

# 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:  
 $\text{Cu}_2\text{S}$ ,  $\text{SnS}$ ,  $\text{Cu}_2\text{SnS}_3$  and  $\text{Cu}_4\text{SnS}_4$ .

# 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?

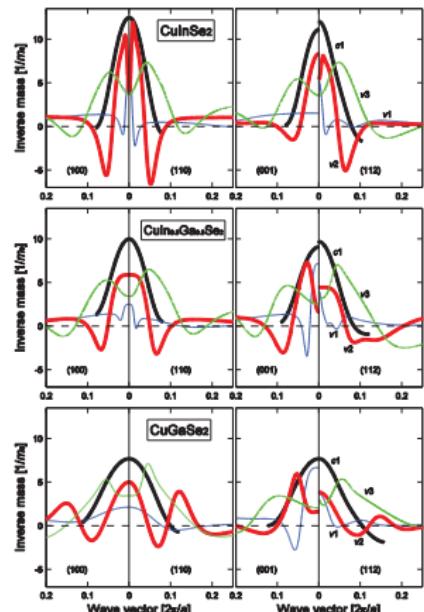
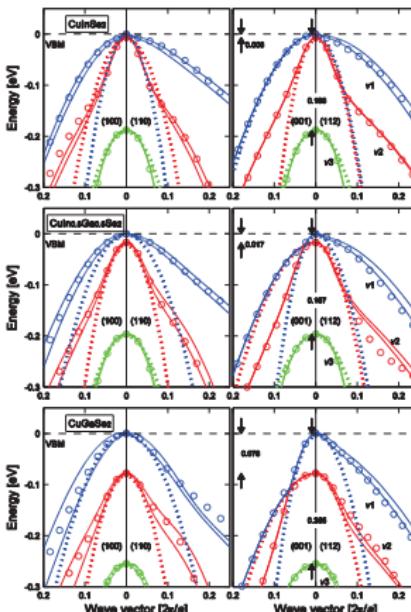
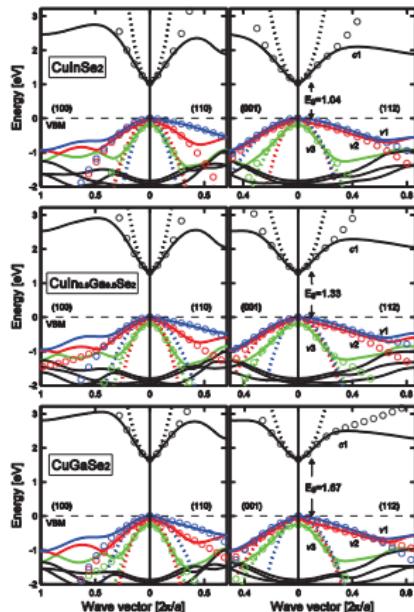
# Computational methods

- 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).

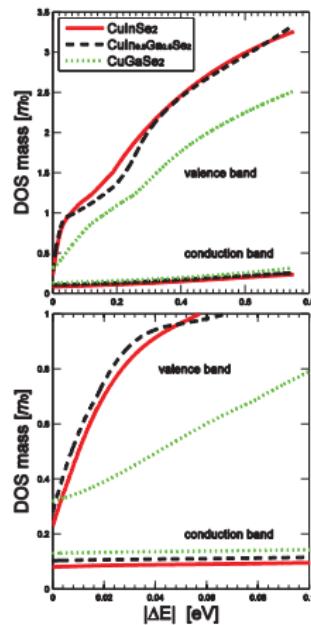
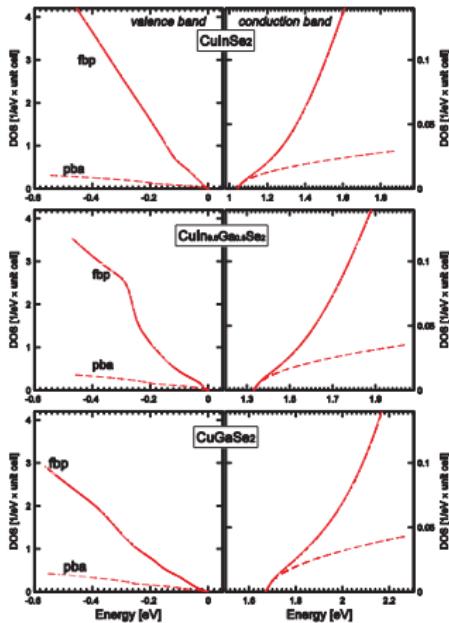
Inverse of electron and hole masses.

