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

PhD student: Rongzhen Chen

Supervisor: Clas Persson

Department of Materials Science and Engineering
Royal Institute of Technology, Stockholm SE-10044, Sweden

14th-May-2015

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

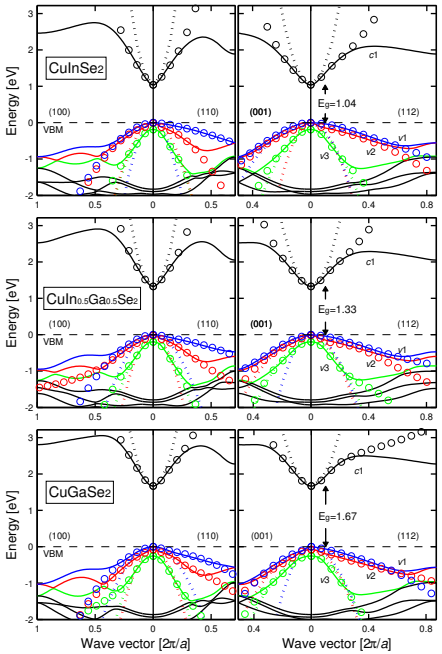
We want to understand materails Cu-based materials for solar cells.

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

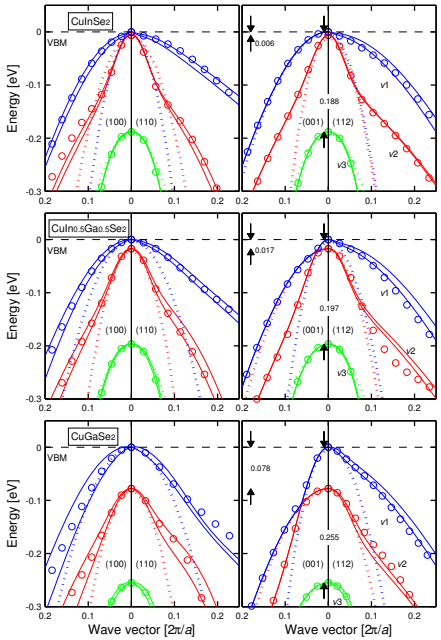
Computational methods

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

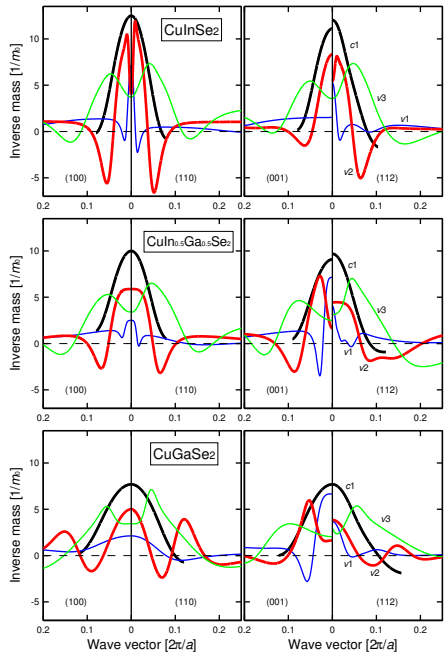
Previous results 1: parameterization of band structure



