

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 $\text{Cu}_2(\text{Zn}, \text{Sn})\text{Se}_4$.
- 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.

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

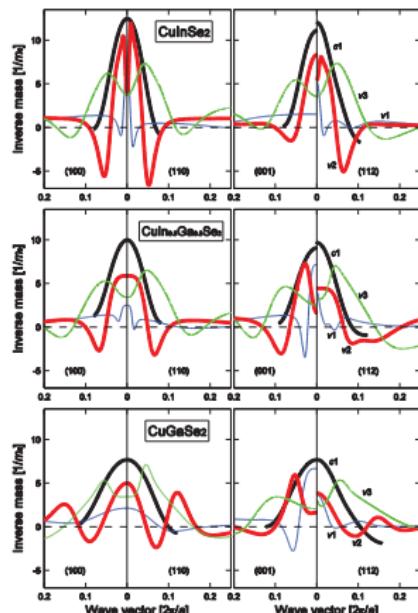
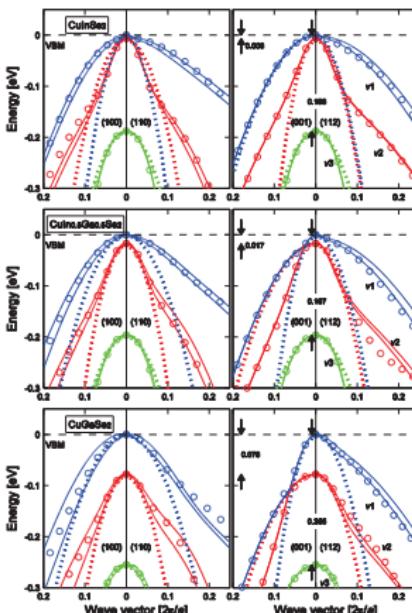
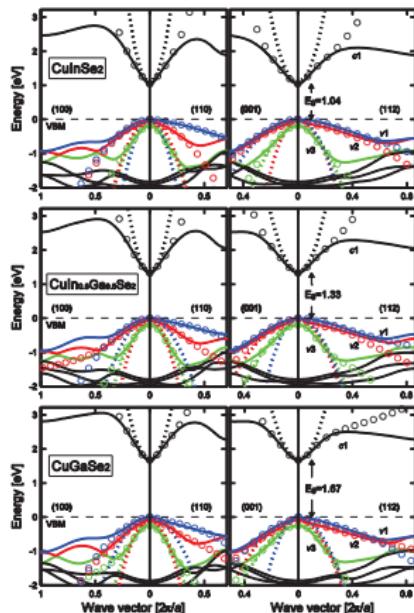
Computational methods

- 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).

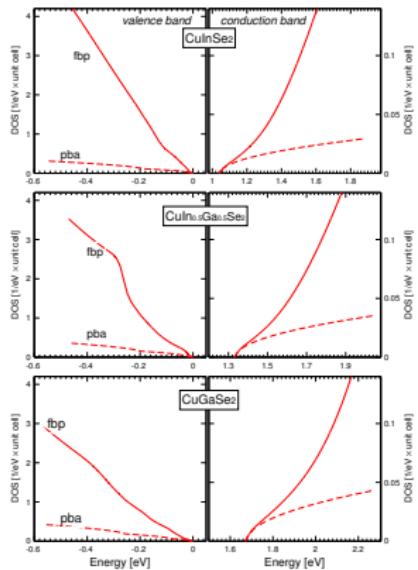
Inverse of electron and hole masses.

