Exploring the Electronic and Optical Properties of $Cu(In,Ga)Se_2$

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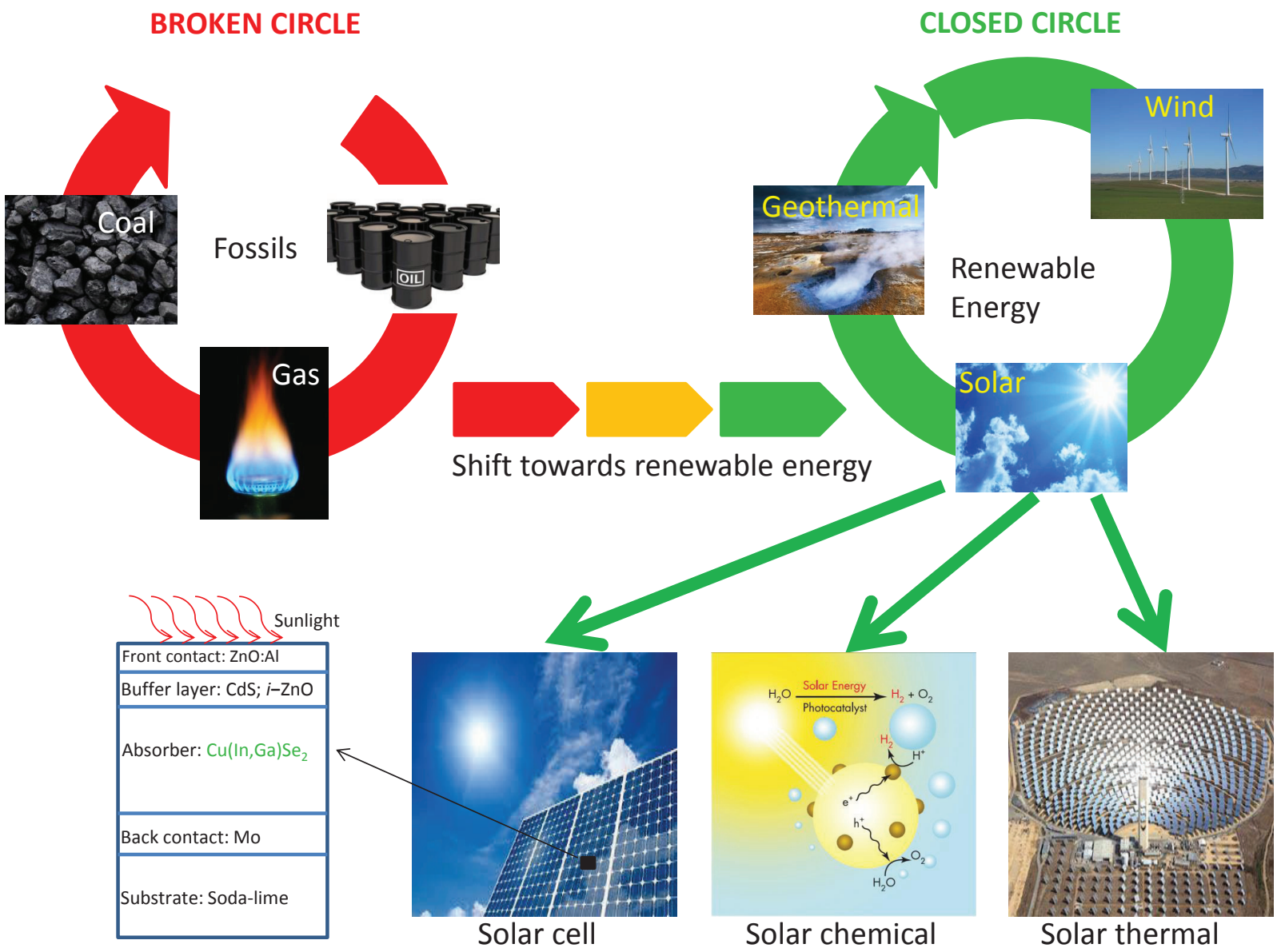
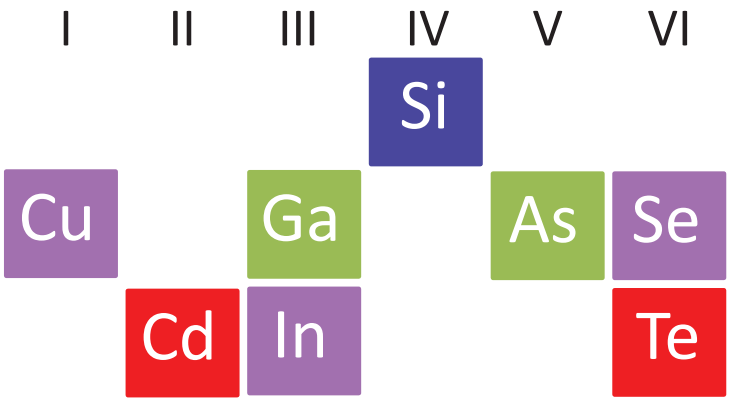
Mar-06-2015

