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:
  $Cu(In,Ga)Se_2$ and $Cu_2(Zn, Sn)Se_4$.
- High absorption materials:
  $Cu(Sb,Bi)(S,Se)_2$ and $Cu_3(Sb,Bi)(S,Se)_3$.
- Noval materials:
  Cu_2S, SnS, Cu_2SnS_3 and Cu_4SnS_4.

Motivation

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

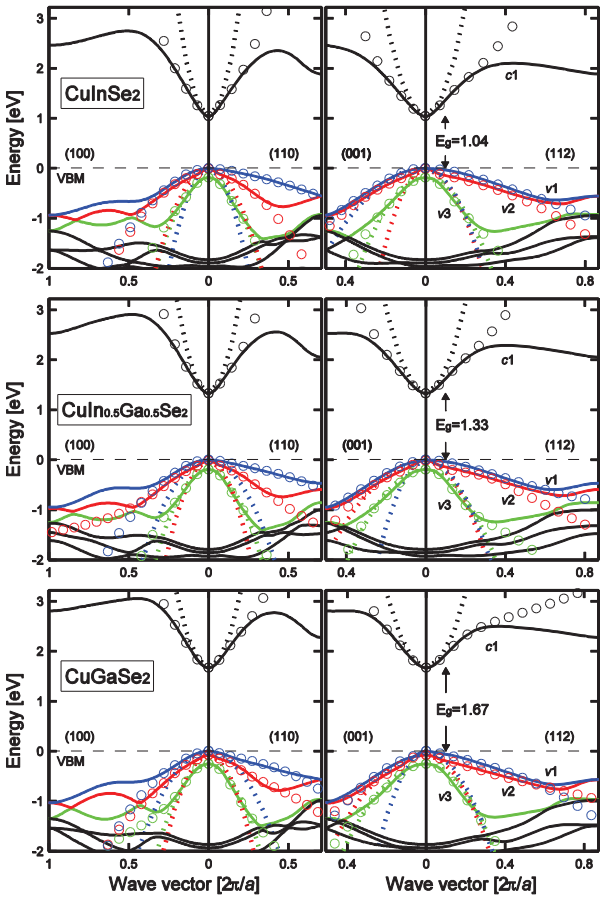
- Why some materials have high or low absorption coefficient?
- How good band-gap can we obtain using theoretical calculation?

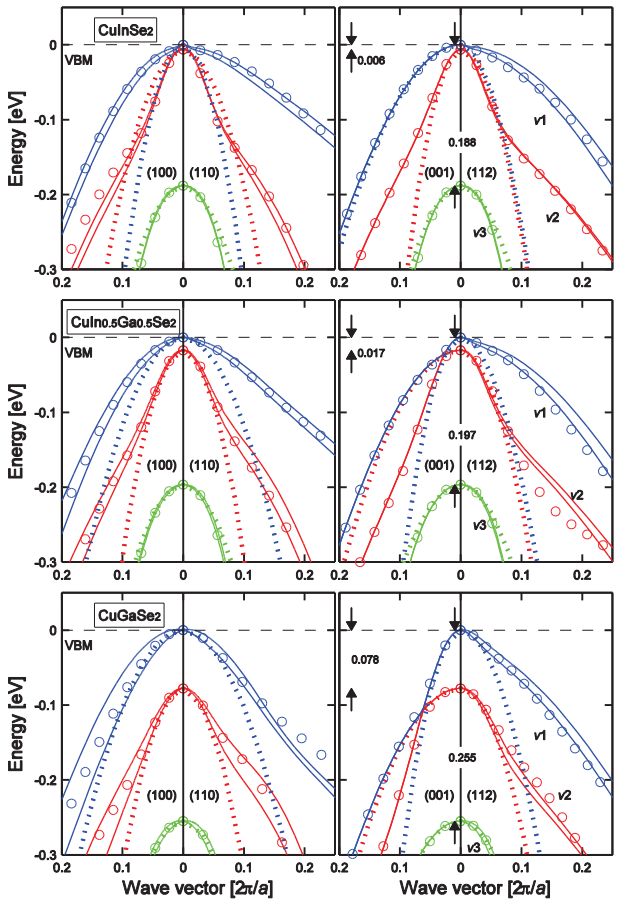
Computational methods

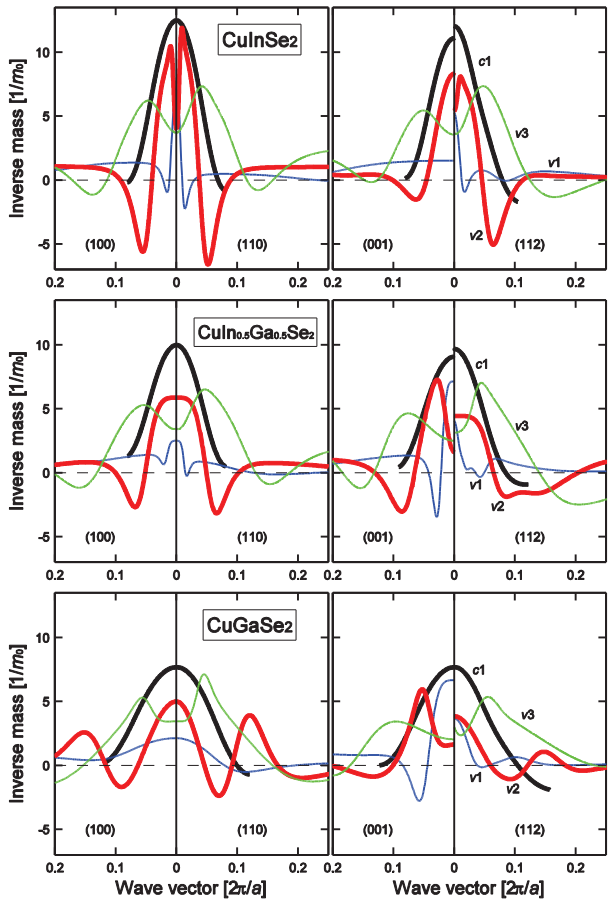
- Fundamental methods
  - Density-functional theory (DFT).
  - Kohn-Sham (KS) equation.
- Beyond DFT
  - GW approximation.
  - Heyd-Scuseria-Ernzerhof (HSE) hybrid functional.

