

Electronic and Optical Properties in Cu-based Materials for Thin-film Solar Cells

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What materials am I working on?

- Commercial materials:
 $\text{Cu}(\text{In},\text{Ga})\text{Se}_2$ and $\text{Cu}_2\text{ZnSn}(\text{Se},\text{S})_4$.
- High absorption materials:
 $\text{Cu}(\text{Sb},\text{Bi})(\text{S},\text{Se})_2$ and $\text{Cu}_3(\text{Sb},\text{Bi})(\text{S},\text{Se})_3$.
- Novel materials:
 Cu_2S , SnS , Cu_2SnS_3 and Cu_4SnS_4 .

Motivation

We want to understand Cu-based materials for solar cells.

- What materials have relatively high absorption coefficient?
- Why some materials have high or low absorption coefficient?
- How good band-gap can we obtain using theoretical calculations?

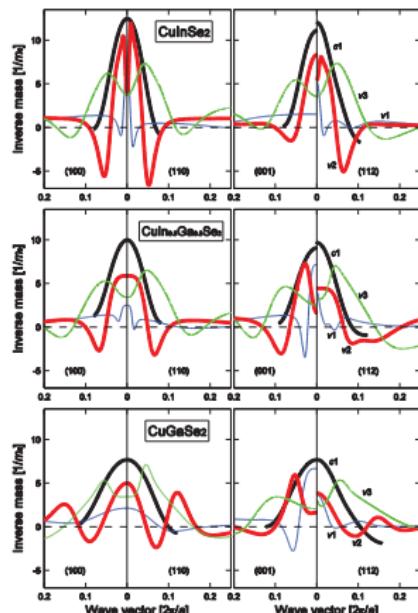
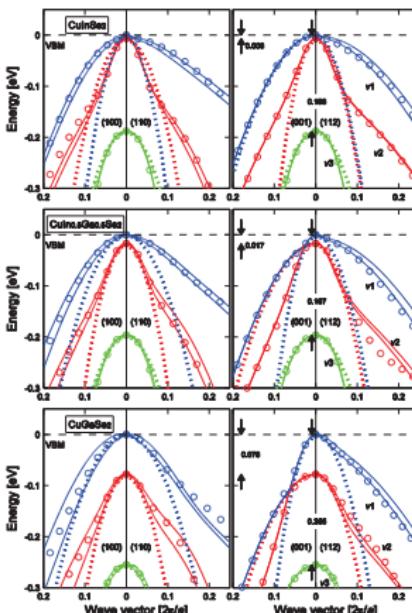
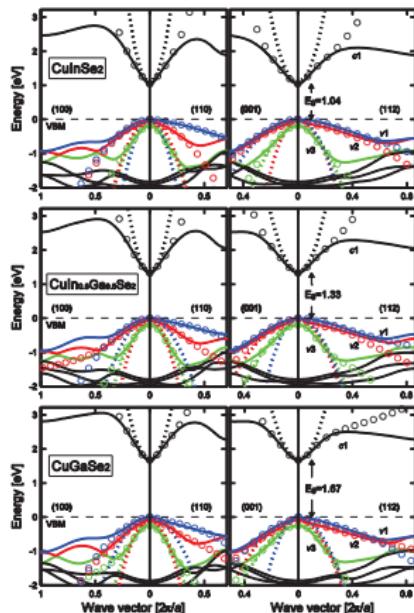
Computational methods

- Fundamental methods
 - Density-functional theory (DFT).
 - Kohn-Sham (KS) equation.
- Beyond DFT
 - GW approximation.
 - Heyd-Scuseria-Ernzerhof (HSE) hybrid functional.

Previous results 1: parameterization of band structure

Thin Solid Films **519**, 7503 (2011).

Journal of Applied Physics **112**, 103708 (2012).



Band structure along four directions. Circles(fbp), Dotted(pba), and solid lines (calculation).