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

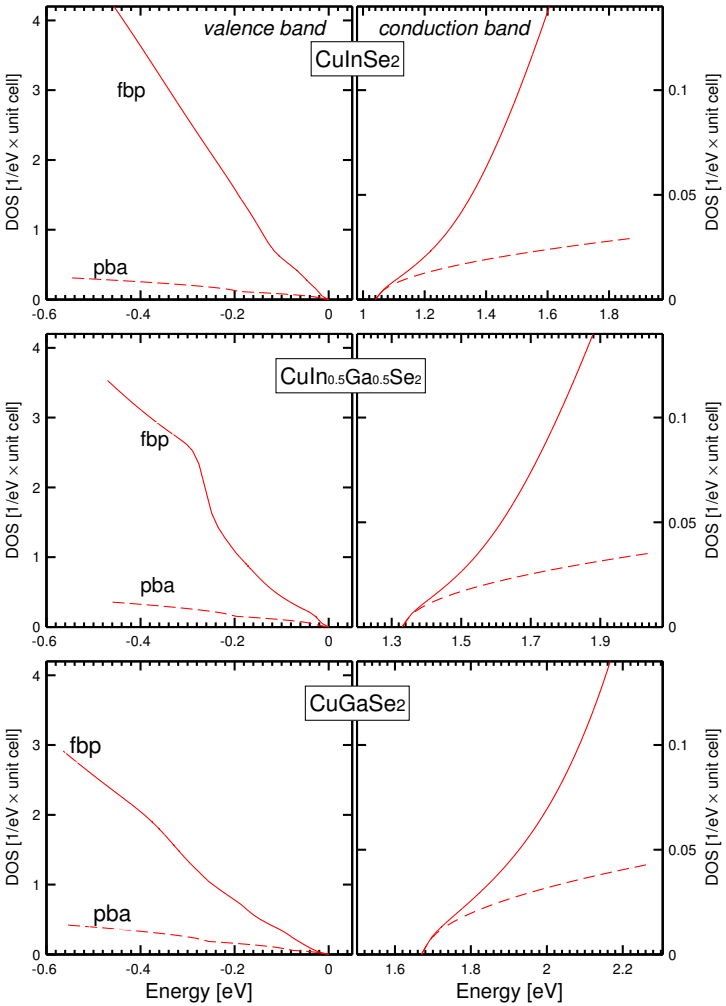


Close-up of electronic band structure.

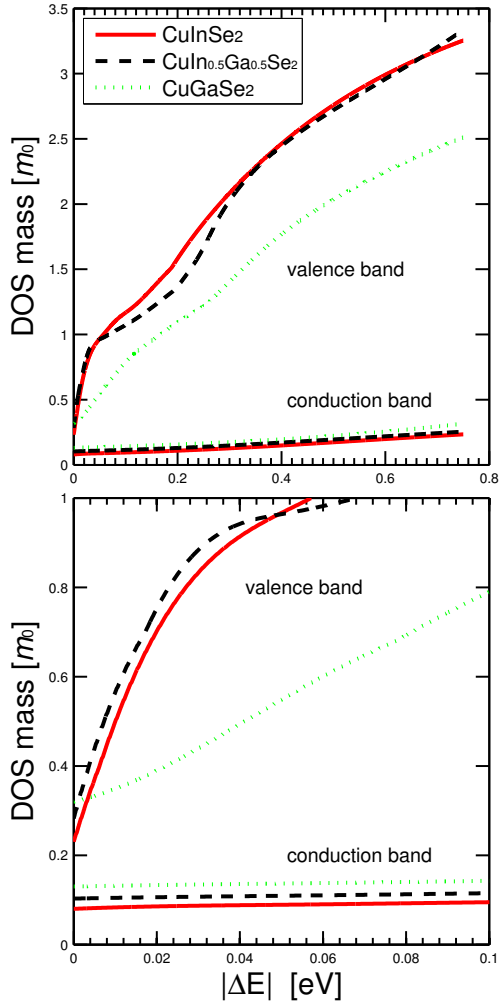


Inverse of effective electron and hole masses.