Previous results 1: parameterization of band structure

Thin Solid Films **519**, 7503 (2011).
Journal of Applied Physics **112**, 103708 (2012).







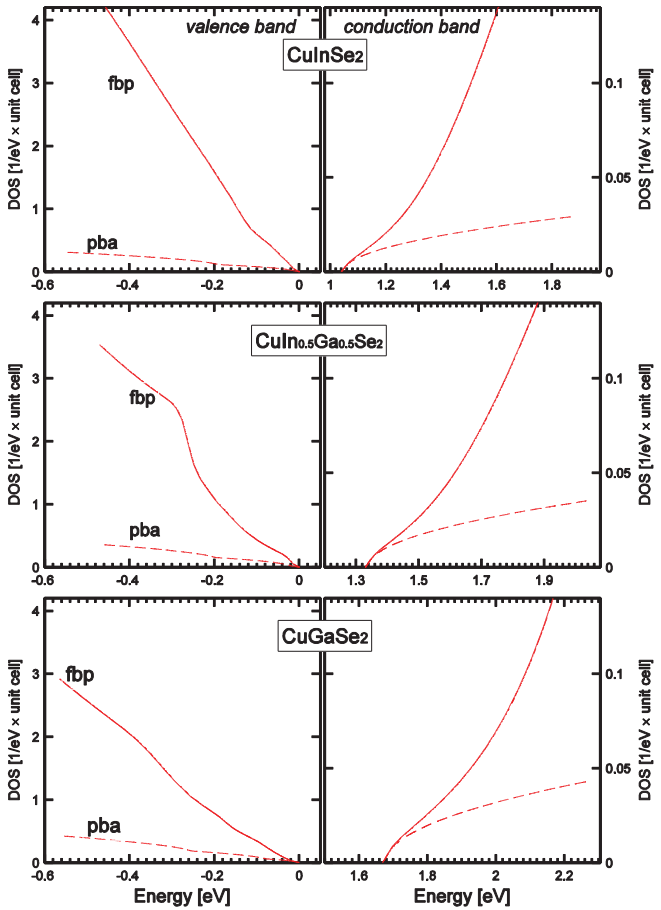
Band structure along four directions. Circles(fbp), Dotted(pba), and solid lines (calculation).

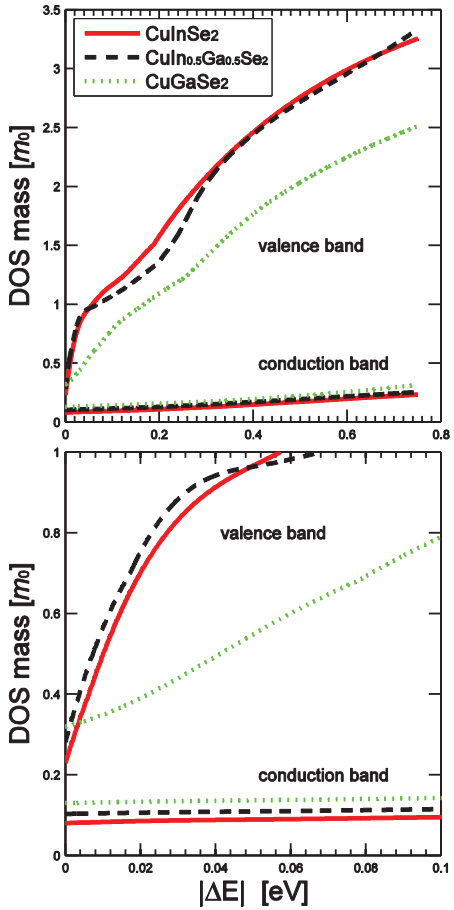
Inverse of electron and hole masses.

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).