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).



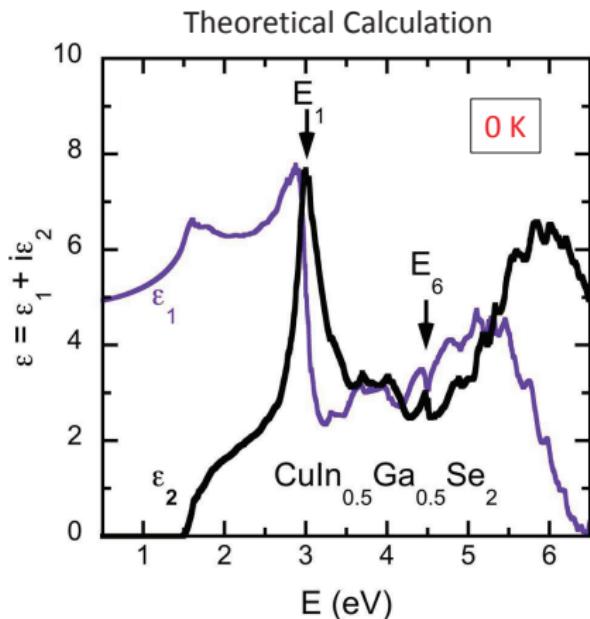
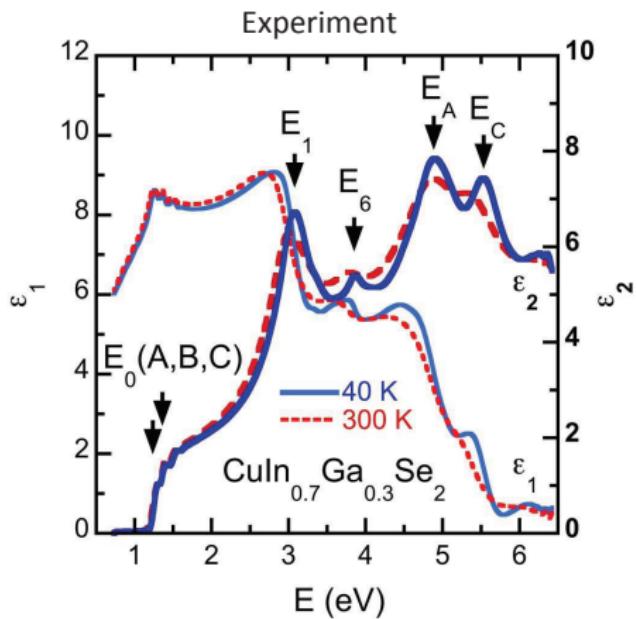
Others:

Fermi level and band-gap with temperature.

Carrier concentration in intrinsic and *p*-type Cu(In, Ga)Se<sub>2</sub>.

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

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

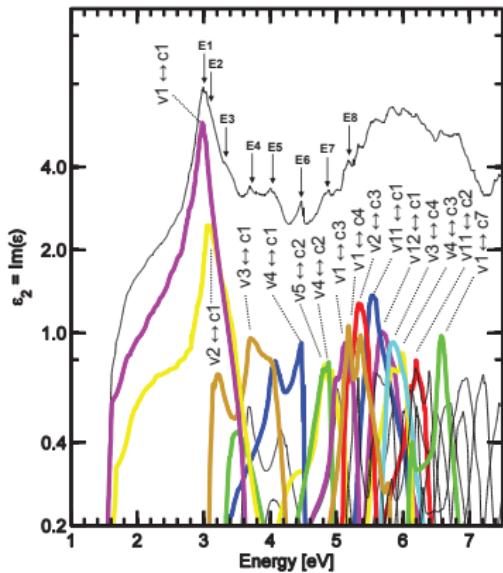


The real ( $\epsilon_1$ ) and imaginary ( $\epsilon_2$ ) part of dielectric function spectra for  $\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$  at 40 K (solid lines) and 300 K (dashed lines).