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

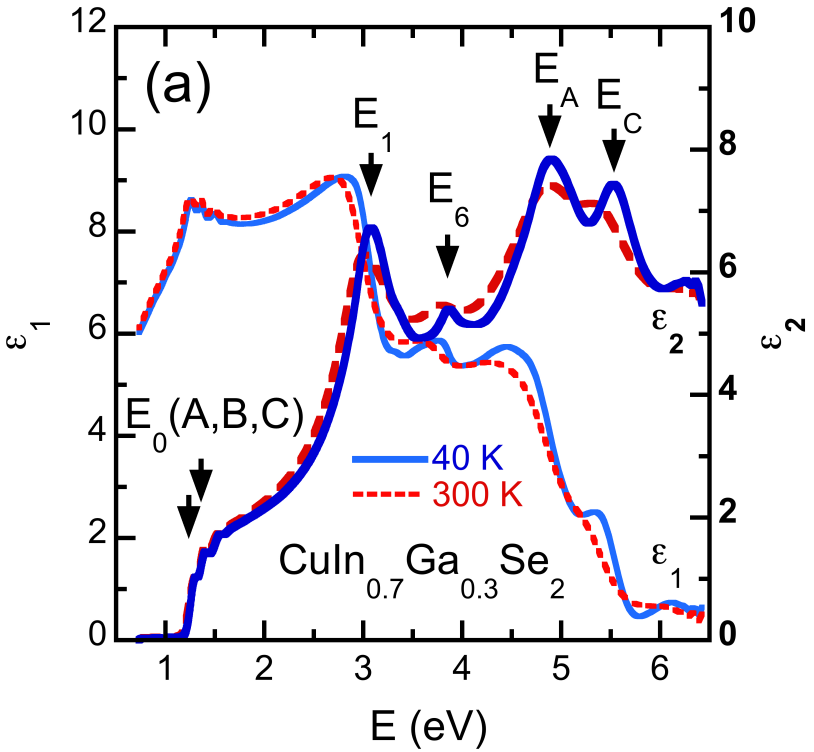


Total DOS of the VBs and CB.

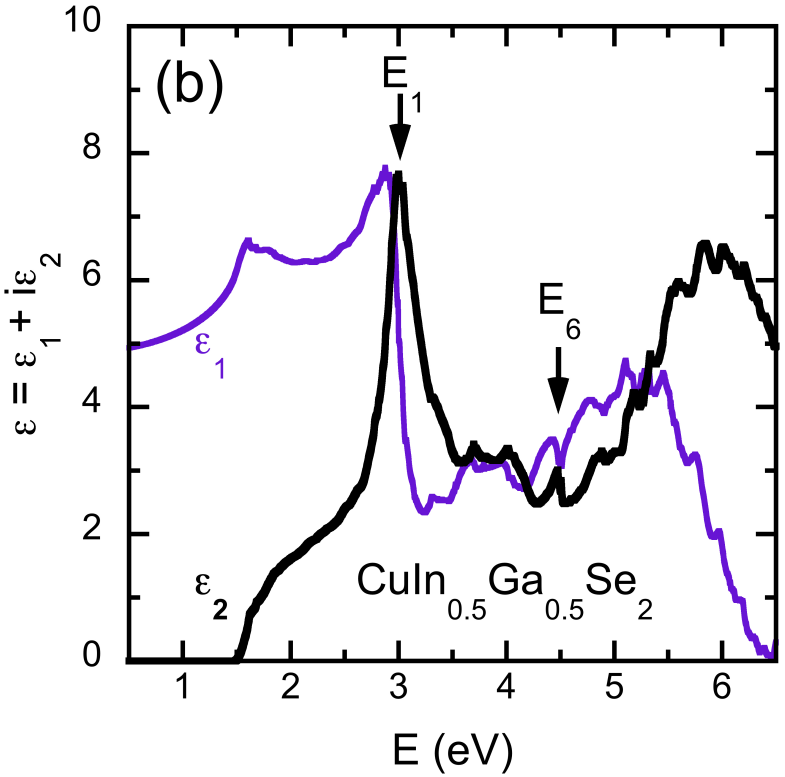


DOS mass.