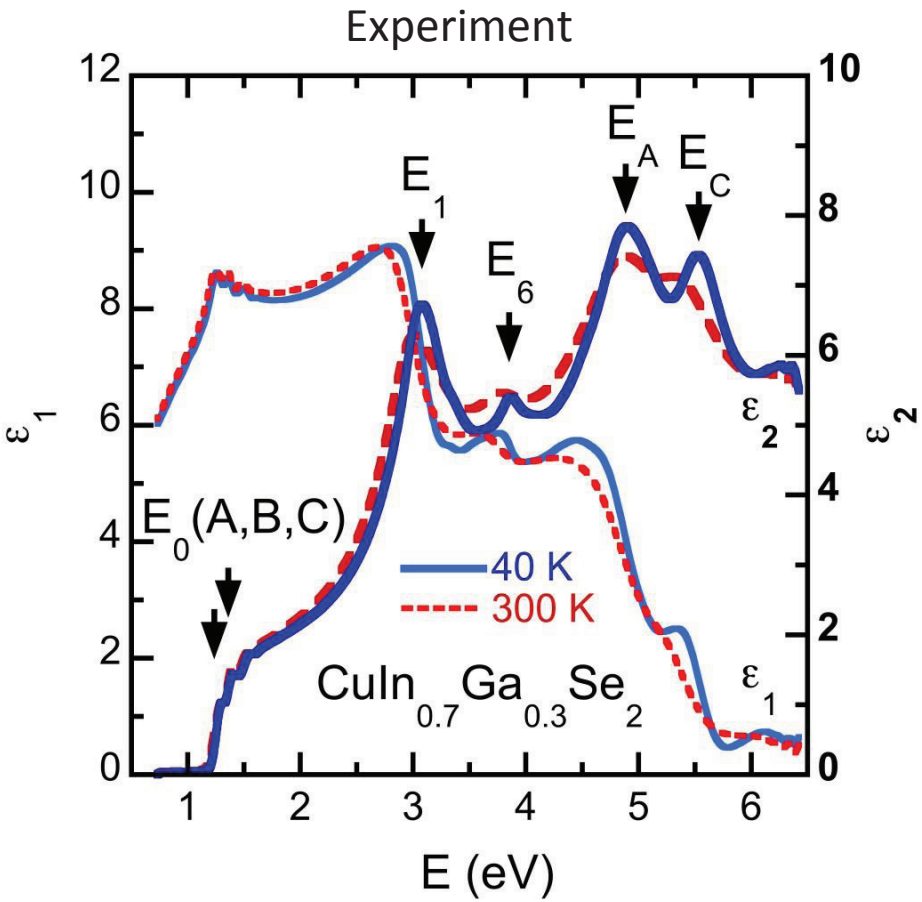




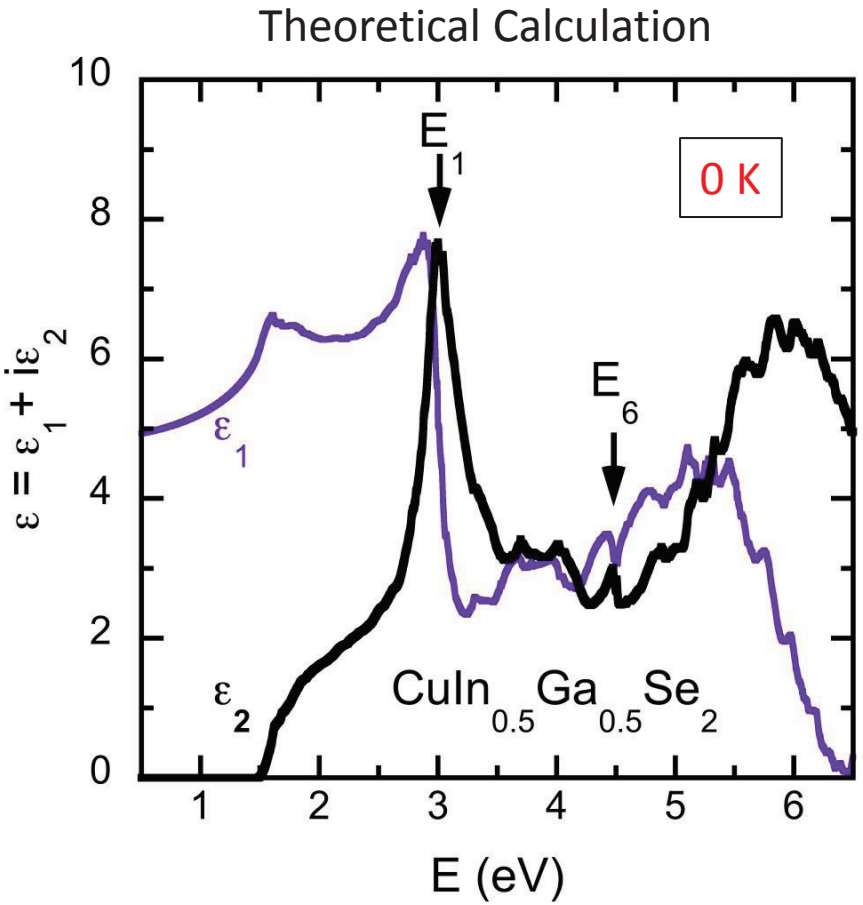
Others:
Fermi level and band-gap with temperature.
Carrier concentration in intrinsic and *p*-type Cu(In, Ga)Se_2.

Previous results 2: dielectric function for $CuIn_{0.5}Ga_{0.5}Se_2$

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



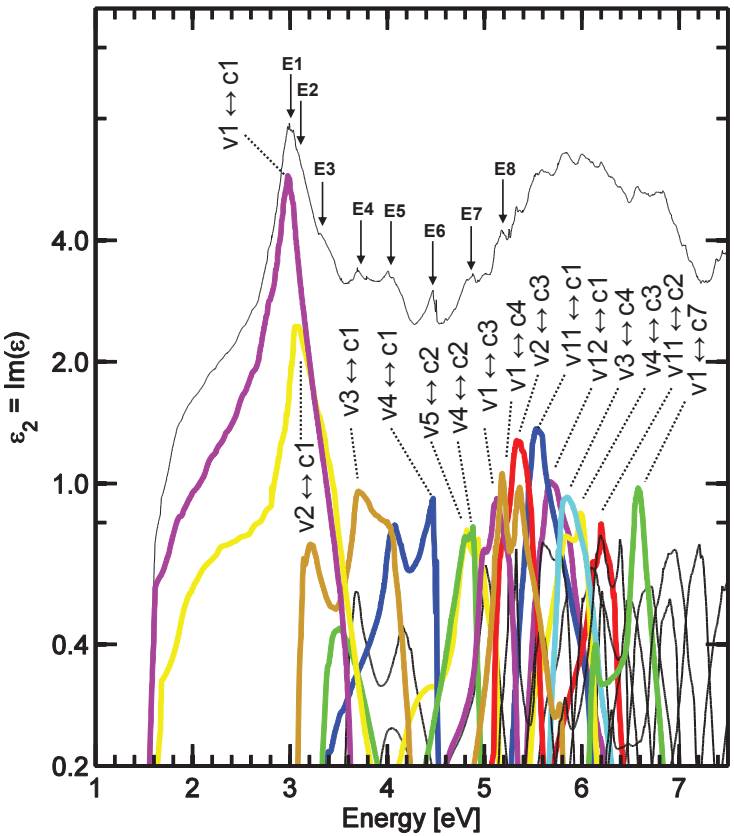
The real (ε_1) and imaginary (ε_2) part of dielectric function spectra for $CuIn_{0.7}Ga_{0.3}Se_2$ at 40 K (solid lines) and 300 K (dashed lines).



