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Increasing the band gap of iron pyrite by alloying with oxygen
MATTHEW LAW, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of California, Irvine, California 92697, JUN HU, YANNING ZHANG, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, California 92697 — Systematic density functional theory studies and model analyses have been used to show that the band gap of iron pyrite (FeS_2) can be increased from $\sim$ 1.0 to 1.2 -1.3 eV by replacing $\sim$ 10% of the sulfur atoms with oxygen atoms (i.e., $\sim$ 10% O_S impurities). O_S formation is exothermic, and the oxygen atoms tend to avoid O-O dimerization, which favors the structural stability of homogeneous $FeS_{2-x}O_x$ alloys and frustrates phase separation into FeS_2 and iron oxides. With an ideal band gap, absence of $O_S$induced gap states, high optical absorptivity, and low electron effective mass, $FeS_{2-x}O_x$ alloys are promising for the development of pyrite-based heterojunction solar cells that feature large photovoltages and high device efficiencies. Acknowledgement: We thank the NSF SOLAR Program (Award CHE-1035218) and the UCI School of Physical Sciences Center for Solar Energy for support of this work. Calculations were performed on parallel computers at NERSC and at NSF supercomputer centers.

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