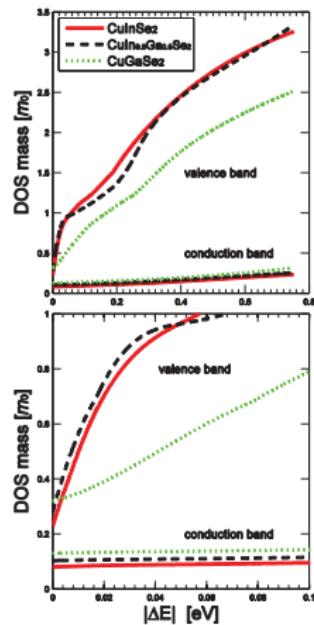
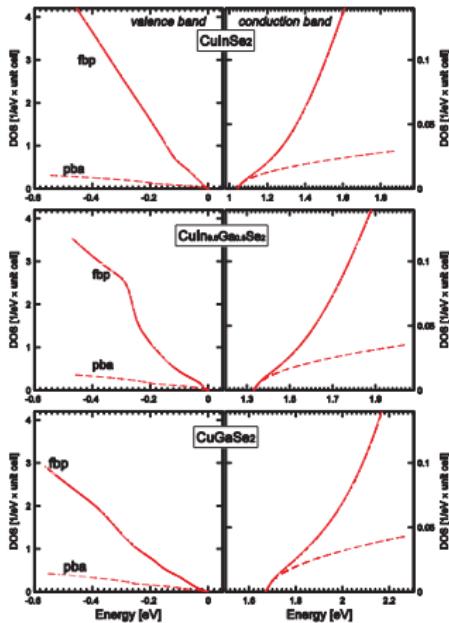
Inverse of electron and hole masses.

full band parameterization: fbp; parabolic band approximation: pba.

Previous results 1: density-of-states (DOS) and DOS mass

Thin Solid Films **519**, 7503 (2011).

Journal of Applied Physics **112**, 103708 (2012).



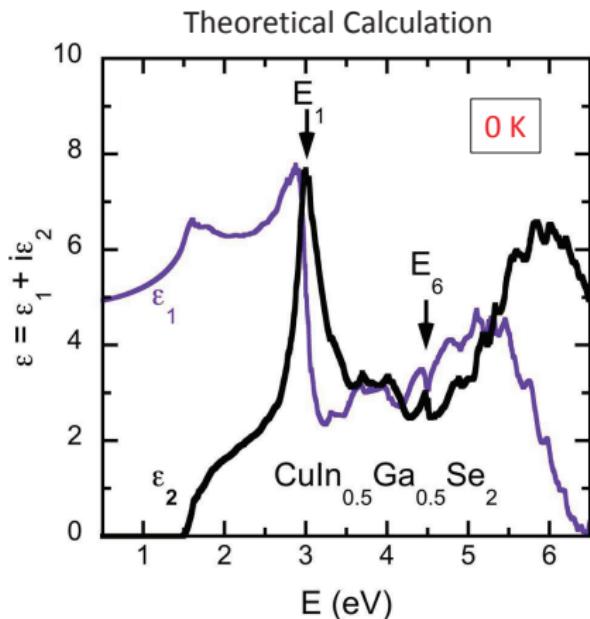
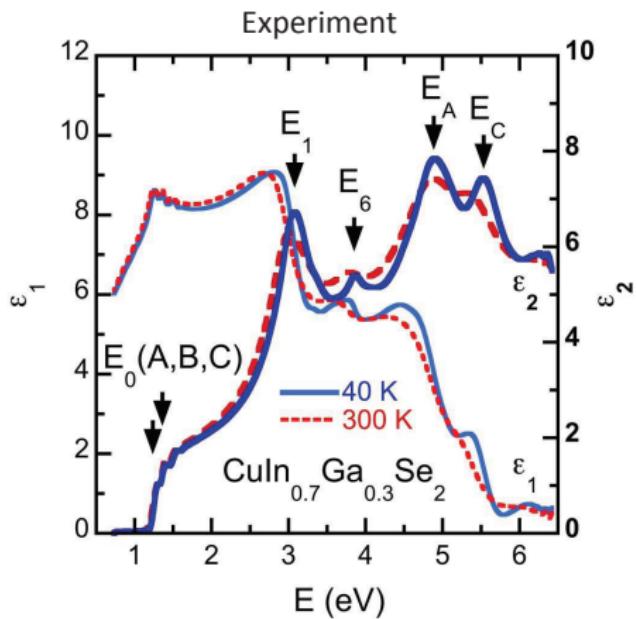
Others:

Fermi level and band-gap with temperature.