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

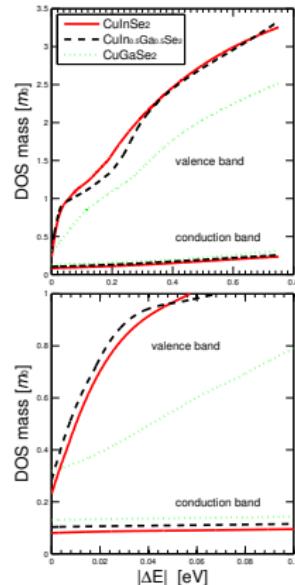
Previous results 1: density-of-states (DOS) and DOS mass

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

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



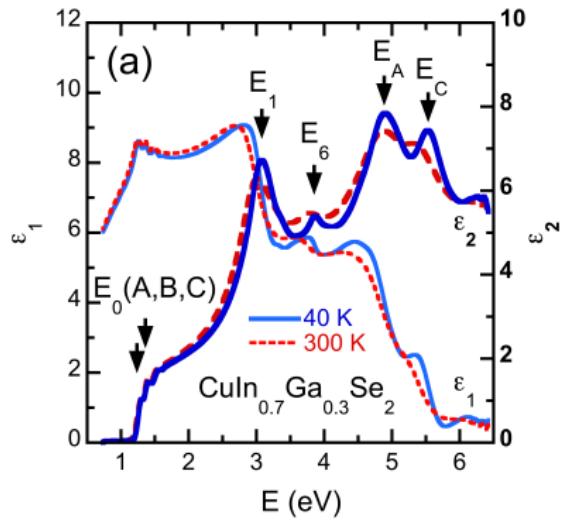
Total DOS of the VBs and CB by pba and fbp.



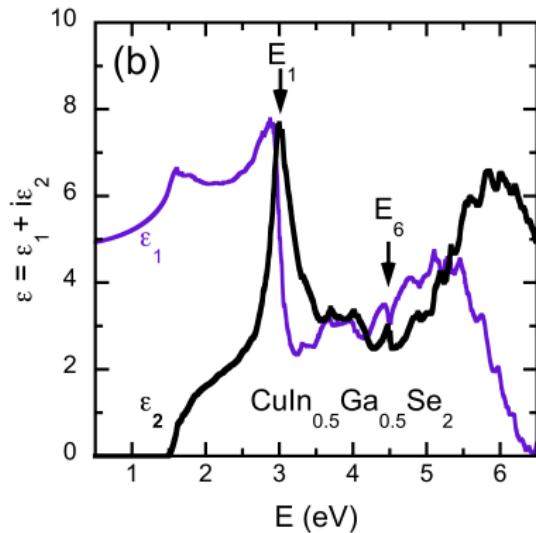
DOS mass by fbp.

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

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



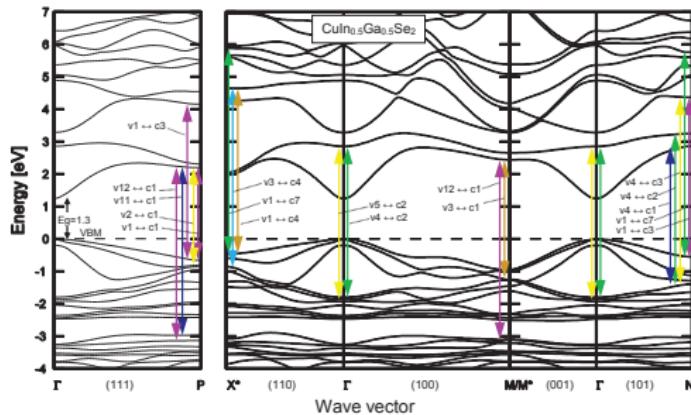
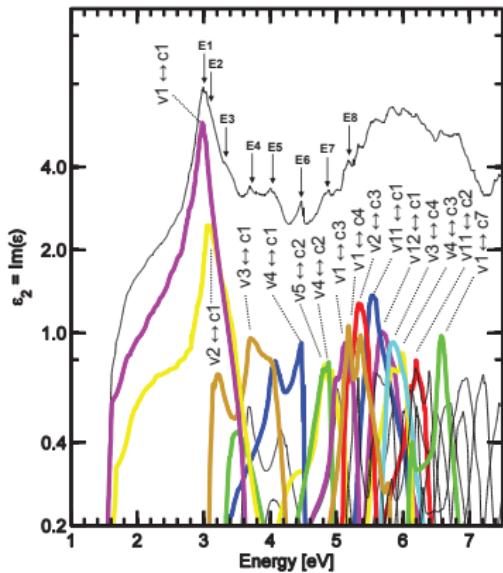
The real (ϵ_1) and imaginary (ϵ_2) part of dielectric function spectra for $\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$ at 40 K (solid line) and 300 K (dashed lines).



