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Possible reasons for low open circuit voltage in pyrite (FeS_2) PREDRAG LAZIC, DMSE, MIT, MA, USA, RICKARD ARMIENTO, IFM, Linkoping University, Sweden, WILLIAM HERBERT, DMSE, MIT, MA, USA, RUPAK CHAKRABORTY, DME, MIT, MA, USA, RUOSHI SUN, DMSE, MIT, MA, USA, MARIA CHAN, Centre for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA, KATHERINE HARTMAN, DMSE, MIT, MA, USA, TONIO BUONASSISI, DME, MIT, MA, USA, BILGE YILDIZ, NSE, MIT, MA, USA, GERBRAND CEDER, DMSE, MIT, MA, USA — Pyrite (FeS_2), being a promising material for future solar technologies, has so far exhibited in experiments an open-circuit voltage (OCV) of around 0.2 V, which is much lower than the frequently quoted "accepted" value for the fundamental bandgap of 0.95 eV. Absorption experiments show large subgap absorption, commonly attributed to defects or structural disorder. However, computations using density functional theory with a semi-local functional predict that the bottom of the conduction band consists of a very low intensity sulfur p-band that may be easily overlooked in experiments. The intensity of absorption into the sulfur p-band is found to be of the same magnitude as contributions from defects and disorder. Our findings suggest the need to re-examine the value of the fundamental bandgap of pyrite presently in use in the literature. If the contribution from the p-band has so far been overlooked, the substantially lowered bandgap would partly explain the discrepancy with the OCV. Also, we show that more states appear on the surface within the low energy sulfur p-band, which suggests a mechanism of thermalization into those states that would further reducing the OCV.

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