Carrier concentration in intrinsic and *p*-type $\text{Cu}(\text{In}, \text{Ga})\text{Se}_2$.

Previous results 2: dielectric function for $\text{CuIn}_{0.5}\text{Ga}_{0.5}\text{Se}_2$

Applied Physics Letters **101**, 261903 (2012).

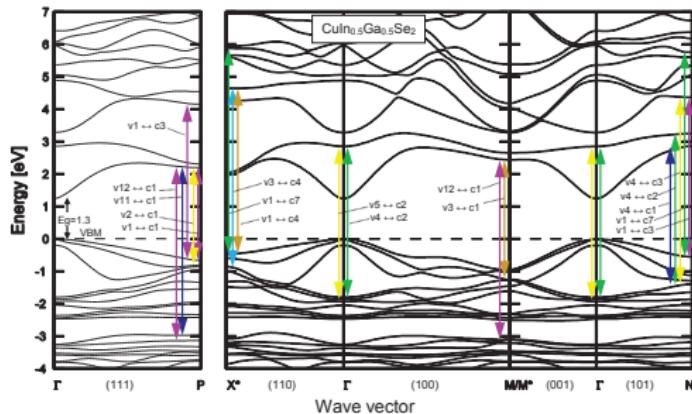
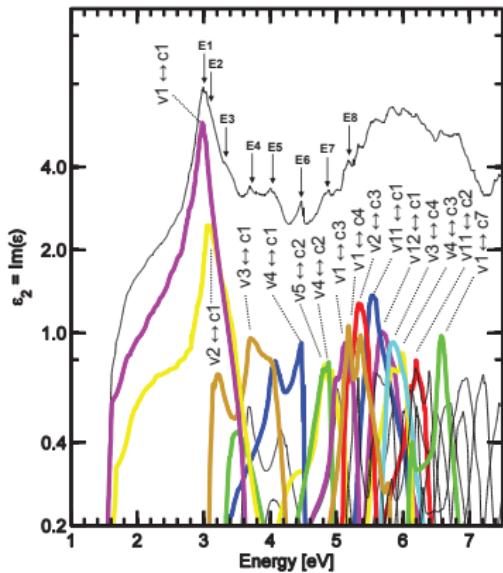


The real (ϵ_1) and imaginary (ϵ_2) part of dielectric function spectra for $\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$ at 40 K (solid lines) and 300 K (dashed lines).

The dielectric function spectra for $\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$ calculated at 0 K.

Previous results 2: analysis of the imaginary part of dielectric function

Applied Physics Letters **101**, 261903 (2012).

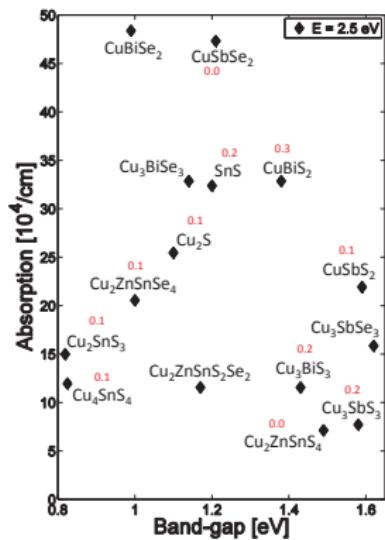
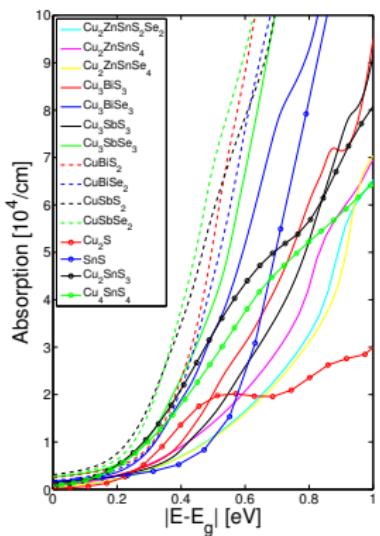
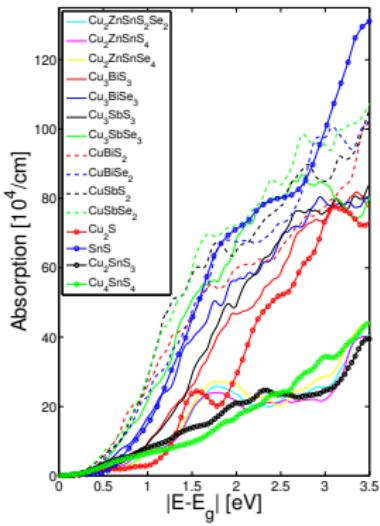