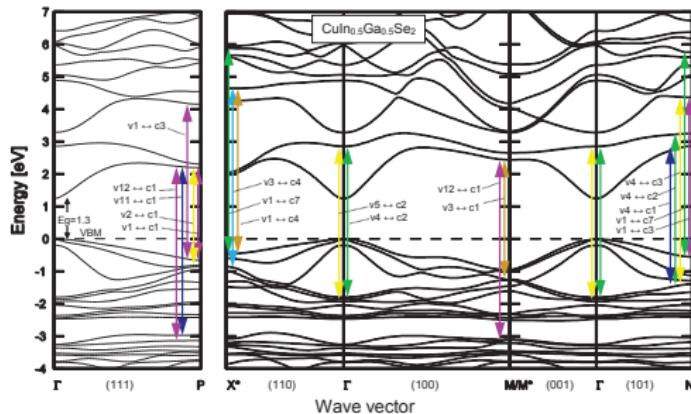
The dielectric function spectra for  $\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$  calculated at 0 K.

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

Applied Physics Letters 101, 261903 (2012).



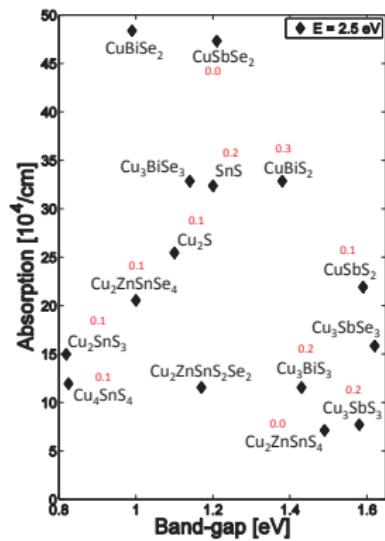
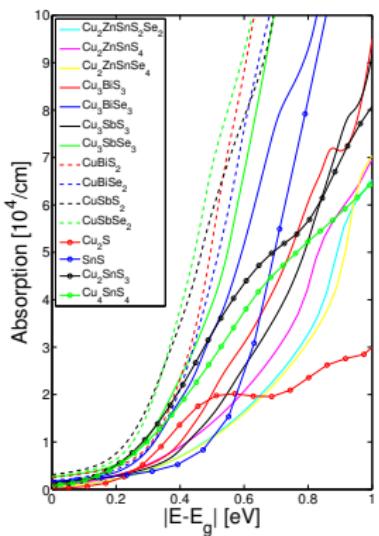
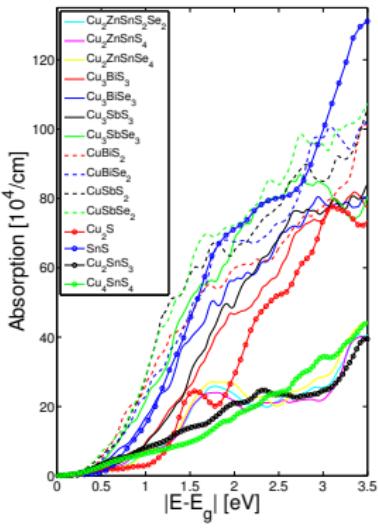
Band-to-band analysis of the contribution to the total  $\varepsilon_2$  spectrum. The vertical axis is in the log scale.



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.

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

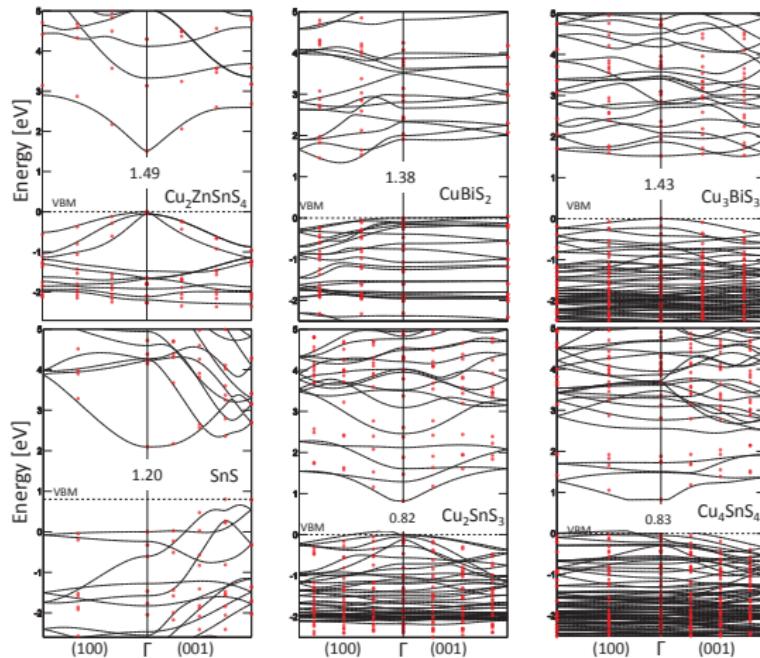
Submitted.



