Parameterization of Energy Bands and Optical Properties in Semiconductor $CuIn_{1-x}Ga_xSe_2$

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October 23, 2013

According to the statistical review of world energy on 2012.

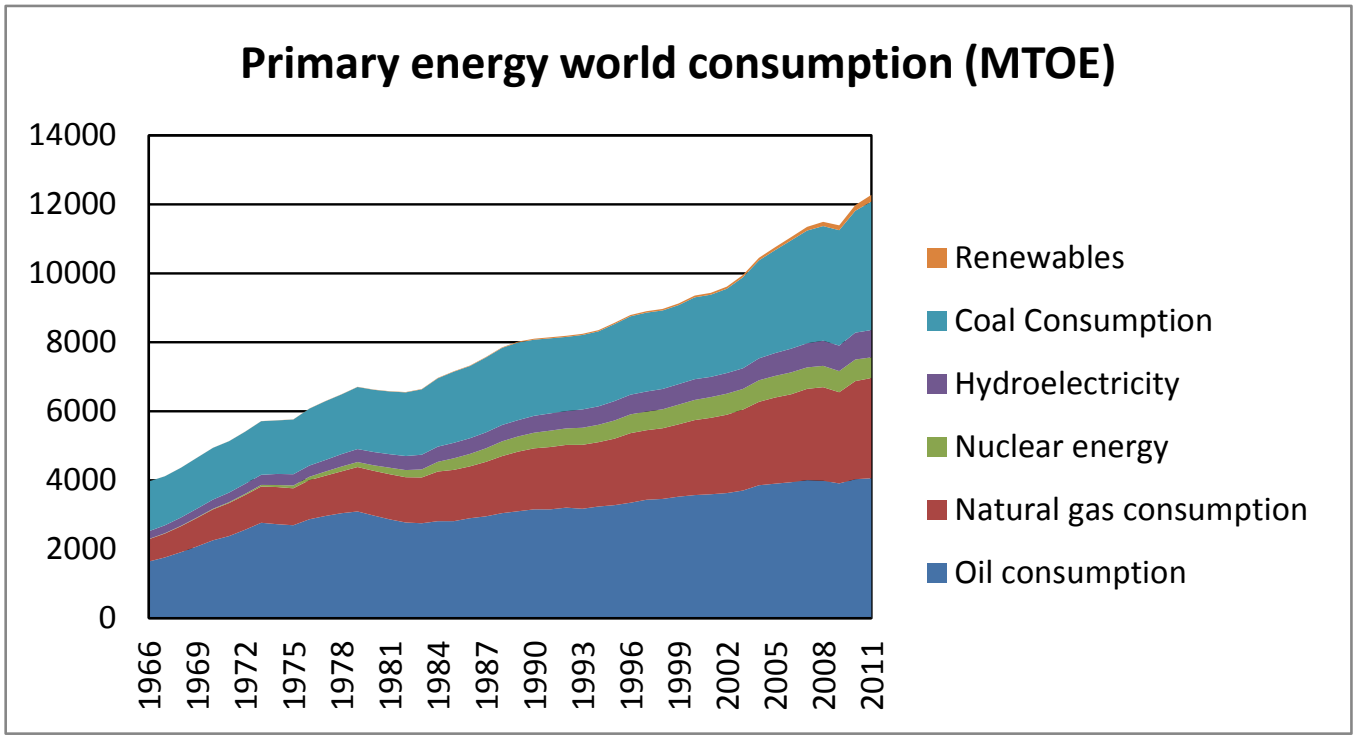

Figure 1: Figure is from BP statistical review of world energy 2012, METO means million tonnes oil equivalent.

