Electronic structure of chalcopyrite CuInSe$_2$: LDA and GW CI-
HAN PARLAK, TANJU GUREL, RESUL ERYIGIT, Abant Izzet Baysal University — 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 calculations 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 crucial 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.