HSE:  $\text{Cu}_2\text{SnS}_3$  and  $\text{Cu}_4\text{SnS}_4$ , GW: others. CSHIFT=0.03.

# Current results: band structure in Cu-based materials

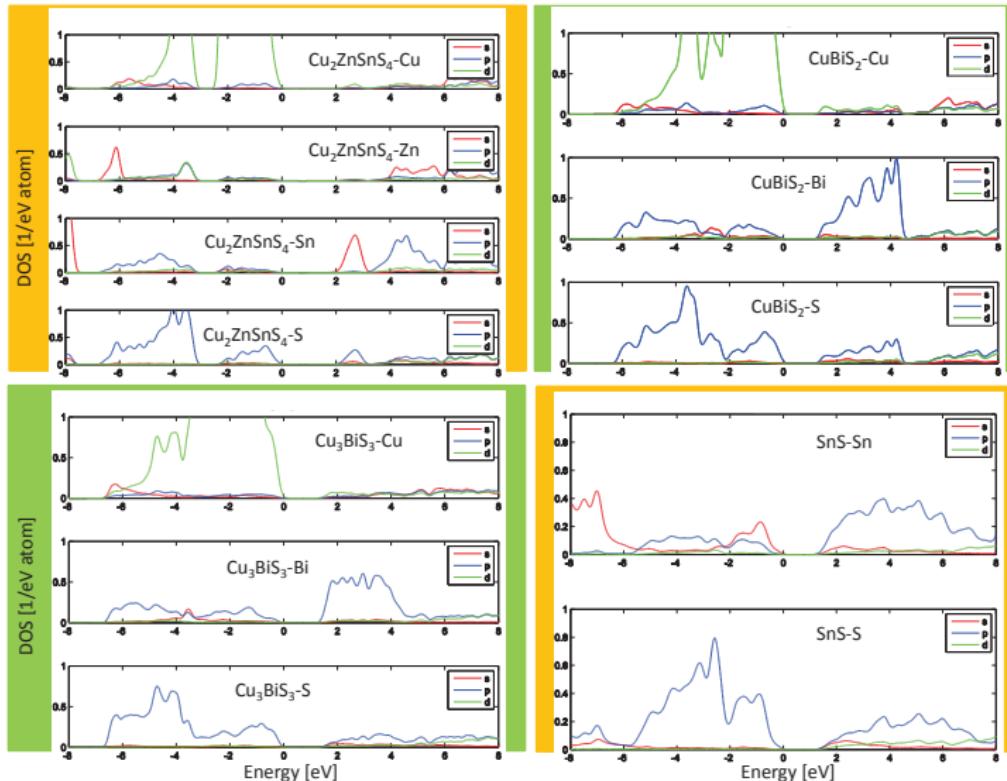
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Circles(HSE:  $\text{Cu}_2\text{SnS}_3$  and  $\text{Cu}_4\text{SnS}_4$ , GW: others), solid lines(PBE).