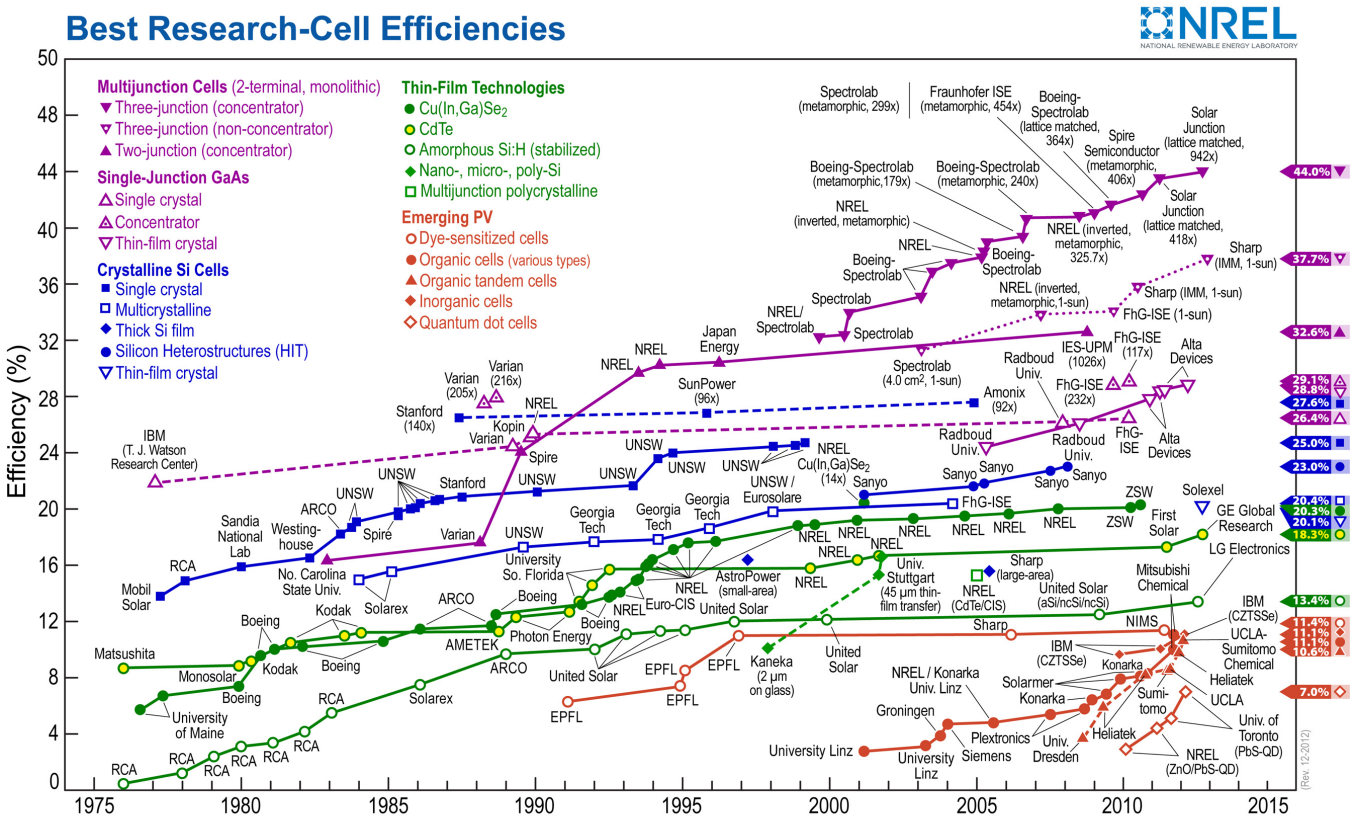

Figure 2: Best research-cell efficiencies. Figure is from National Renewable Energy Laboratory (NREL), Golden, Colorado.

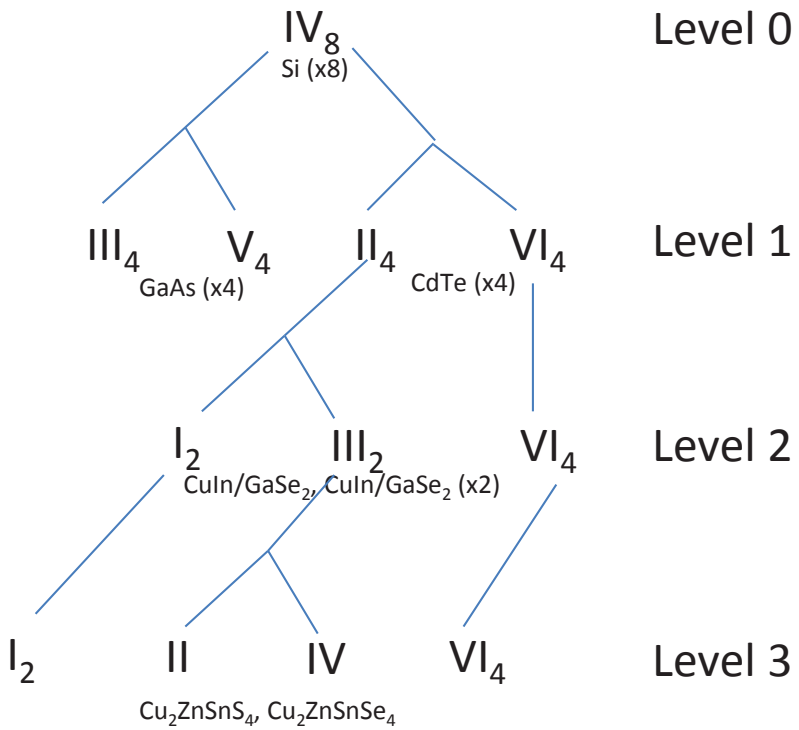

Figure 3: Candidate of solar cell materials (absorption coefficient, band gap range, cost and enviromental safety) .

By considering the electron energy dispersion only around the Γ-point (centre of the Brillouin zone), the parabolic band approximation (pba) is utilized:

$$E_j^{pb}(\mathbf{k}) = E_j(\mathbf{0}) \pm \left[\frac{\tilde{\mathbf{k}}_x^2 + \tilde{\mathbf{k}}_y^2}{m_j^{\perp}} + \frac{\tilde{\mathbf{k}}_z^2}{m_j^{\parallel}} \right] \tag{1}$$

A common way to parameterize the energy bands is within the so called $K \cdot P$ approximation. However, the crystal-field interaction as well as the spin-orbit coupling of $CuIn_{1-x}Ga_xSe_2$ generates rather complex energy dispersions. So we extend the $K \cdot P$ expressions to higher orders.

$$
\begin{aligned}
E_j(\mathbf{k}) = E_j^{pb}(\mathbf{k}) + E_j^0 + \Delta_{j,1} & \left(\delta_{j,1}^2 \left(\frac{\tilde{\mathbf{k}}_x^4 + \tilde{\mathbf{k}}_y^4}{m_0^2} \right) + \delta_{j,2}^2 \left(\frac{\tilde{\mathbf{k}}_x^2 \tilde{\mathbf{k}}_y^2}{m_0^2} \right) + 1 \right)^{1/2} \\
+ \Delta_{j,2} & \left(\delta_{j,3}^3 \left(\frac{\tilde{\mathbf{k}}_x^6 + \tilde{\mathbf{k}}_y^6}{m_0^3} \right) + \delta_{j,4}^3 \left(\frac{\tilde{\mathbf{k}}_x^2 \tilde{\mathbf{k}}_y^4 + \tilde{\mathbf{k}}_x^4 \tilde{\mathbf{k}}_y^2}{m_0^3} \right) + 1 \right)^{1/3} \\
+ \Delta_{j,3} & \left(\delta_{j,5}^2 \left(\frac{\tilde{\mathbf{k}}_z^4}{m_0^2} \right) + 1 \right)^{1/2} + \Delta_{j,4} \left(\delta_{j,6}^3 \left(\frac{\tilde{\mathbf{k}}_z^6}{m_0^3} \right) + 1 \right)^{1/3} \\
+ \Delta_{j,5} & \left(\delta_{j,7}^2 \left(\frac{\tilde{\mathbf{k}}_x^2 \tilde{\mathbf{k}}_z^2 + \tilde{\mathbf{k}}_y^2 \tilde{\mathbf{k}}_z^2}{m_0^3} \right) + 1 \right)^{1/2} \\
+ \Delta_{j,6} & \left(\delta_{j,8}^3 \left(\frac{\tilde{\mathbf{k}}_x^4 \tilde{\mathbf{k}}_z^2 + \tilde{\mathbf{k}}_y^4 \tilde{\mathbf{k}}_z^2}{m_0^3} \right) + \delta_{j,9}^3 \left(\frac{\tilde{\mathbf{k}}_x^2 \tilde{\mathbf{k}}_z^4 + \tilde{\mathbf{k}}_y^2 \tilde{\mathbf{k}}_z^4}{m_0^3} \right) + \delta_{j,10}^3 \left(\frac{\tilde{\mathbf{k}}_x^2 \tilde{\mathbf{k}}_y^2 \tilde{\mathbf{k}}_z^2}{m_0^3} \right) + 1 \right)^{1/3}
\end{aligned}
\tag{2}
$$

Unfortunately, the rather complex VB energy dispersions of $CuIn_{1-x}Ga_xSe_2$ require quite many fitting parameters. The CB, however, needs less parameters.