The dielectric function spectra for $\text{CuIn}_{0.5}\text{Ga}_{0.5}\text{Se}_2$ calculated at 0 K.

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

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

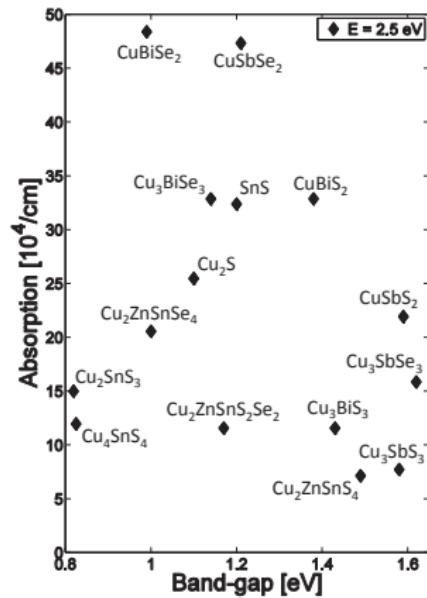
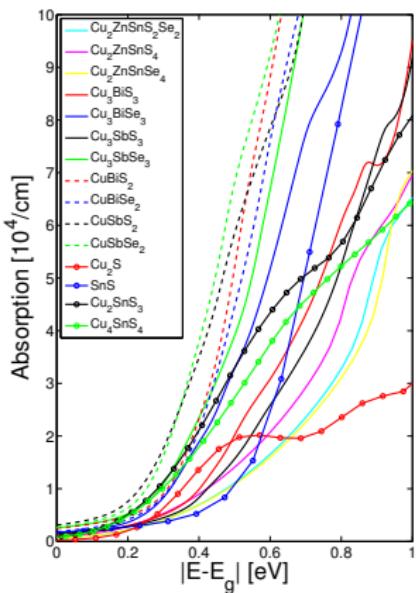
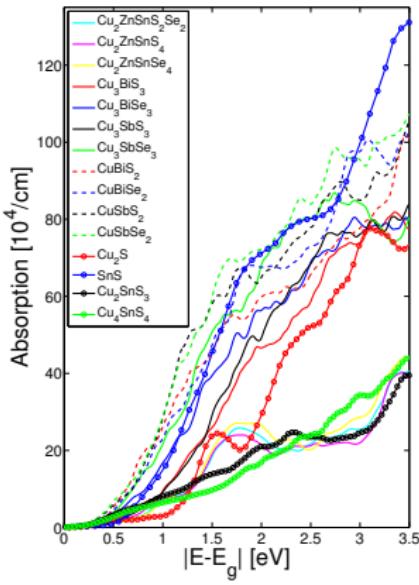


The calculated electronic band structure of $\text{CuIn}_{0.5}\text{Ga}_{0.5}\text{Se}_2$ where the CPs are identified along the main symmetry directions.