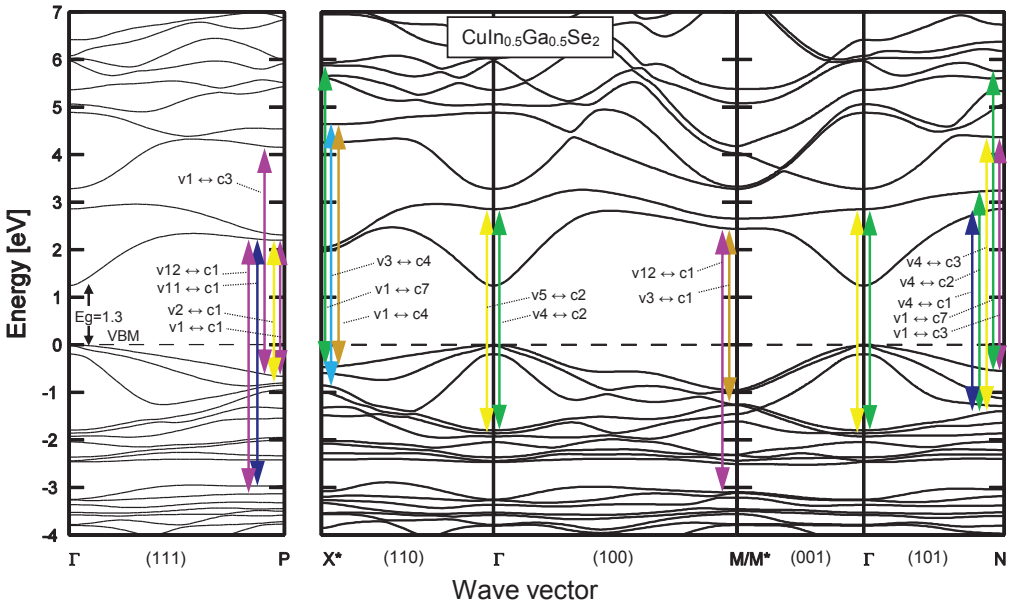
The dielectric function spectra for $CuIn_{0.7}Ga_{0.3}Se_2$ calculated at 0 K.

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

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



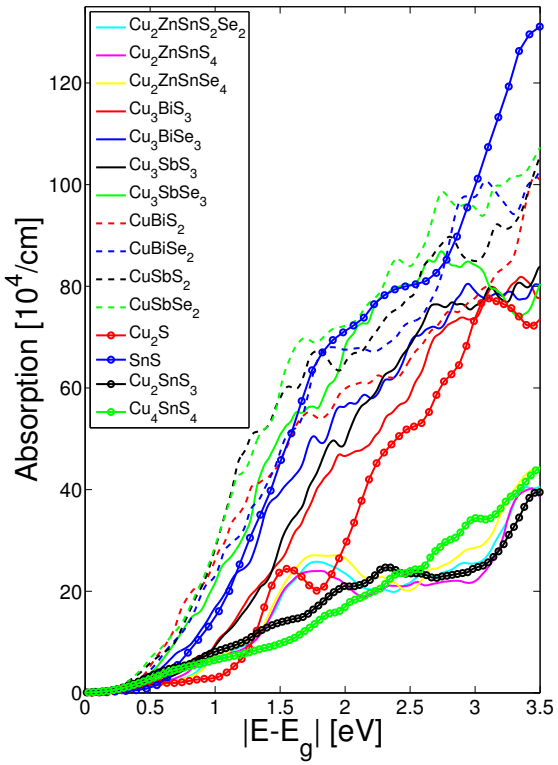
Band-to-band analysis of the contribution to the total ε_2 spectrum. The vertical axis is in the log scale.