The lowest conduction band (CB) and the three uppermost valence bands (VBs) of $CuIn_{1-x}Ga_xSe_2$ (x=0, 0.5, and 1) in order to better describe of the non-parabolic and anisotropic.

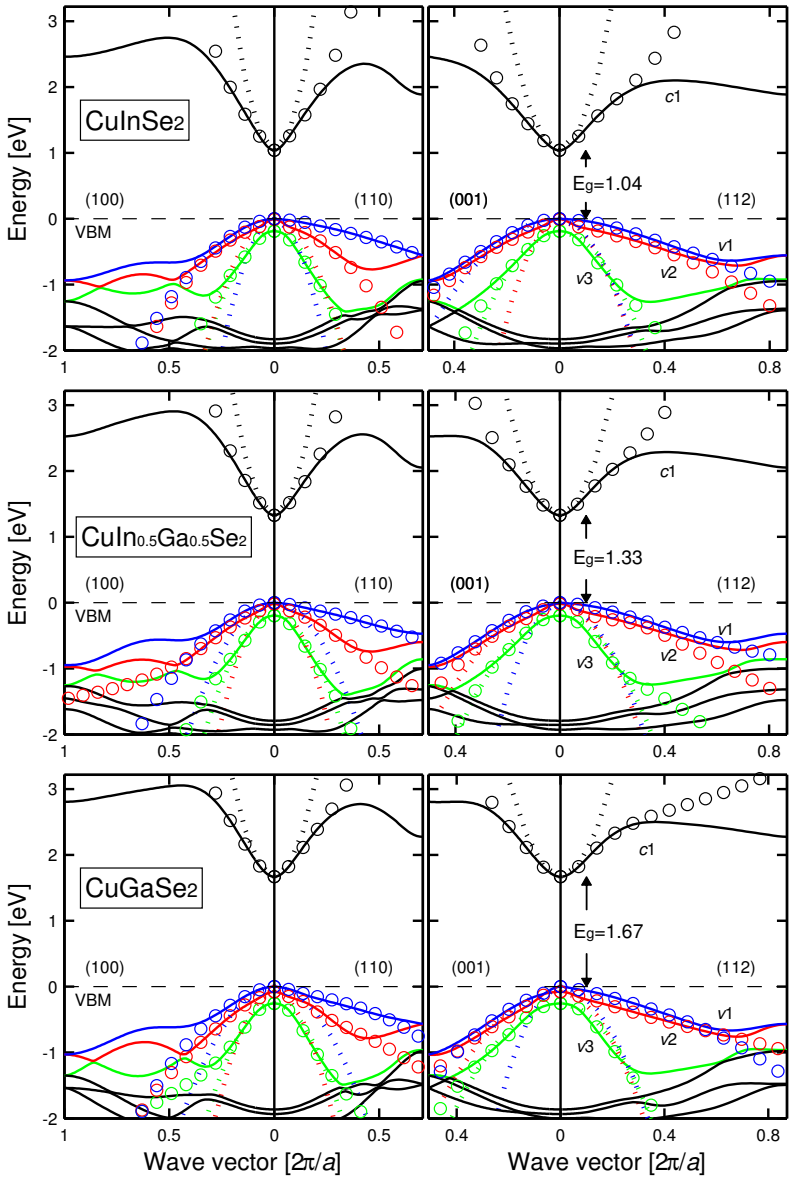

Figure 4: Electronic band structure along four directions. the circles are the results of the full band parameterization (fbp), and the dotted lines represent the parabolic band approximation.

