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Light-induced metastability in the wide-gap ZnO and $CuGaSe_2$ caused by anion vacancies STEPHAN LANY, National Renewable Energy Laboratory, Golden, CO 80401, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — First-principles electronic structure calculations [1] show that anion vacancies in II-VI and chalcopyrite I-III-VI_2 semiconductors are a class of intrinsic defects that can produce metastable behavior and persistent photoconductivity (PPC), arising from a pronounced coupling between electronic and structural degrees of freedom. In ZnO, V_O^0 has a deep localized donor state in the gap, while V_O^{2+} has a shallow level near the CBM. Illumination excites V_O^0 to V_O^++e and to V_O^{2+}+2e, and this transition is accompanied by large lattice relaxation. The latter state is metastable and acts as a shallow donor, leading to persistent *electron* photoconductivity (*n*-type PPC), which persists until it is thermally activated into the deep V_O^0. Comparing the behavior of the anion vacancy in the wide-gap chalcopyrite $CuGaSe_2$ to that in ZnO, we find an interesting asymmetry: V_{Se} produces persistent *hole* photoconductivity in *p*-$CuGaSe_2$, constituting the unusual case where a donor-like defect creates *p*-type PPC.

[1] Stephan Lany and Alex Zunger, Phys. Rev. Lett. **93**, 156404 (2004).

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