, Harvard University, JEFFREY NEATON, Lawrence Berkeley National Lab — In the quest to develop sustainable materials for solar energy conversion, iron pyrite (FeS2) holds great promise as a solar absorber. The electronic band gap of FeS2, however, is not well matched to the solar spectrum. Here we explore chemical doping as a strategy to engineer the band gap of FeS2, as has been successfully demonstrated with other semiconducting materials. Using first-principles calculations, we first establish the relationship between pressure, lattice distortions, and the electronic structure of FeS2, and rationalize the results in terms of distortions in the crystal-field splitting of Fe. We then investigate the effects of doping FeS2 with transition metal elements, wherein our strategy is guided by the knowledge of band gap dependence on local distortions.

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