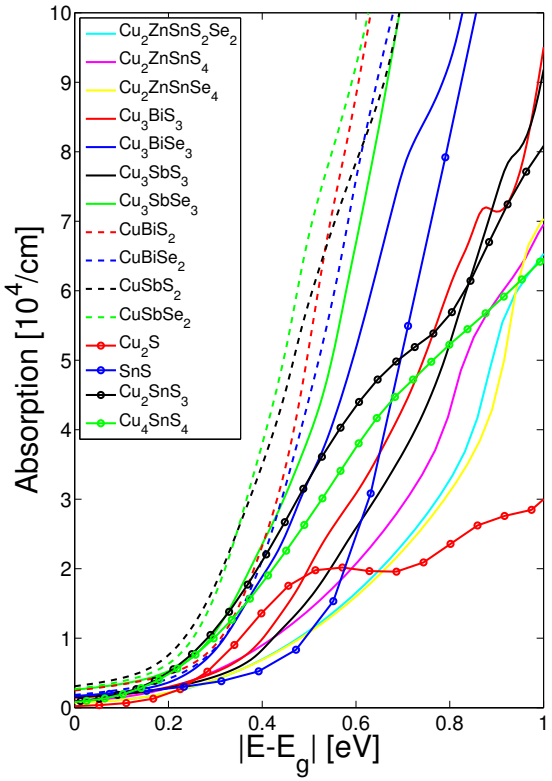


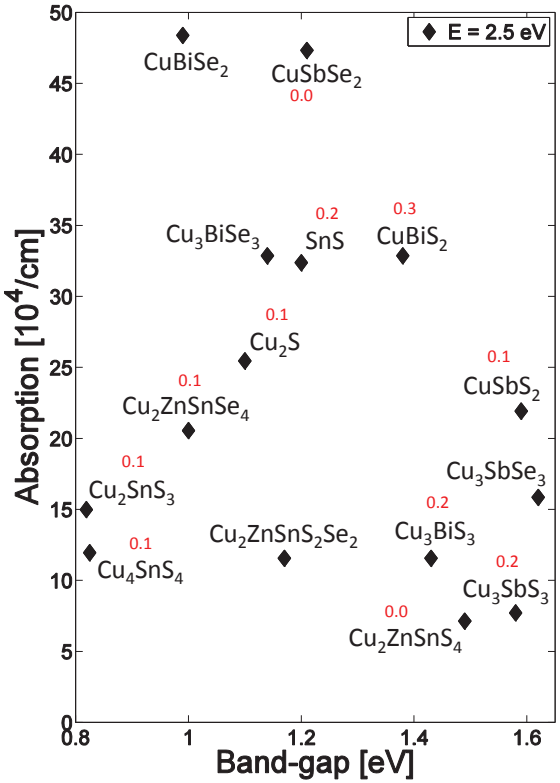
The calculated electronic band structure of $CuIn_{0.5}Ga_{0.5}Se_2$ where the CPs are identified along the main symmetry directions.

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

Submitted.



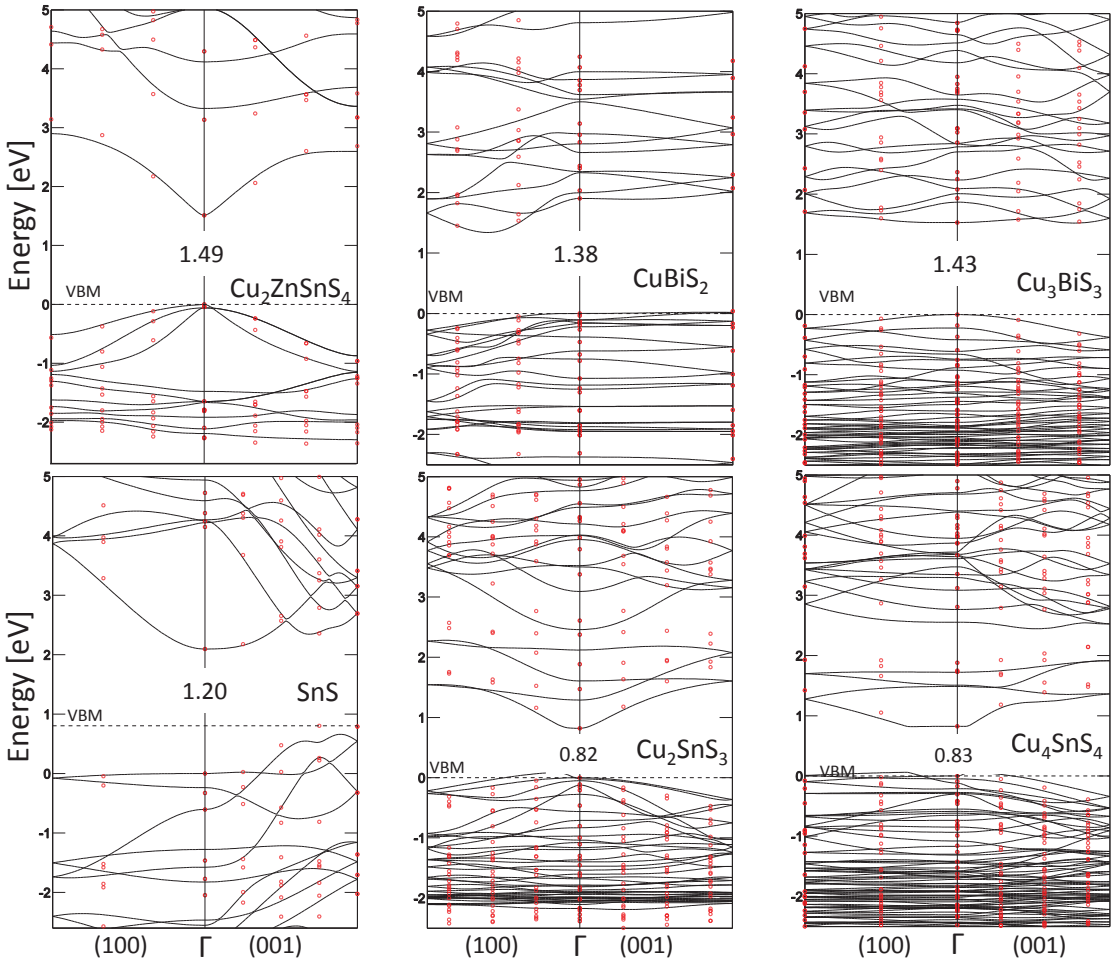




HSE: Cu_2SnS_3 and Cu_4SnS_4, GW: others. CSHIFT=0.03.