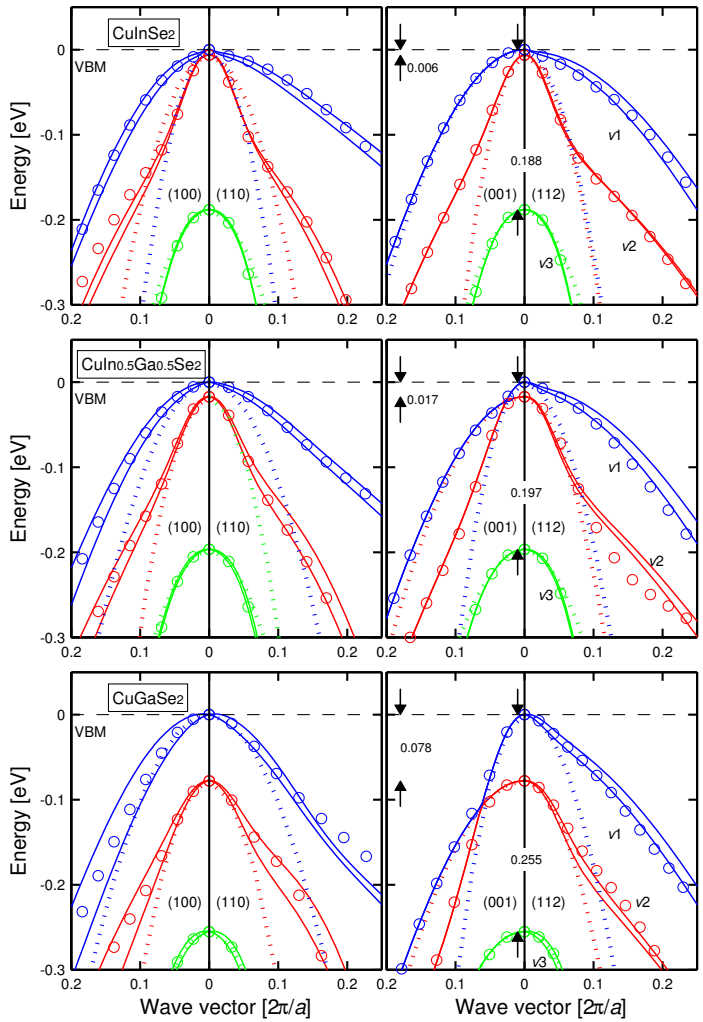

Figure 5: Close-up of above figure

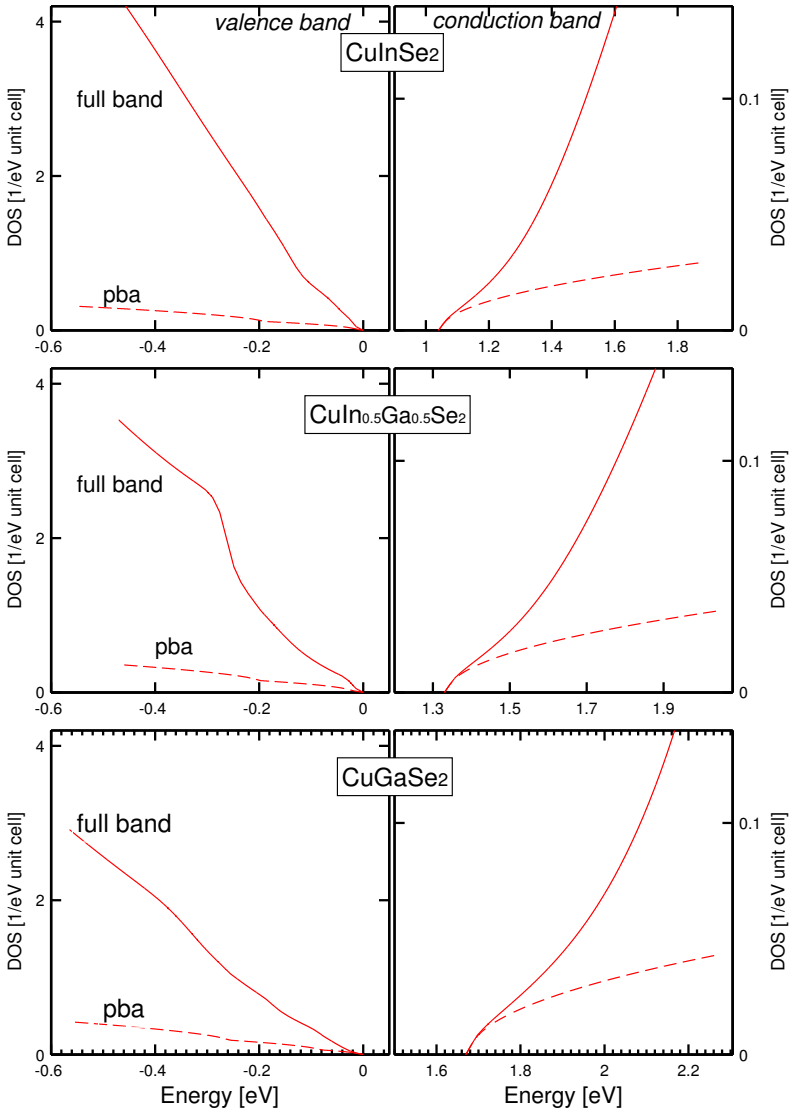

Figure 6: Total DOS ($g_{v/c}(E)$) of the VBs (left panels) and of the CB (right panels) for $CuIn_{1-x}Ga_xSe_2$. The solid lines show the full band parameterization (fbp), and the dashed lines represent the parabolic band approximation (pba).

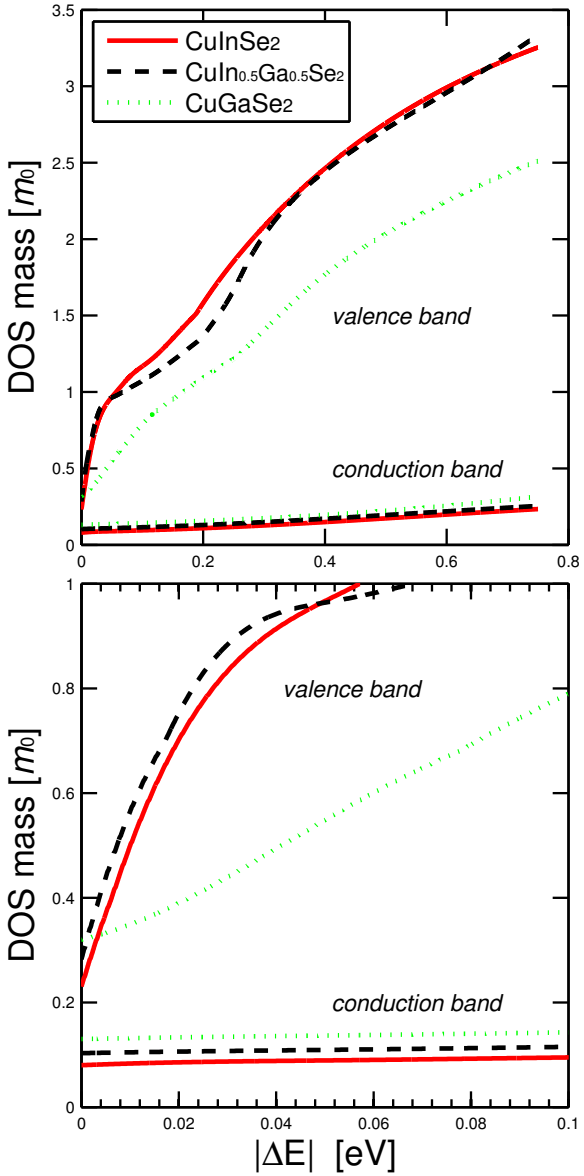

Figure 7: The DOS mass of the VBs and the CB in $CuIn_{1-x}Ga_xSe_2$. The upper (lower) panel shows in a wider (narrower) energy region.

