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Energy bands and point defects in $CuInSe_2$ and $CuGaSe_2$ calculated by Quasiparticle Self-Consistent *GW* MARK VAN SCHILFGAARDE, TAKAO KOTANI, Arizona State University — $CuIn_xGa_{1-x}Se_2$, or CIGS, is emerging as a leading candidate for second-generation solar cell applications. Here we present the bulk energy band properties and dielectric response of $CuInSe_2$ and $CuGaSe_2$, computed within the Quasiparticle Self-Consistent *GW* (QS*GW*) approximation. QS*GW* has been proven to be a very reliable, true *ab initio* predictor of QP levels in a wide variety of materials systems; it is expected to be similarly reliable for chalcopyrite semiconductors. The fundamental gap agrees well with experiment. Also, the electron and hole effective masses are evaluated. Various kinds of point defects were considered using certain approximations to QS*GW*. Of particular interest are low-energy cation defects (antisites and vacancies). Rather unusual properties of these levels are found, owing to the unique role that shallow Cu *d* states play in CIGS.

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