Current results: band structure in Cu-based materials

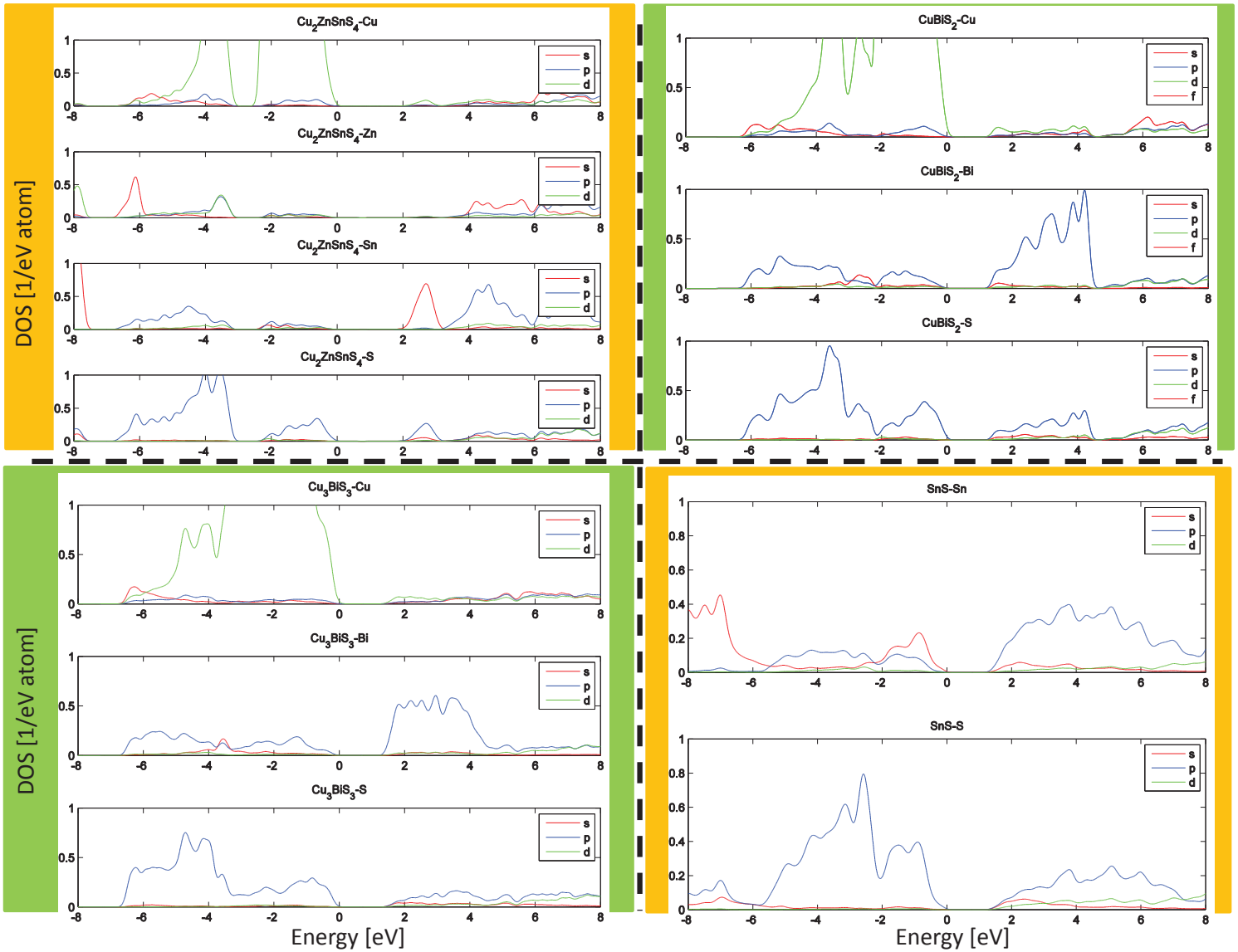
Submitted.



Circles(HSE: Cu_2SnS_3 and Cu_4SnS_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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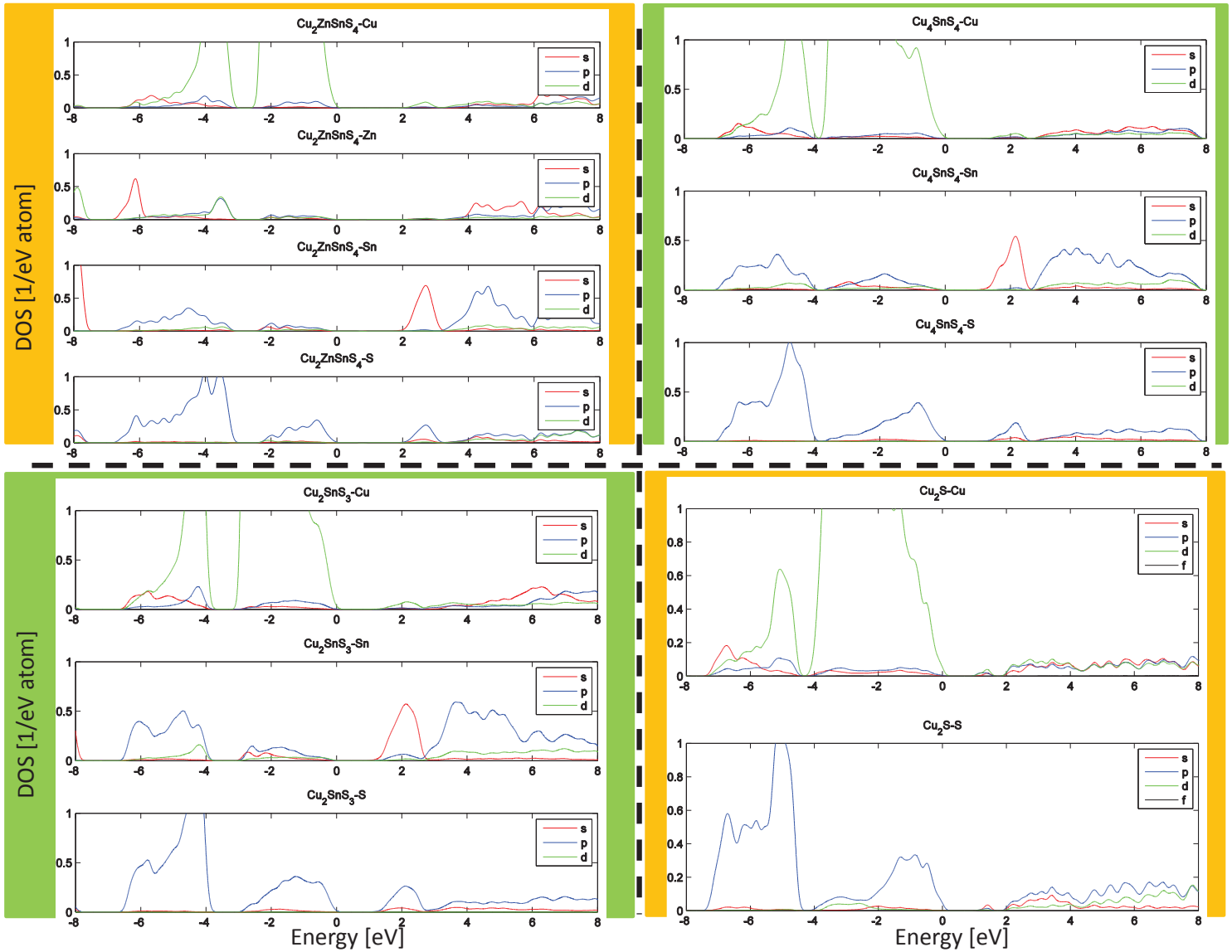


