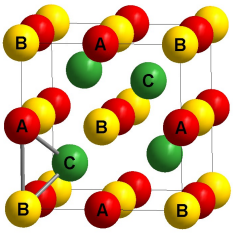
10. January 2017 at 2:00 pm, Galilei room

Simulation of Semiconductor Materials for Solar Cells within the projects PINET and comCIGS

by Maria Tissen

All those interested are warmly invited to this presentation, which is given within the scope of a application procedure for a PhD position in the TWIST group.

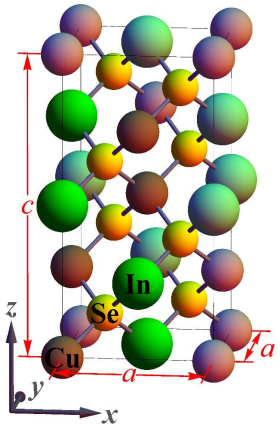
I made my Bachelor and Master theses within the cooperative projects PINET and comCIGS, which concentrated on finding alternative semiconductor materials for PIN solar cells and optimization of the efficiency of CIGS thin film solar cells.
A promising strategy was the use of Ab intio calculations. This means here, structural and electronic properties of semiconductor materials were derived from first principles like electrostatic laws and quantum mechanics. A short introduction will be given, how to do this beginning from the Schrödinger equation and taking into account some simplifications and approximations.



Cell of a semi-Heusler compound

The calculations in the Bachelor thesis concentrated on selected groups of semi-Heusler structures and its further electronic properties. This work followed the one of Thomas Gruhn, who investigated semi-Heusler compounds with eight valence electrons. The total number of valence electrons of the constituents in my work was 18, which is the next possible way to reach the noble gas configuration. Some examples of electronic properties, like the density distribution of the valence electrons, will be shown.

The calculation in the Bachelor thesis used a primitive cell of three atoms, whereas the Master thesis took aim on Monte Carlo simulation on nanometer scale. Thus 10000 and more atoms where taken into account to get the thermodynamic properties of the pseudo-binary structure $Cu(In,Ga)Se_2$.
The energy difference after every simulation step was needed. Cluster expansion, which is based on the Ising model, is a good method to lead back the calculation of the energy to atomic scale. The different atomic size of Indium and Gallium leads to tension in the structure. This Constituent strain has also to be taken into account. The main part of my work was to derive a model for the tension in structures with tetragonal symmetry. Only models for cubic and hcp structures were known from the literature.



Cell of the Chalcopyrite compound $CuInSe_2$