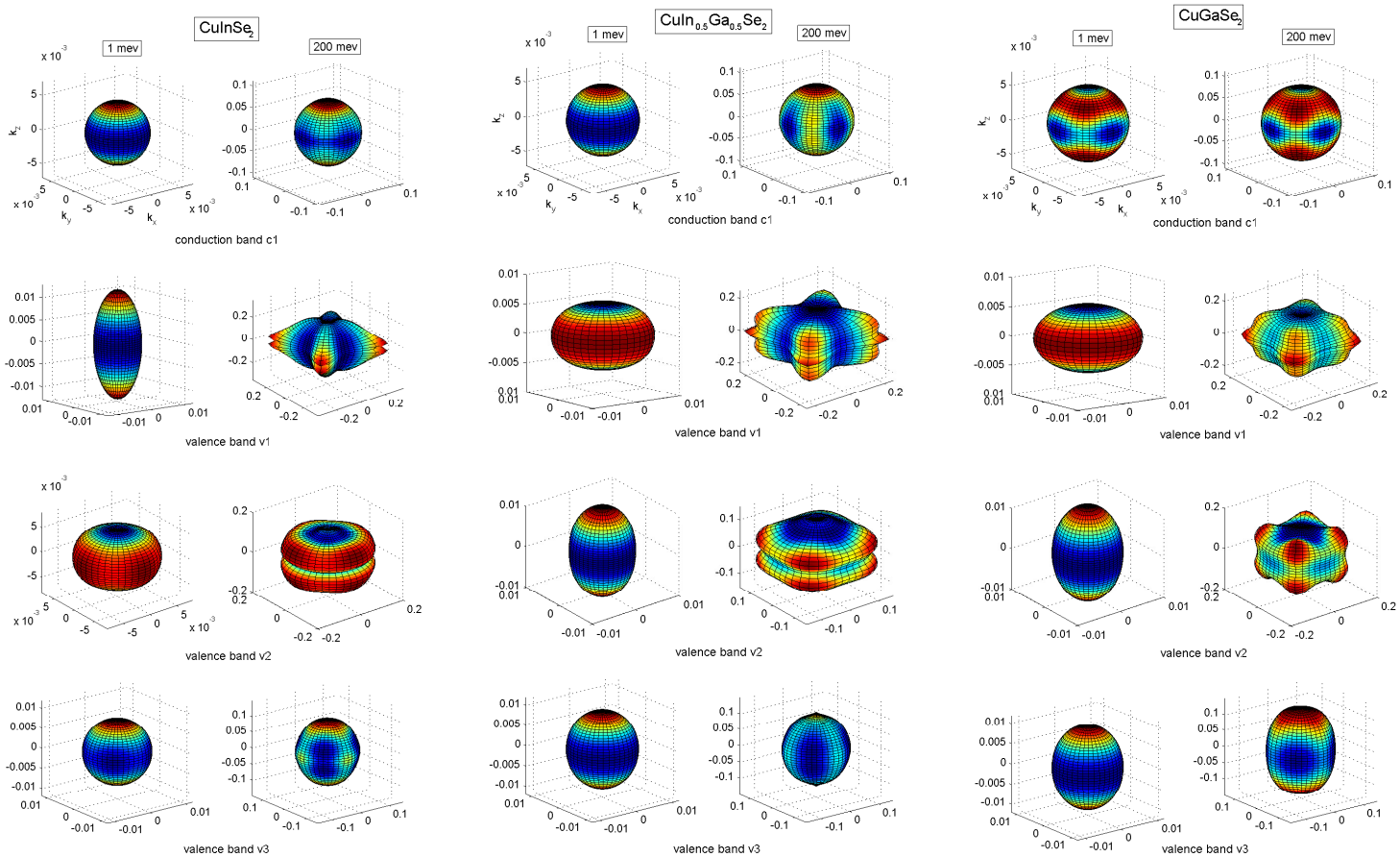

Figure 8: Constant energy surfaces for the three uppermost VBs and the lowest CB for the energies E = 1 meV (left column ellipsoidal) and E = 200 meV (right column).