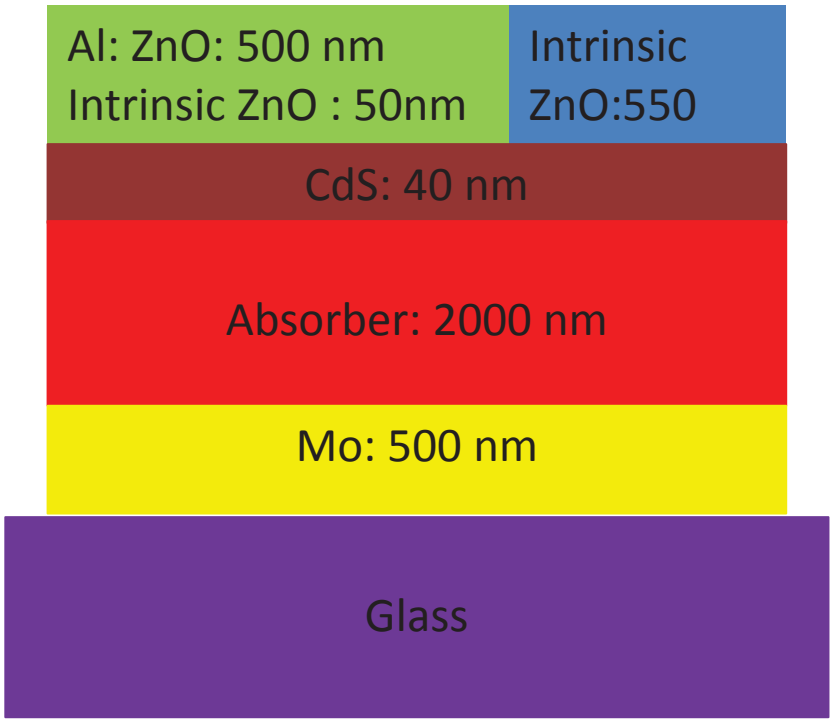
Current results: quantum efficiency in Cu-based materials solar cells

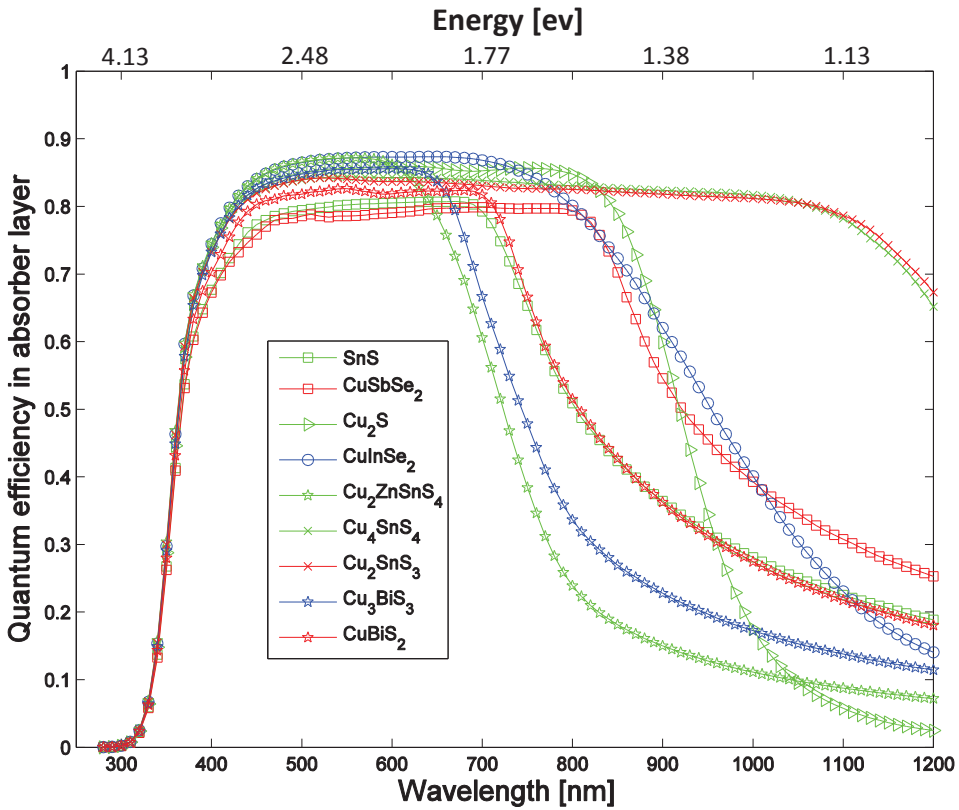
add a model figure

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

Submitted.