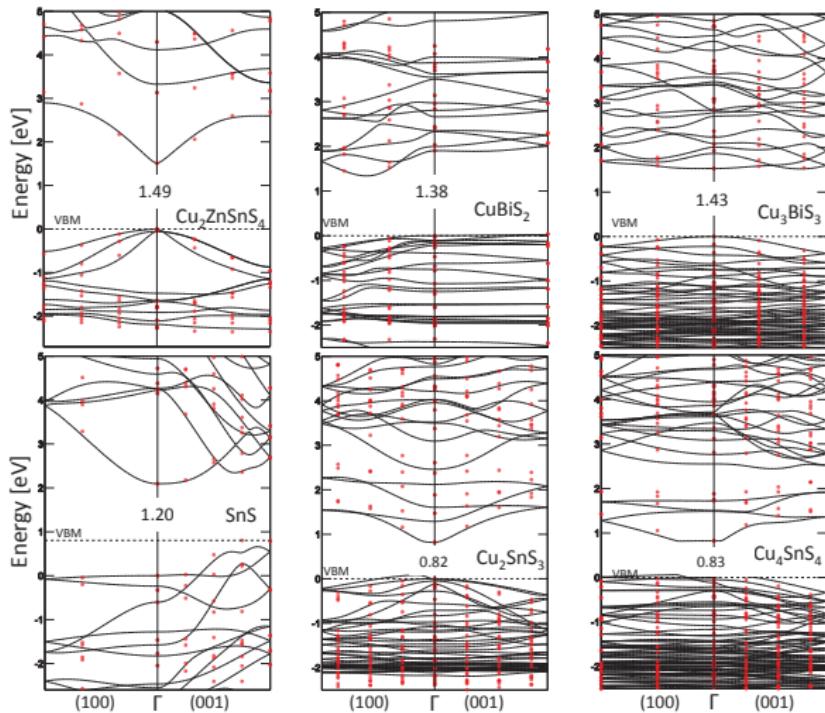
Band-to-band analysis of the contribution to the total ϵ_2 spectrum. The vertical axis is in the log scale.