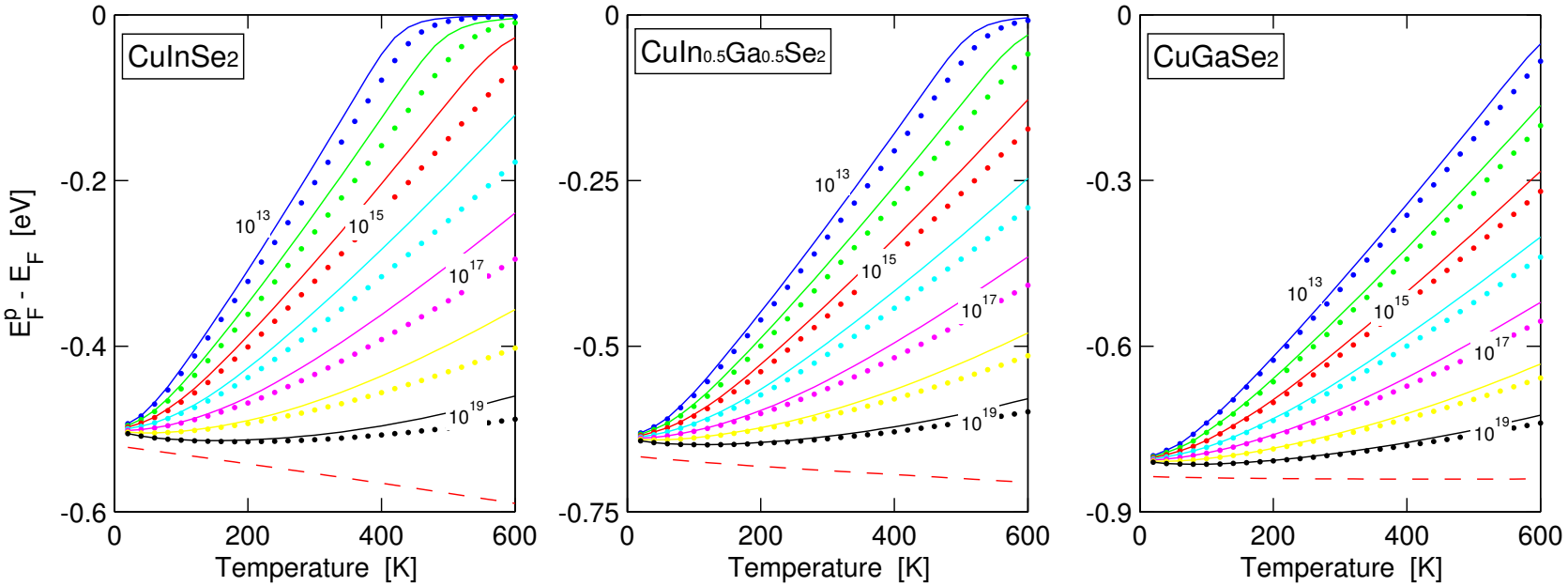

Figure 9: Fermi level as functon of the temperature fo p-type $CuIn_{1-x}Ga_xSe_2$ for the effective doping concentration $N_A = 10^{13}, 10^{14}, 10^{15}, ...,$ and 10^{19} acceptors/cm^3. Solid and dotted lines represent the full band parameterization and the parabolic band approximation, respectively.

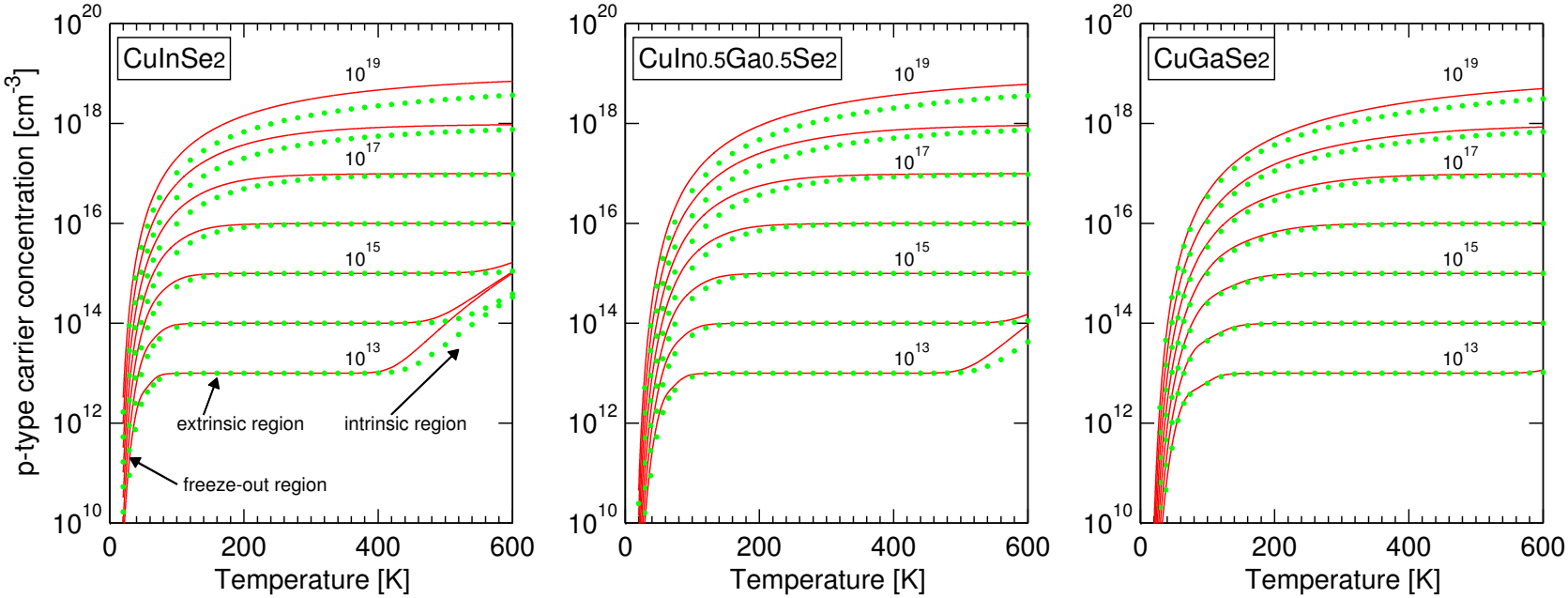

Figure 10: Free carrier concentration as function for the temperature in $p-type$ for the effective doping concentration $N_A = 10^{13}, 10^{14}, 10^{15}, ...,$ and 10^{19} acceptors/cm^3. Solid and dotted lines represent the full band parameterization and the parabolic band approximation, respectively.

The dielectric function spectra of $CuIn_{0.5}Ga_{0.5}Se_2$ is calculated with full-potential linearized augmented plane wave method (Wien2k) using the generalized gradient approximation plus an onsite Coulomb interaction U of the Cu d states, it is compared with experiment as well. Probable electronic origins of the interband critical features (CPs) observed are discussed.