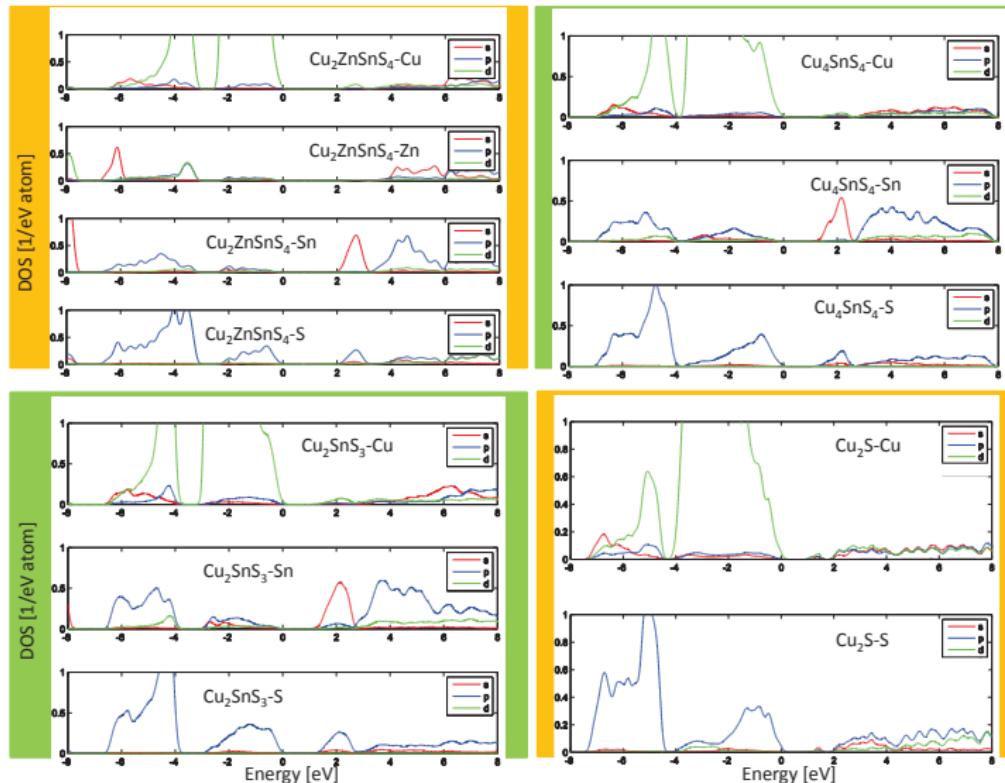
# Current results: density-of-states in Cu-based materials

Submitted.

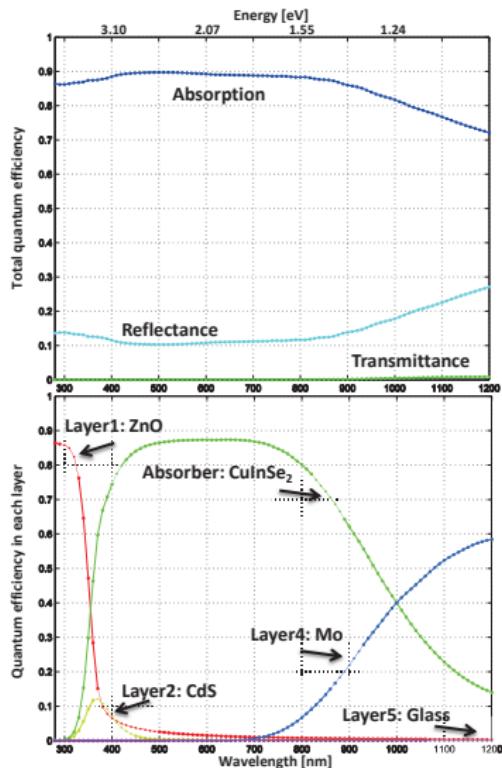
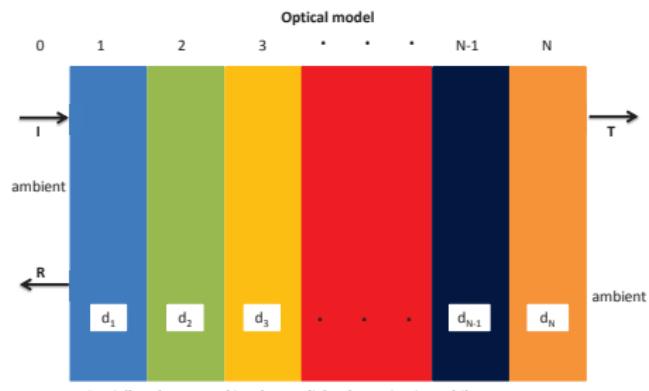