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

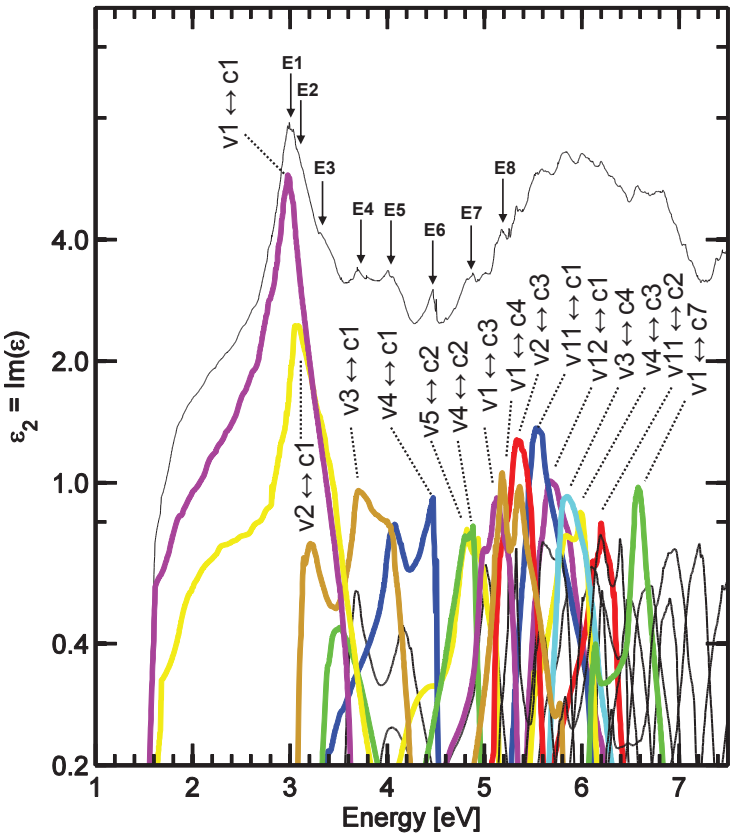


The real (ε_1) and imaginary (ε_2) part of dielectric function spectra for $CuIn_{0.7}Ga_{0.3}Se_2$ at 40 K (solid line) and 300 K (dashed lines).

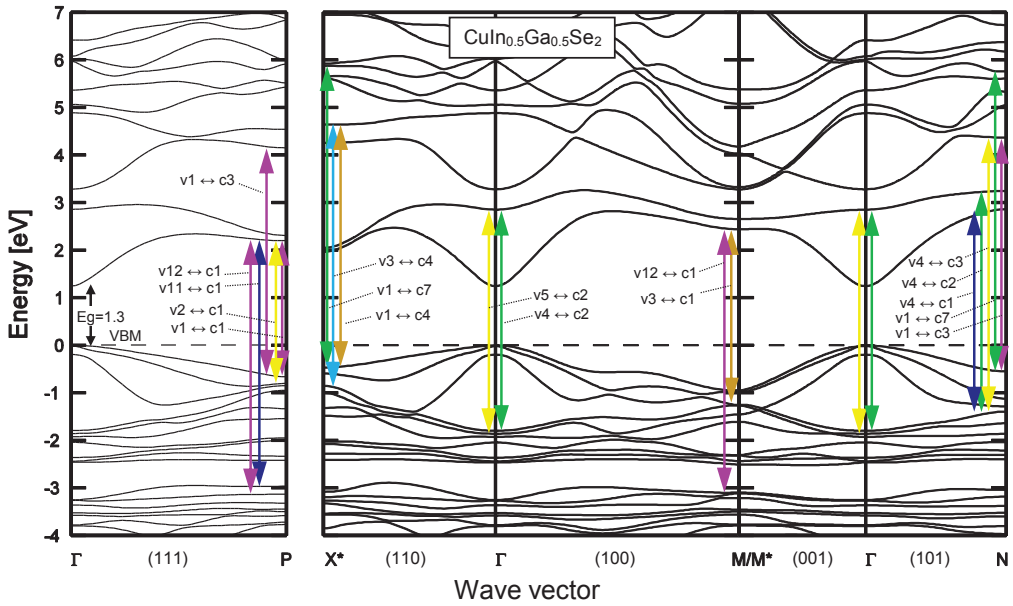


The dielectric function spectra for $CuIn_{0.5}Ga_{0.5}Se_2$ calculated by FPLAPW method at 0 K.

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



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.

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

New results: band structure and density-of-states in Cu-based materials

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

1 Summary

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.
- 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.

Acknowledgements

- I would like to express my sincere appreciation to my supervisor Prof. Clas Persson for his academic encouragement and professional guidance.
- I would like to thank all the group colleagues in Stockholm and Oslo for helpful research discussions and chatting. I would like to thank all other people at the Department of Material Sciences and Engineering at KTH for creating a nice working atmosphere.
- The China Scholarship Council, the Swedish Energy Agency, the Swedish Research Council, Stiftelsen Axel Hultgrens fond, Olle Erikssons stiftelse for materialteknik, and KTH Computational Science and Engineering Centre (KCSE) are acknowledged for financial support.