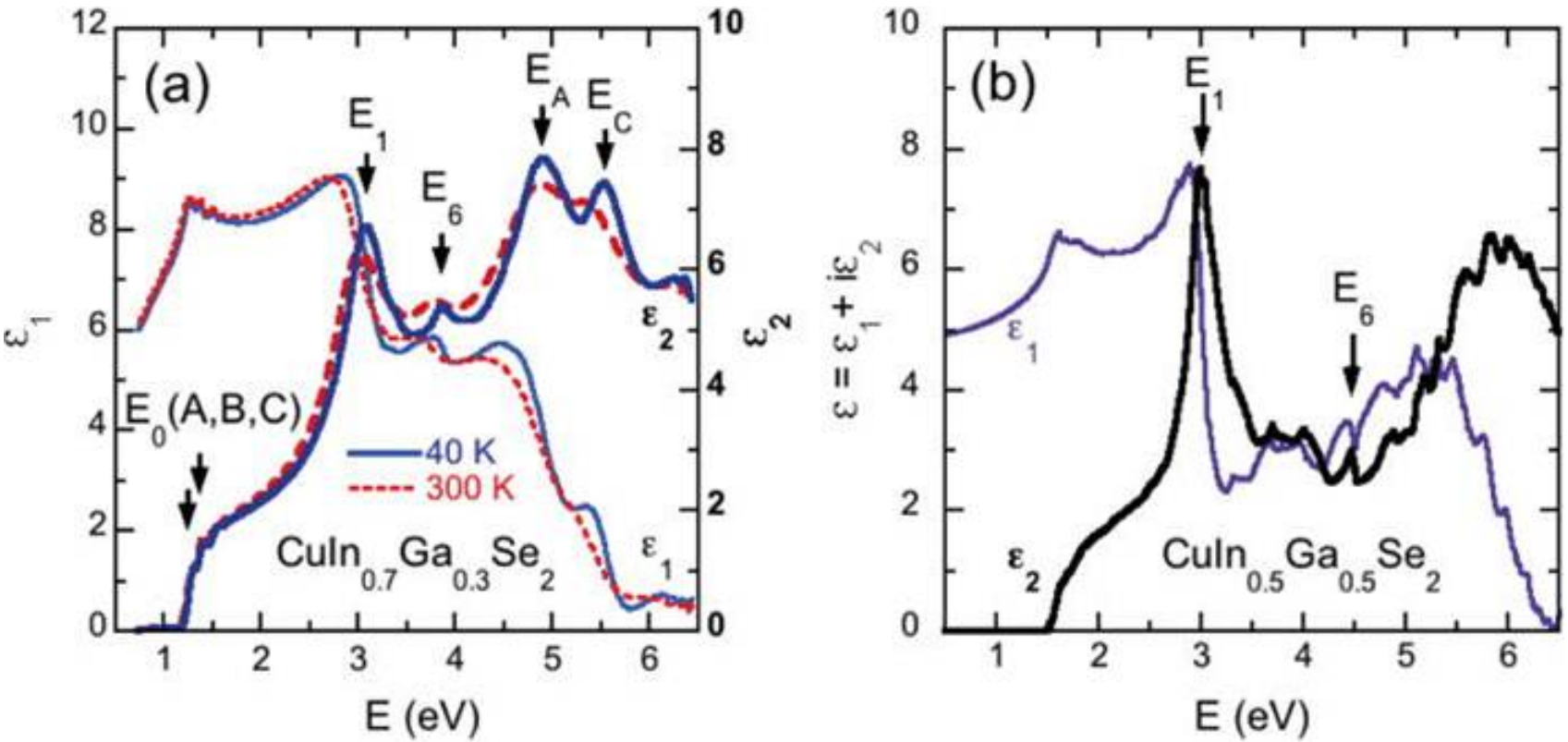

Figure 11: (a) Modeled dielectric function spectra for $CuIn_{0.7}Ga_{0.3}Se_2$ taken at 40 K and 300 K. The dielectric function for $CuIn_{0.5}Ga_{0.5}Se_2$ calculated by the FPLAPW using the GGA+U

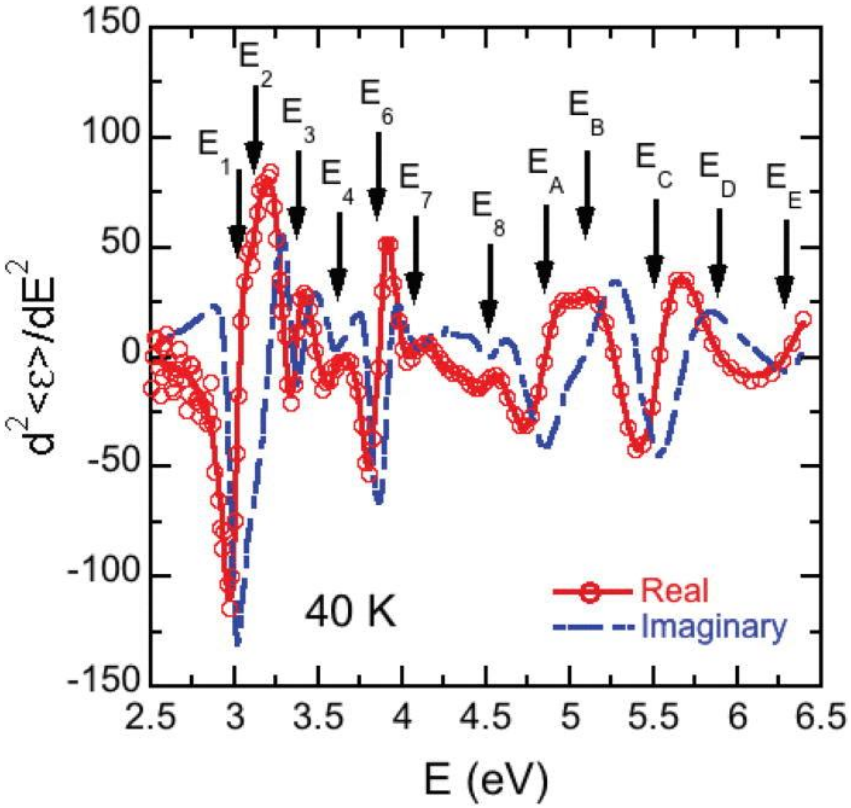

Figure 12: Solid red are standard CP lineshapes bet fit to $d^2 < \varepsilon_1 > /dE^2$ (open circles) and dashed-dotted blue lines are $d^2 < \varepsilon_2 > /dE^2$. Energies of each CP are indicated by arrows and labeled in a numeric and alphabetic order.