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

submitted

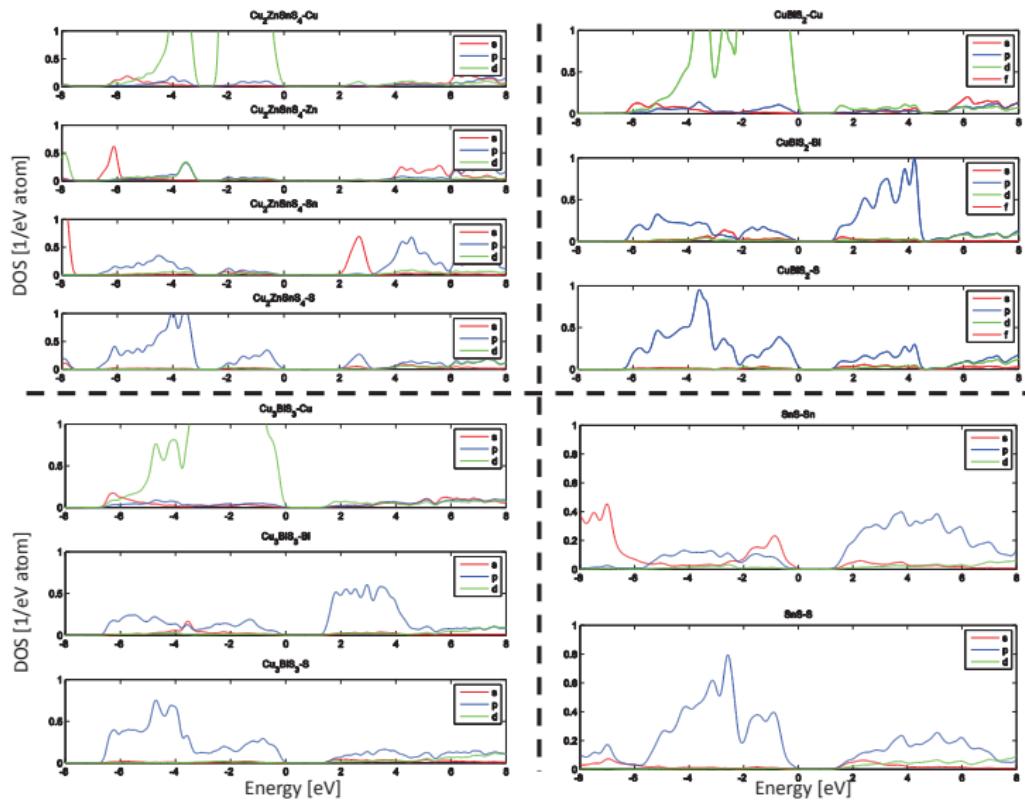


New results: band structure in Cu-based materials

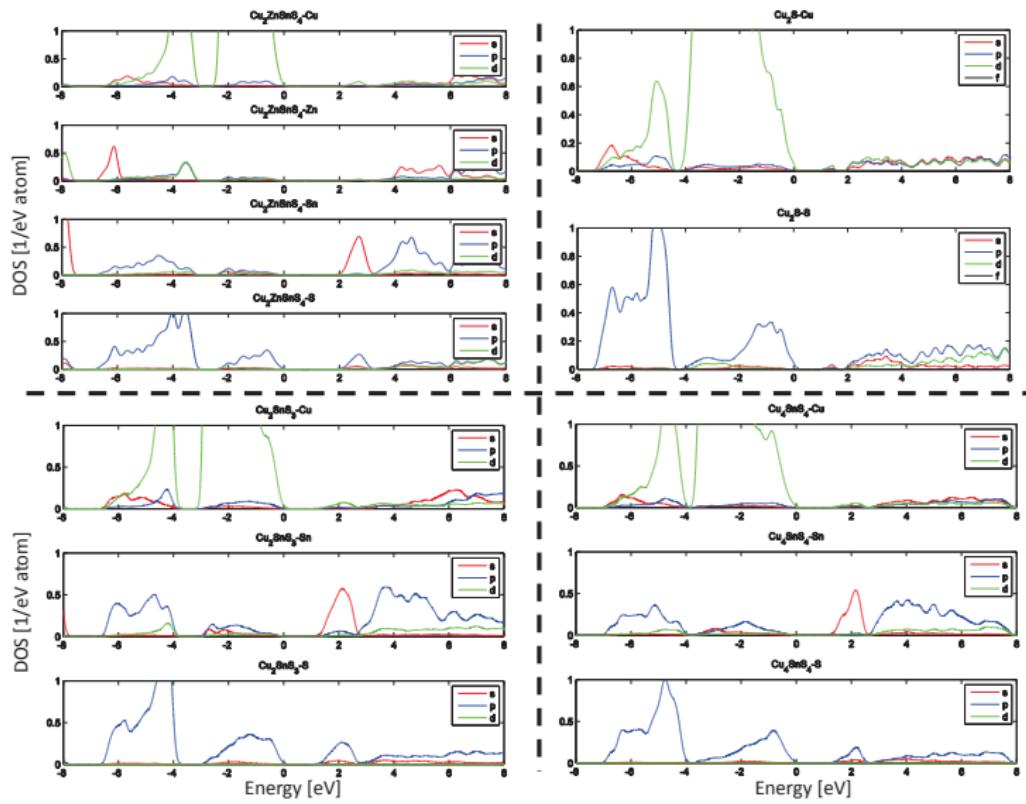


Circles(HSE: Cu_2SnS_3 and Cu_4SnS_4 , GW: others), solid lines(PBE).

