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

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# Outline

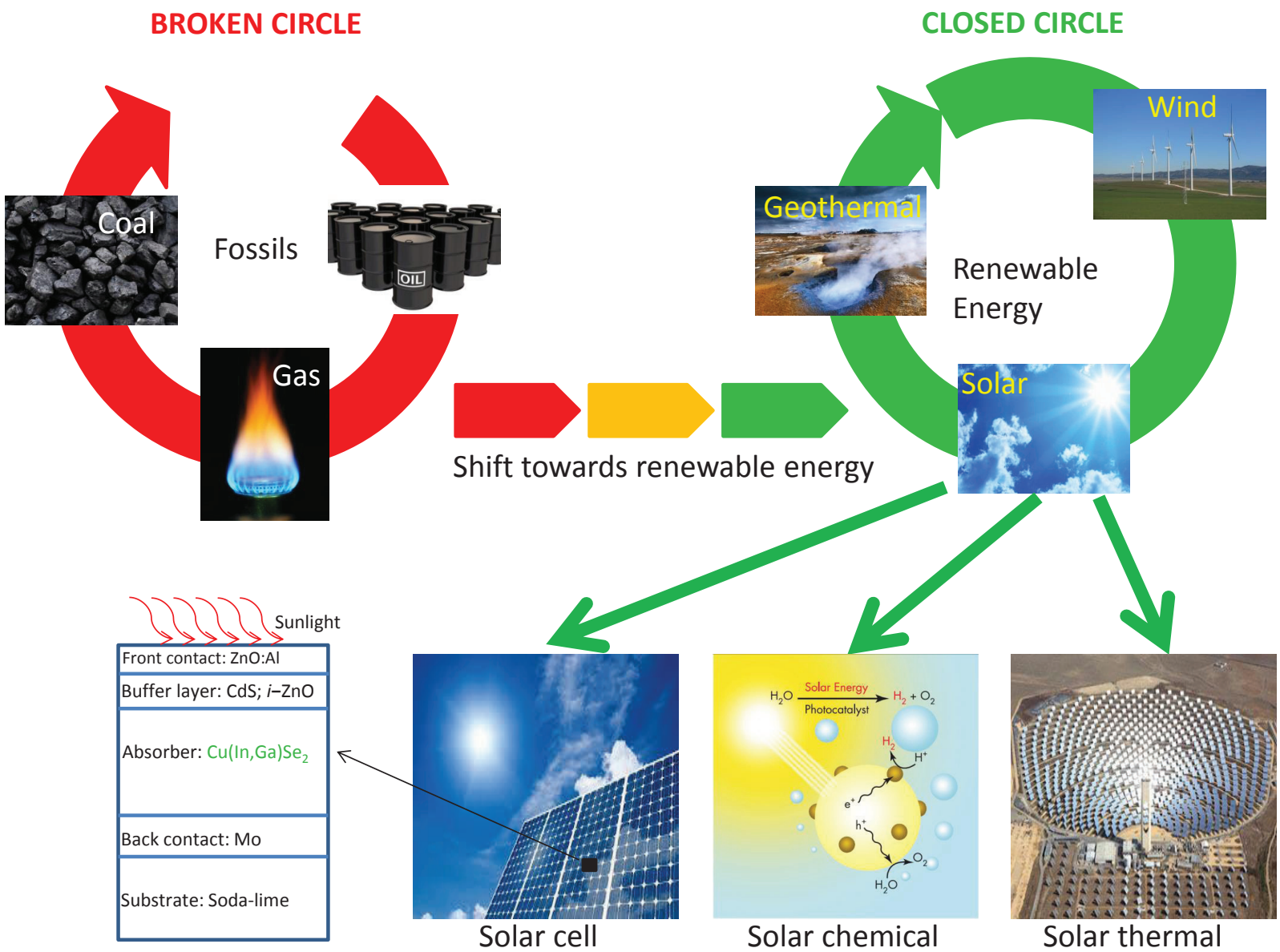

1. Background

2. *Ab initio* alloy theory
   - Density functional theory

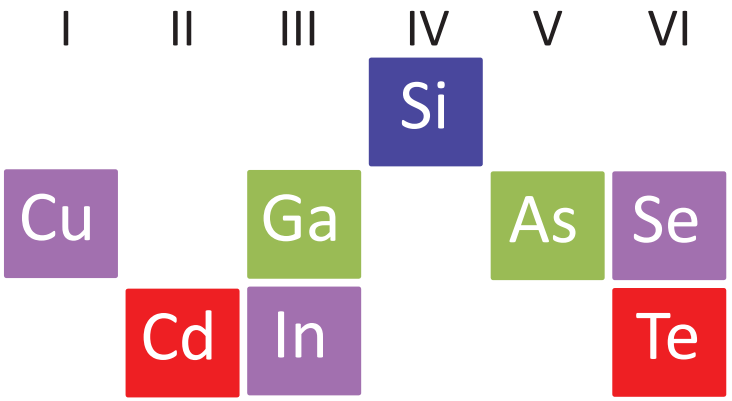
1 Background

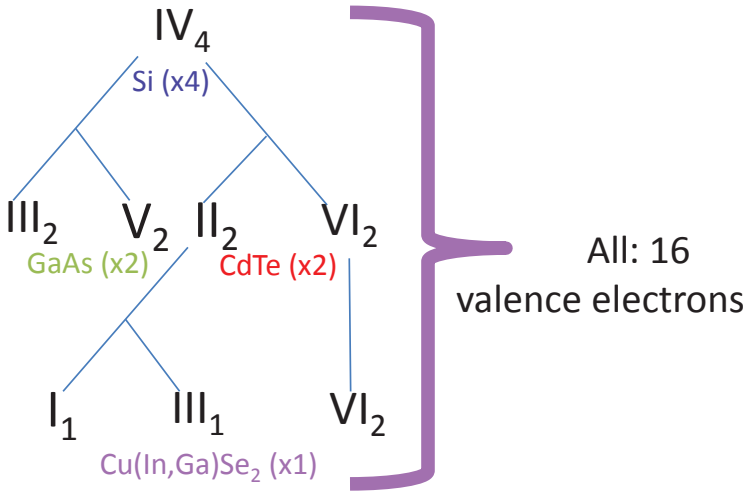
2 *Ab initio* alloy theory

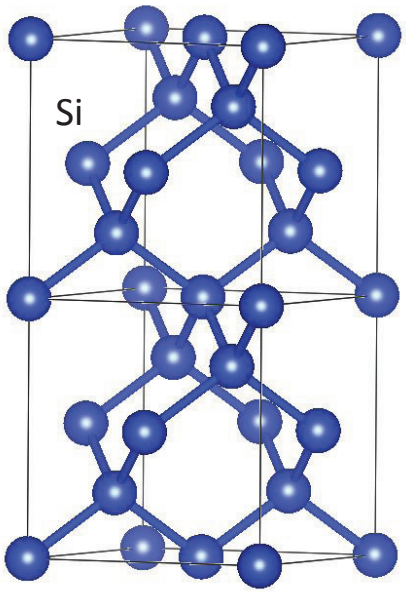