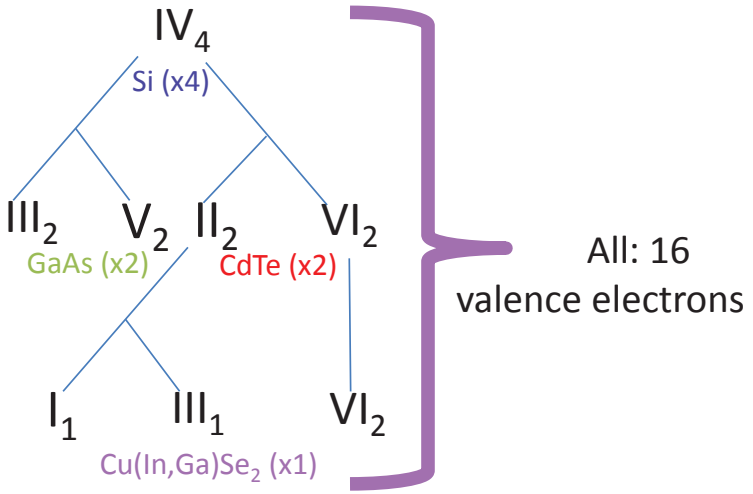
Outline

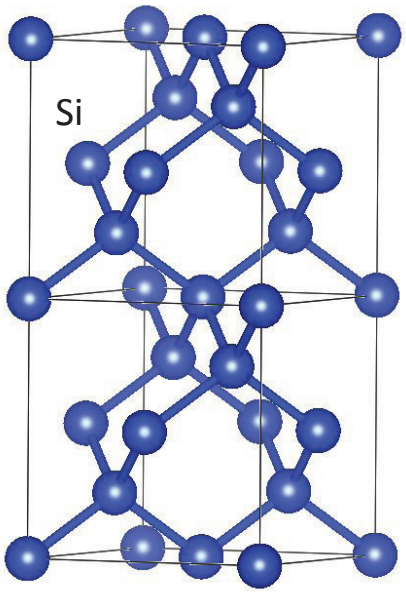
What material am I working on?



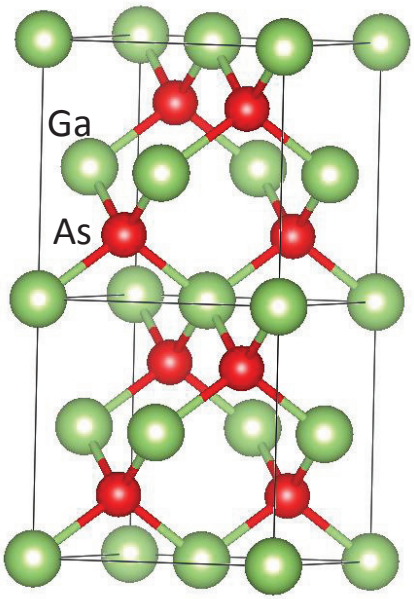
Why $Cu(In,Ga)Se_2$?



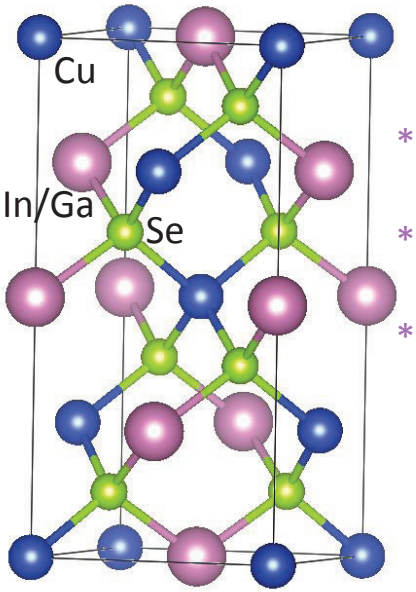




Diamond: Si



Zinc blende: GaAs



Chalcopyrite: $Cu(In,Ga)Se_2$

* Direct and tunable band-gap
* High optical coefficient
* Efficiency 23.3% in lab

Which aspects of $Cu(In,Ga)Se_2$ have I been working on?

- Energy bands of $CuInSe_2$, $CuIn_{0.5}Ga_{0.5}Se_2$, and $CuGaSe_2$ are calculated by means of theoretical calculations. Parameterization of the lowest conduction (CB) and the three uppermost valence bands (VBs) are expored based on the calculated energy bands. Carrier concentration, Fermi level, and many other aspects are analyzed based on the parameterization.
- Optical properties of $CuIn_{0.5}Ga_{0.5}Se_2$ are explored by means of theoretical calculations.

Motivation for the parameterization

Motivation for calculation of optical properties

1. Background
2. Motivation
3. *Ab initio* alloy theory
   - Density functional theory

Density functional theory (DFT)

- the ground state of an interacting electron system is uniquely described by an energy functional of the electron density,
- the true ground state electron density minimizes the energy functional and the minimum gives the total energy.

$$[-\nabla^2 + V_{eff}(\mathbf{r})]\psi_i^k = \epsilon_i^k \psi_i^k, \tag{1}$$

$$V_{eff}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r}), \tag{2}$$

$$\mu_{xc} \equiv \delta E_{xc}[n(\mathbf{r})]/\delta n(\mathbf{r}). \tag{3}$$

$$E_{tot} = T_s + \int v_{ext}(\mathbf{r}) n(\mathbf{r}) d^3r + \frac{1}{2} \int \int \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' + E_{xc} \tag{4}$$


KTH
VETENSKAP
OCH KONST

Thank you for your attention!

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