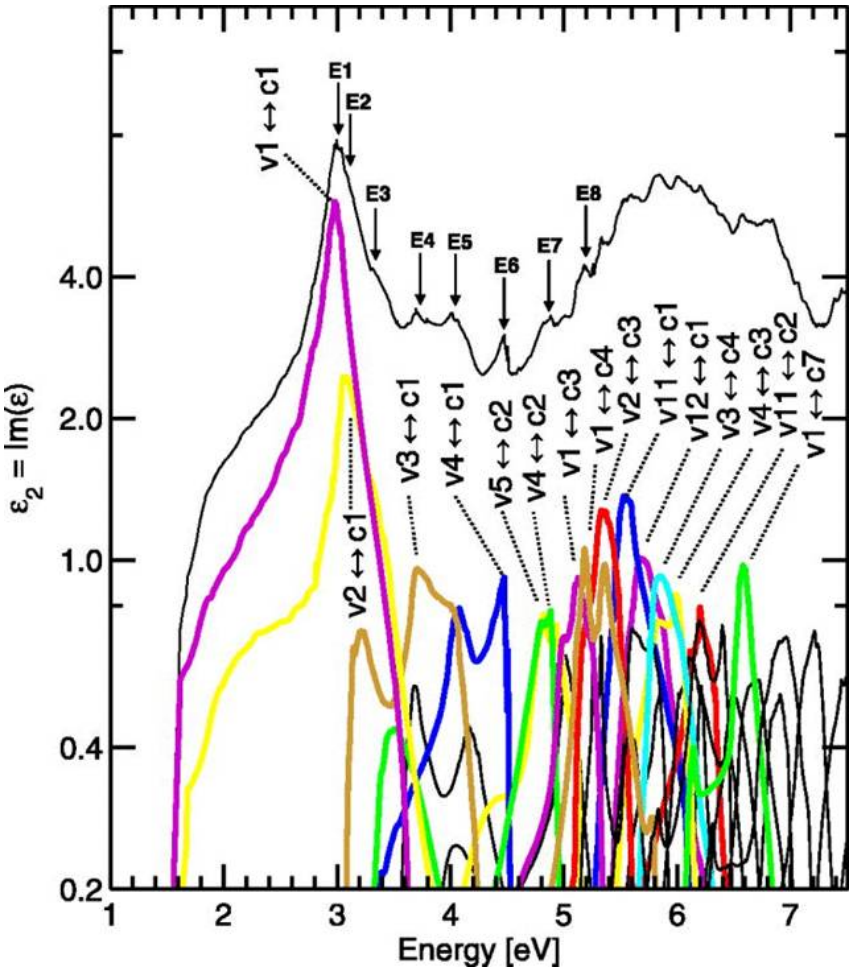

Figure 13: Band-to-band analysis of the contribution to the total ε_2 spectrum. The most important valence-to-conduction band transitions are marked. Spin-orbit coupling is included.

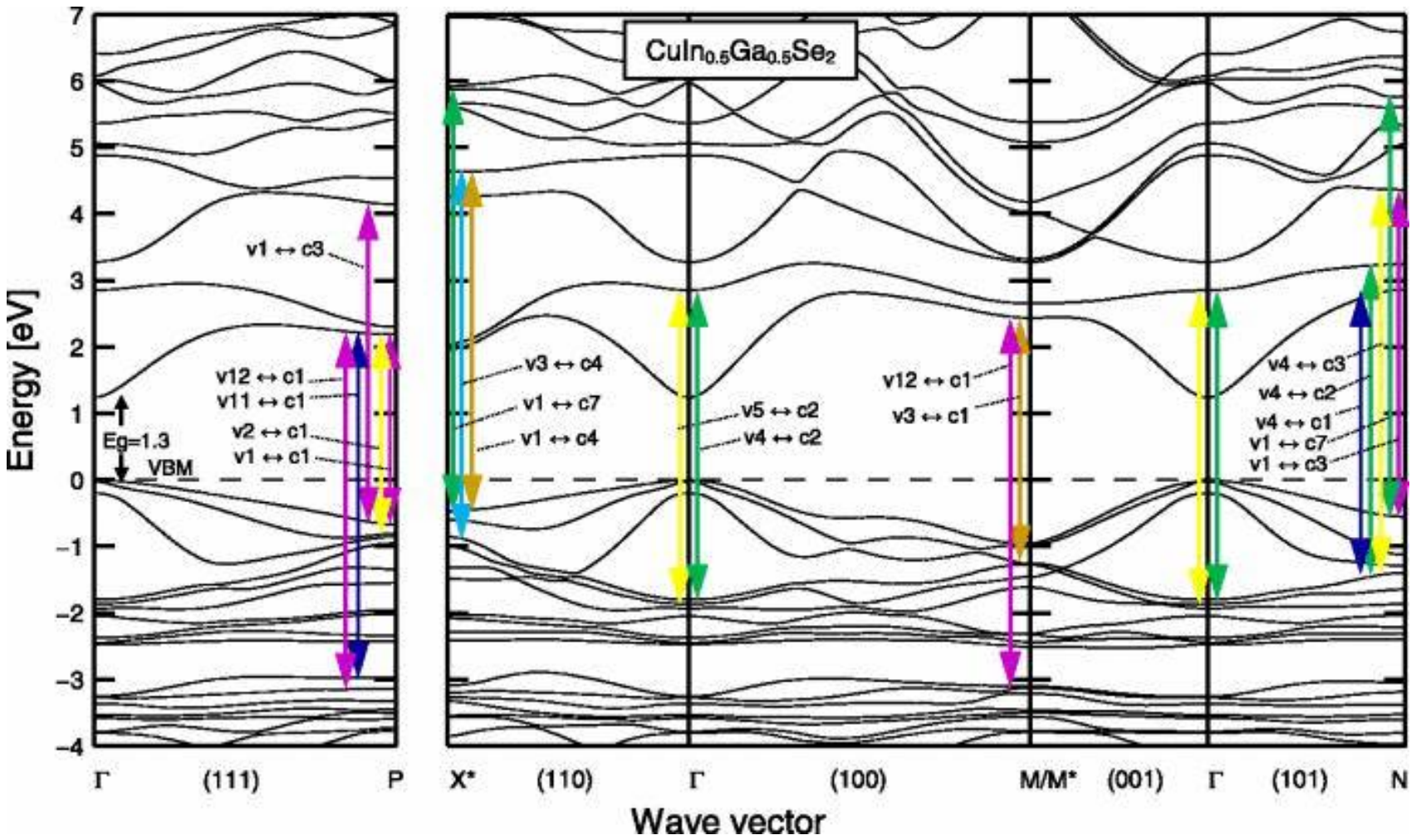

Figure 14: The calculated electronic band structure of $CuIn_{0.5}Ga_{0.5}Se_2$ where the CPs are identified along the main sysmetry directions.

I am involved in the implementation of the Exciting Code (Prof. Claudia Draxl), which is full-potential all-electron density-functional-theory (DFT) package implementing the families of linearized augmented planewave (LAPW) methods. The main work is about scalar relativistic approximation, spin-orbit coupling and new $K \cdot P$ method. Everything is under development now.

The code mainpage is http://exciting-code.org/, which has many features (TDDFT, GW and BSE ...).

Thank you for your time!