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**GW calculations of the bandgap of pyrite under various conditions** BRIAN KOLB, ALEXIE KOLPAK, Massachusetts Institute of Technology — Iron pyrite holds great promise as a solar cell material because of its near optimal bandgap (0.95 eV) and its high optical absorbance. Nevertheless, real solar cells made from this material suffer from poor performance. In particular, the low open circuit voltage of around 200 meV precludes pyrite's use in effective solar cell devices. Several theories have been proposed to explain this low open-circuit voltage including bulk defects, intrinsic surface states within the gap, and surface defects. Careful DFT calculations have shown that bulk defects are exceedingly rare. Further, the calculations do not exhibit intrinsic surface states within the gap. Researchers disagree about the effect of surface defects, particularly sulfur deficiencies, on the bandgap. This work combines DFT with GW calculations of the bandgap to address some of the most fundamental and important questions about the cause of the low open-circuit voltage of pyrite solar cells including the true role of surface defects, the nature of the interface with metal electrodes, and the effect of phonons on the bandgap. This investigation is undertaken with an eye toward engineering a pyrite-based material that can perform well in real solar cell applications.

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