The calculated electronic band structure of $\text{CuIn}_{0.5}\text{Ga}_{0.5}\text{Se}_2$ where the CPs are identified along the main symmetry directions.

Band-to-band analysis of the contribution to the total ϵ_2 spectrum. The vertical axis is in the log scale.

Current results: absorption and band-gap in Cu-based materials

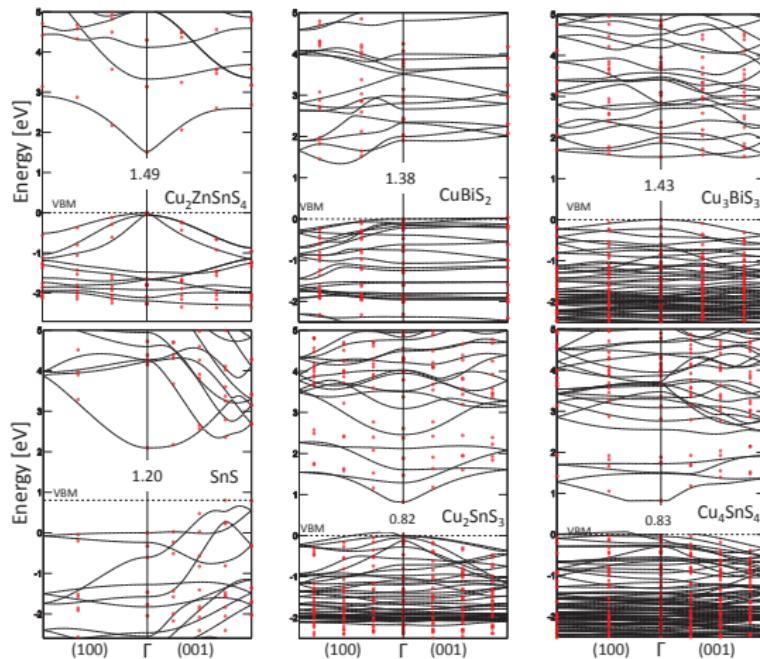
To be submitted.



HSE: Cu_2SnS_3 and Cu_4SnS_4 , GW: others. CSHIFT=0.03.