# Current results: density-of-states in Cu-based materials

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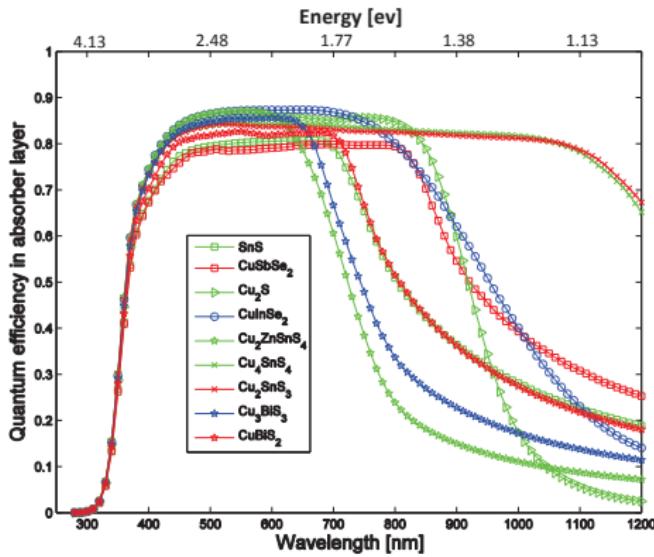
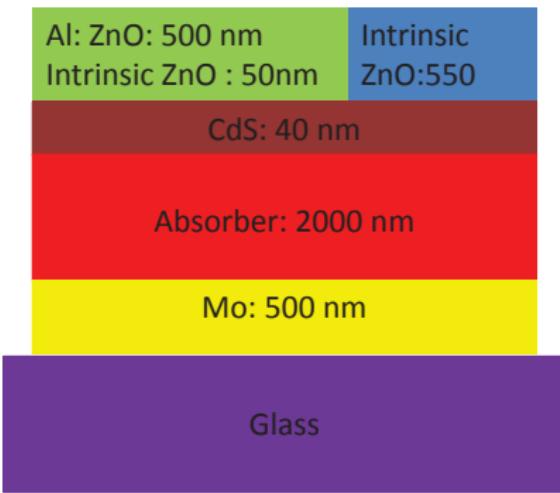
# Current results: quantum efficiency in Cu-based materials solar cells



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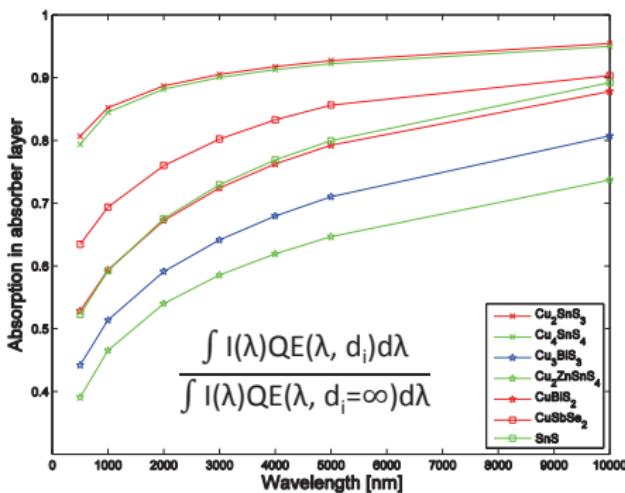
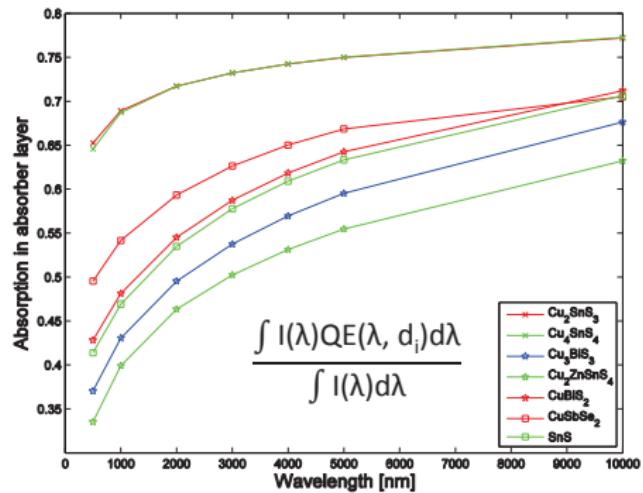
Submitted.

Simulation solar cell structure



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

Submitted.



Here,  $I(\lambda)$  is the spectral power density of the AM1.5 solar spectrum with wavelength  $\lambda$ .  $QE(\lambda, d_i)$  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  $\text{Cu}_m\text{SnS}_n$  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 much localized  $p$ -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!