# What material am I working on?



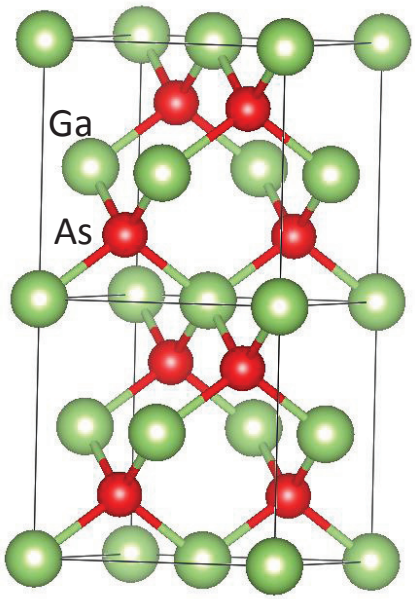
# Why $Cu(In,Ga)Se_2$?



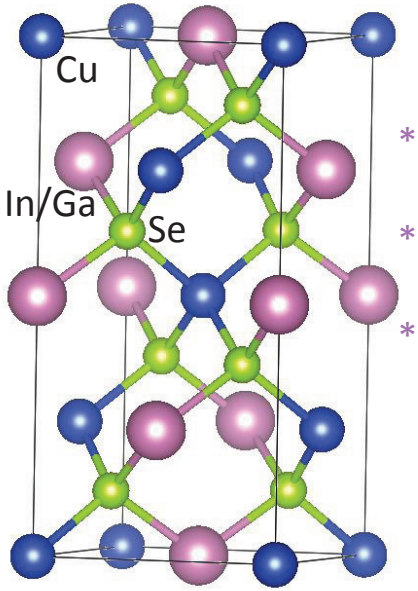




**Diamond: Si**




**Zinc blende: GaAs**




**Chalcopyrite: $Cu(In,Ga)Se_2$**

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

1 Background

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# 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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