Electronic structure of chalcopyrite CuInSe$_2$: LDA and GW CI-
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— CuInSe$_2$ is an important ternary semiconductor for solar cell applications with
the highest demonstrated conversion efficiency. We have investigated its electronic
structure by using pseudopotential density functional theory at the local density
approximation (LDA) as well as by Hedin's GW approximation schemes. GW cal-
culations are performed in self- consistent form as well as at the static COHSEX
approximation level. The COHSEX approach results are found to be in reasonable
agreement with the experimental data. The role of Copper semicore states ($3s^2 3p^6$)
in the band structure is found to be negligible for the LDA calculations while its cru-
cial for obtaining a correct ordering of the bands at the GW level. The overall GW
band structure is found to be similar to the LDA one with an almost dispersionless
scissor shift along the $Z - \Gamma - X$ direction of the Brillouin zone.

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