Current results: band structure in Cu-based materials

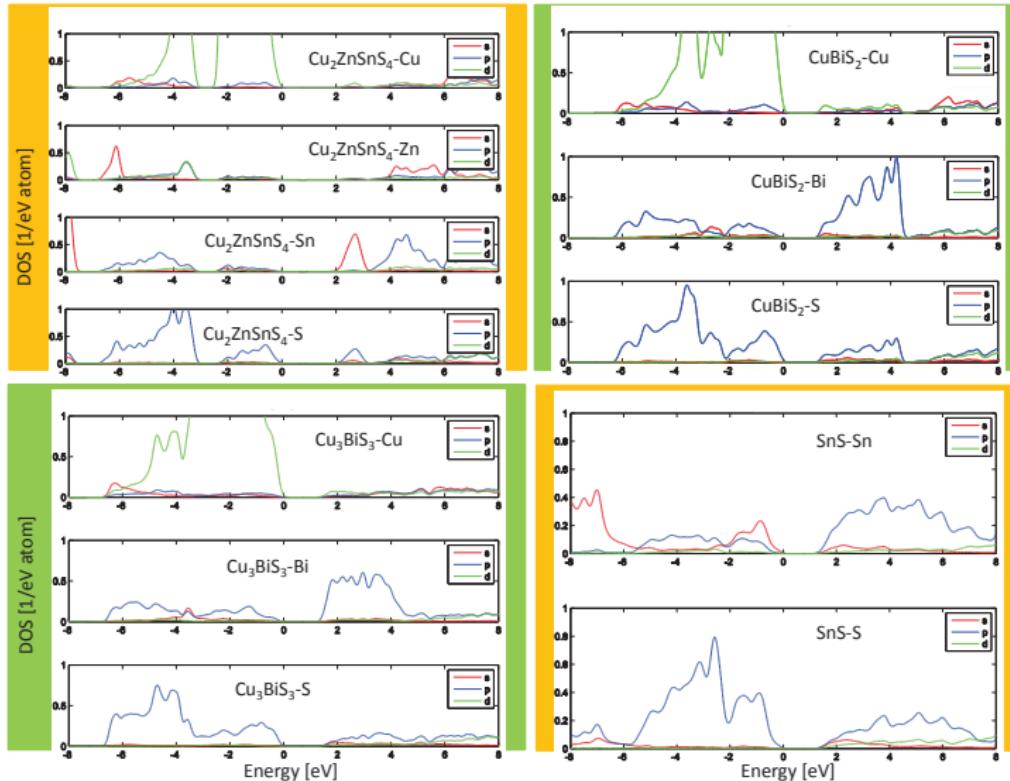
To be submitted.



Circles(HSE: Cu_2SnS_3 and Cu_4SnS_4 , GW: others), solid lines(PBE).

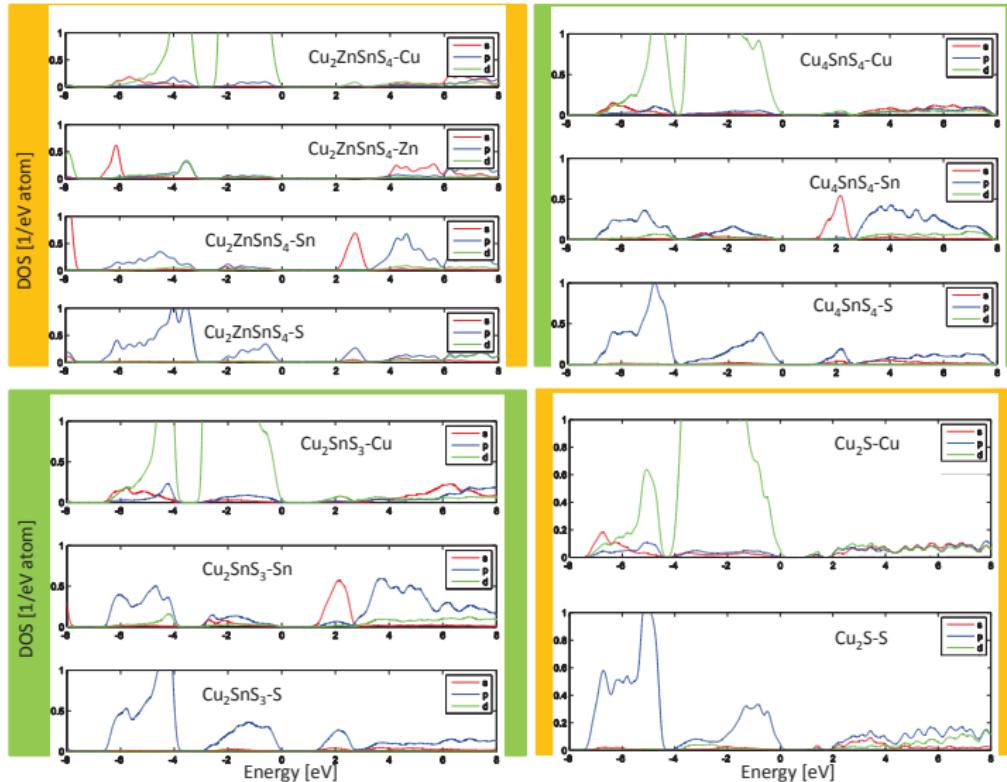
Current results: density-of-states in Cu-based materials

To be submitted.