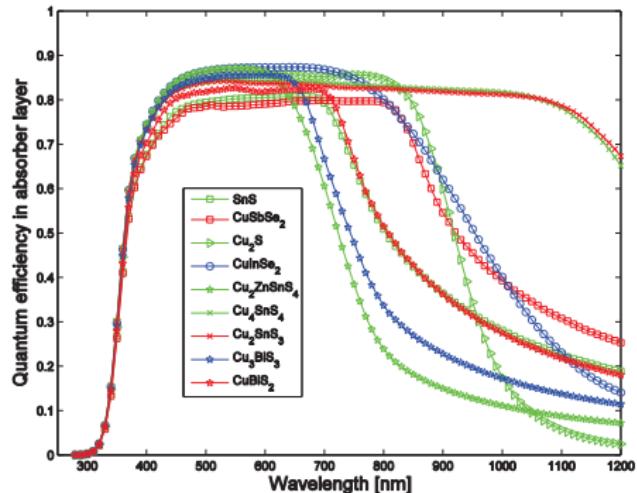
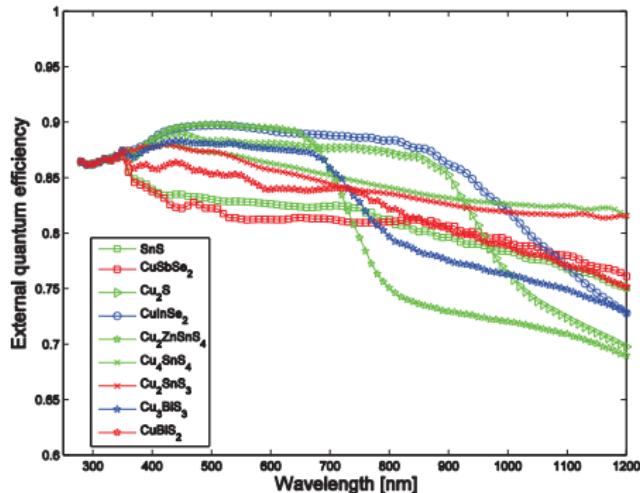
New results: density-of-states in Cu-based materials



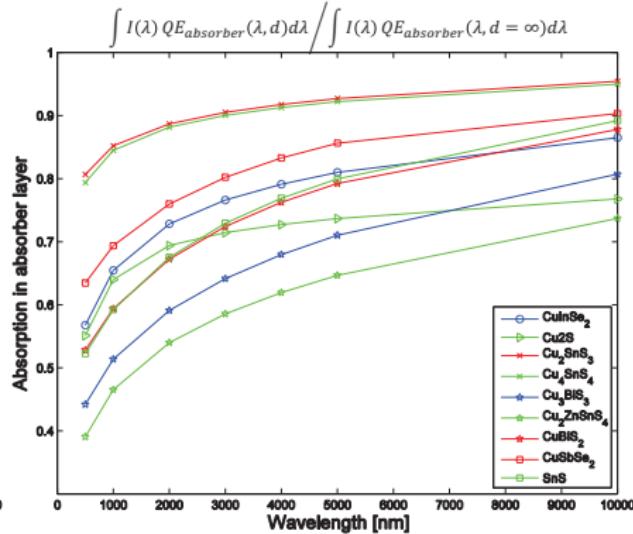
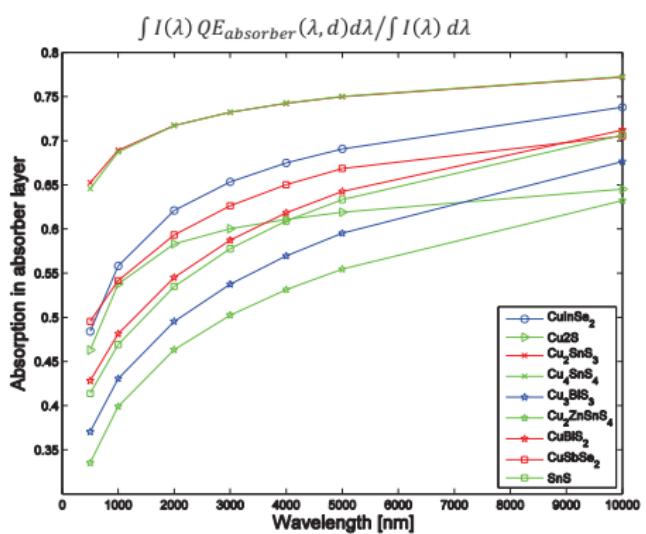
New results: density-of-states in Cu-based materials



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



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



Summary

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

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