Relativistic electronic structure and photovoltaic performance of K_2CsSb

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Antimony-based materials have emerged as promising non-toxic and earth-abundant photovoltaic candidates with similar electronic properties to the lead hybrid perovskites. The family of Heusler alloys X_2YZ and XYZ have attracted considerable attention due to their highly symmetric structure, compositional flexibility, low thermal conductivity and remarkable transport properties. Among them, the full-Heusler K_2CsSb has shown its potential application as a photocathode and thermoelectric, while its possibility to serve as a photovoltaic remains unexplored. In this project, using hybrid DFT calculations with spin-orbit coupling, K_2CsSb is found to exhibit an ideal direct bandgap, dispersive conduction band, strong optical absorption, and a competitive theoretical efficiency of over 28% at a thickness of 200nm. The point defect study will be included in this project to further understand the trap-limited efficiency of this promising photovoltaic candidate.

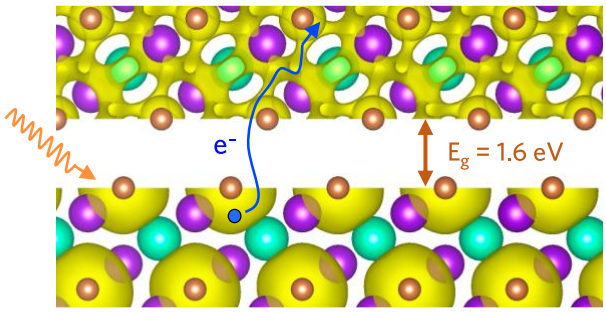

Figure 1:Partial density distribution at K2CsSb valence band maximum and conduction band minimum.