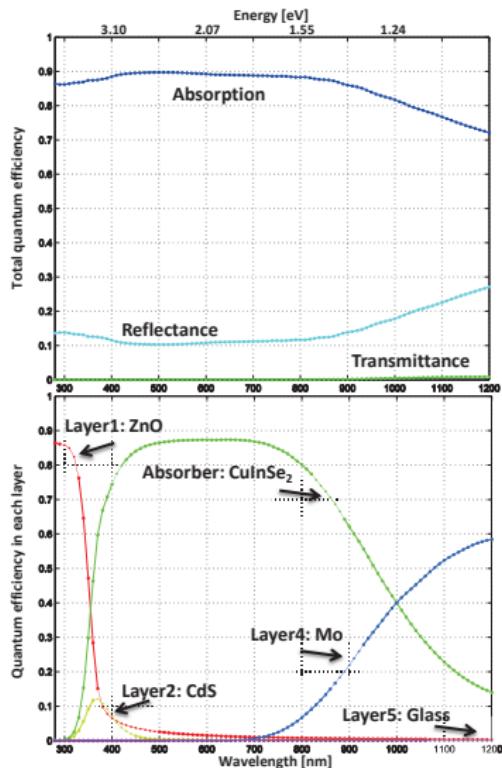
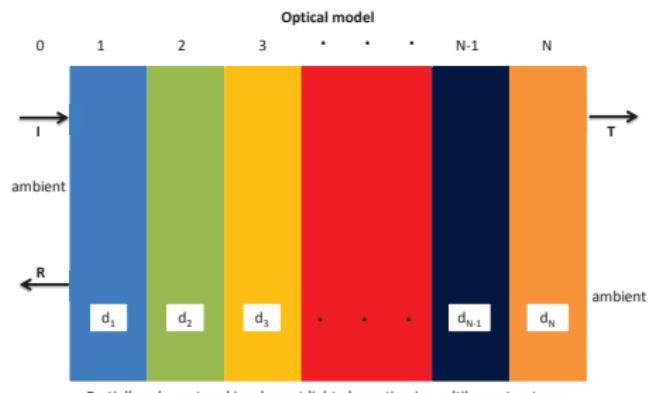


Current results: density-of-states in Cu-based materials

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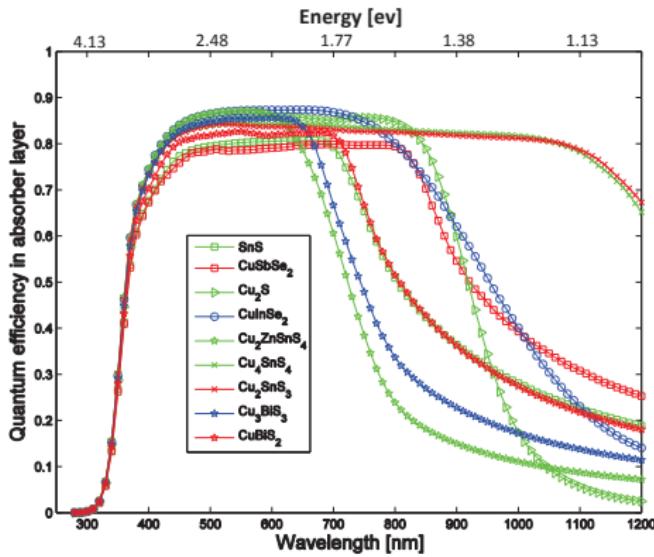
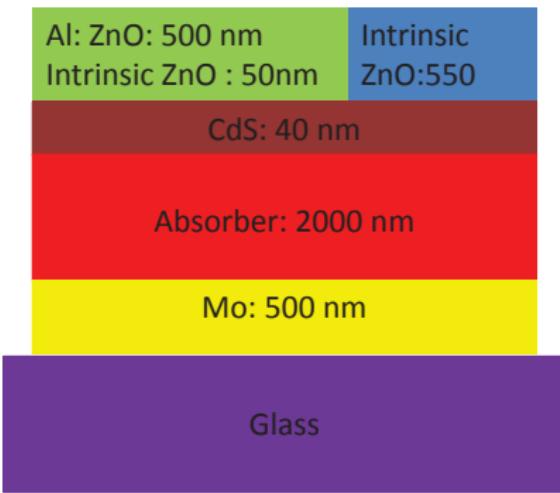
Current results: quantum efficiency in Cu-based materials solar cells