Simulation solar cell structure





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

Optical efficiency in each layer:

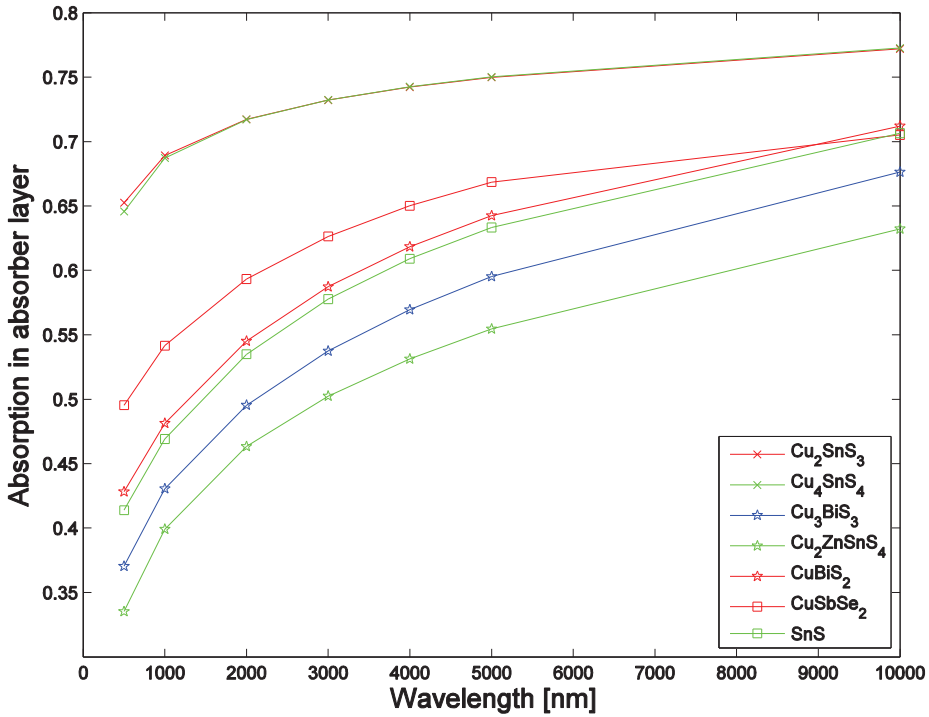
$$A(d_i) = \frac{\int I(\lambda) QE(\lambda, d_i) d\lambda}{\int I(\lambda) d\lambda} \tag{1}$$

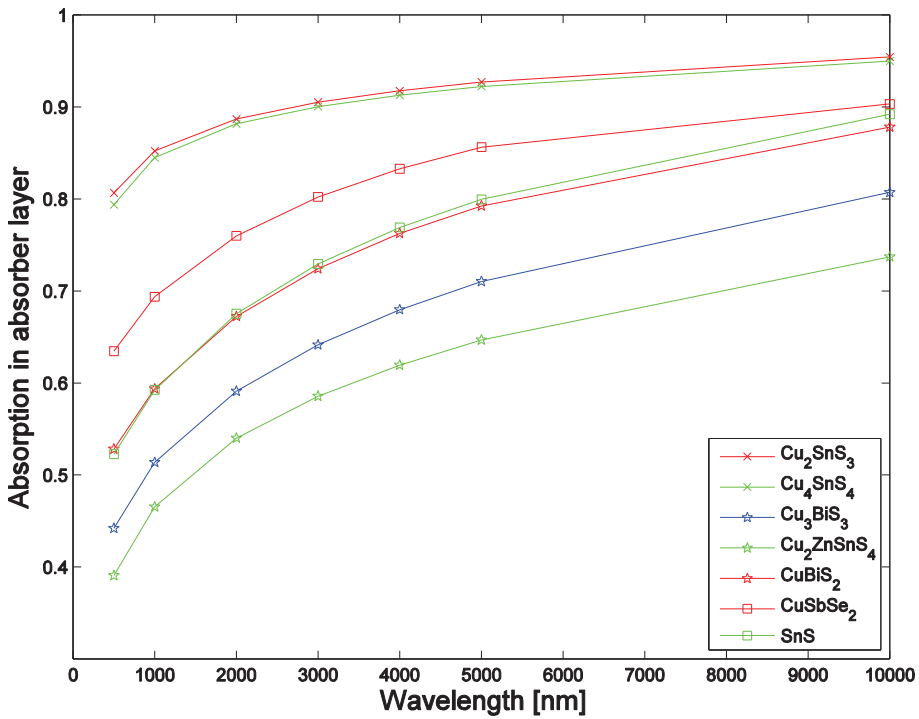
$$A'(d_i) = \frac{\int I(\lambda) QE(\lambda, d_i) d\lambda}{\int I(\lambda) QE(\lambda, d_i = \infty) d\lambda} \tag{2}$$

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

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

Submitted.





Summary

- Previous work:
  - Eergy bands are non-parabolic even very close to the Γ-point, and the effective masses are **k**-dependency.
  - The dielectric function calculated by our theoretical method shows a good agreement with the result of experiment.
- Current work:
  - ...
  - ...

Acknowledgements

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