EXPLORING PHOTOVOLTAIC POTENTIAL OF CZTS: AN AB INITIO STUDY OF KESTERITIC SOLID SOLUTIONS

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CZTS (copper-zinc-tin-sulfide) is being extensively studied as an alternative to CIGS (copper-indium-gallium-selenide) for thin film solar cell applications. [1] This interest is due to the greater abundance of the elemental components of CZTS in the Earth's crust compared to CIGS. Additionally, CZTS has a crystal structure similar to chalcopyrite, albeit slightly different (space group of kesterite, I-4), and is thus expected to have comparable properties.

Like chalcopyrites, kesterites can form solid solutions that influence their electronic and photovoltaic properties. Investigating this impact is essential to predict the potential of a specific kesteritic material for photovoltaic applications.

We conducted an ab initio study of kesteritic solid solutions relevant to photovoltaic applications and calculated their electronic properties. Additionally, we performed many-body perturbation theory (MBPT) calculations to obtain absorption spectra and analyze their dependence on elemental concentrations. Special attention was given to including excitonic effects in the calculations and evaluating their impact on the final spectra.

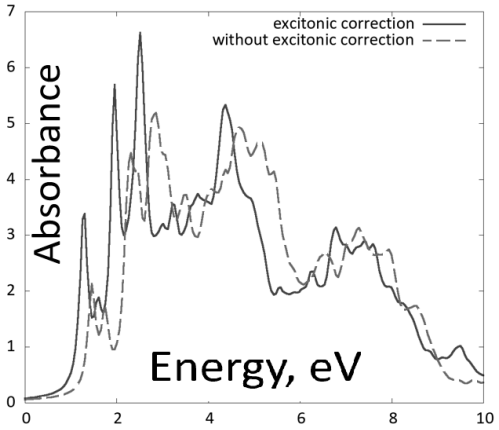

Fig.1 Example of CZTS *calculated absorption spectra with (solid line) and without (dashed line) excitonic correction.*

For the initial density functional theory (DFT) computation, we used the plane-wave-based PWSCF utility from Quantum Espresso. [2] The resulting wave functions were subsequently used in MBPT calculations with the Yambo code, where excitonic effects were modeled using the Bethe-Salpeter equation. [3]

We successfully predict the optical absorption and electronic structure of the given kesteritic materials, and hence our results enhance the understanding of this class of materials and could significantly contribute to future solar cell design.

References

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