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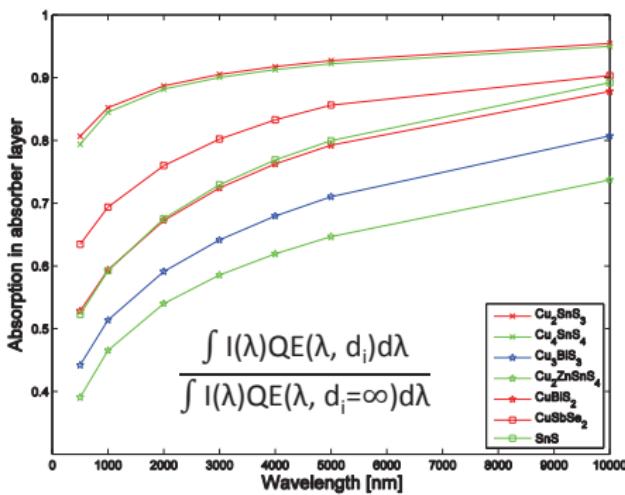
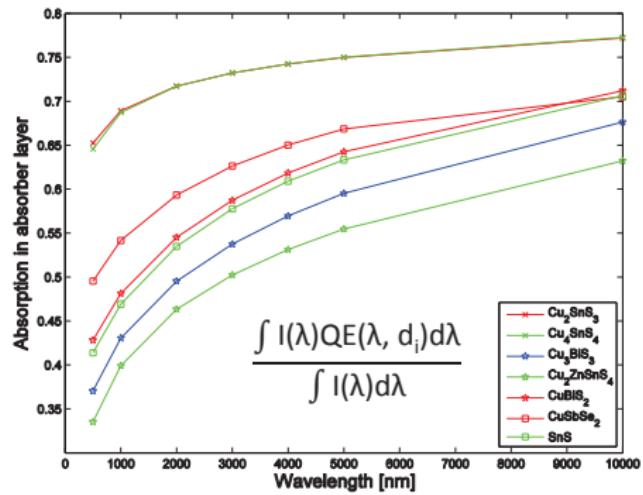
To be submitted.

Simulation solar cell structure



Current results: quantum efficiency in Cu-based materials solar cells

To be submitted.



Here, $I(\lambda)$ is the spectral power density of the AM1.5 solar spectrum with wavelength λ . $QE(\lambda, d_i)$ is the quantum efficiency in the corresponding layer with thickness d_i .

Summary for current work

- $\text{Cu}_x(\text{Bi},\text{Sb})(\text{Se},\text{S})_y$ and SnS materials have high absorption coefficient compared with $\text{CuZnSn}(\text{Se},\text{S})_4$, and Cu_mSnS_n materials have similar absorption coefficient compared with $\text{CuZnSn}(\text{Se},\text{S})_4$.
- The high absorption coefficients can be explained by the flat valence and conduction bands, as well as stronger p -states of Bi, Sb for $\text{Cu}_x(\text{Bi},\text{Sb})(\text{Se},\text{S})_y$ and Sn for SnS.
- GW and HSE are valuable methods to calculate band-gap for semiconductor. The absolute value of band-gap error is around 0.2 eV compared with experimental values.

Thank you for your attention!