LIÈGE université Sciences
SPIN
UHASSELT

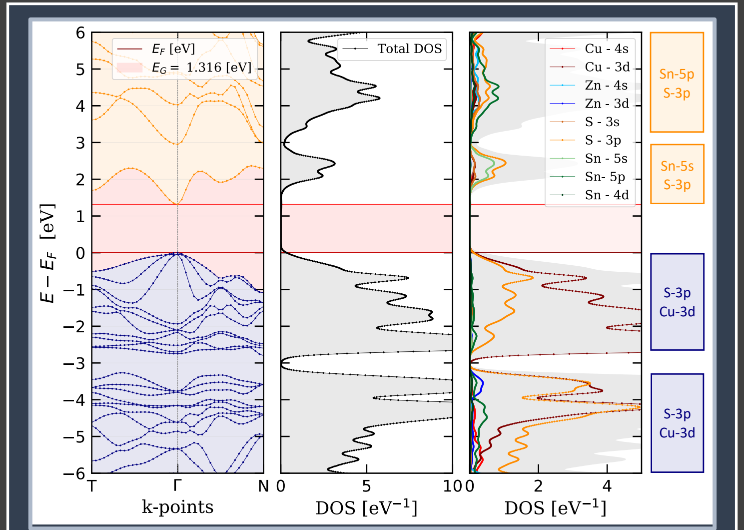
thomas.ratz@uliege.be

Submitted to *Solar Energy Materials and Solar Cells journal*

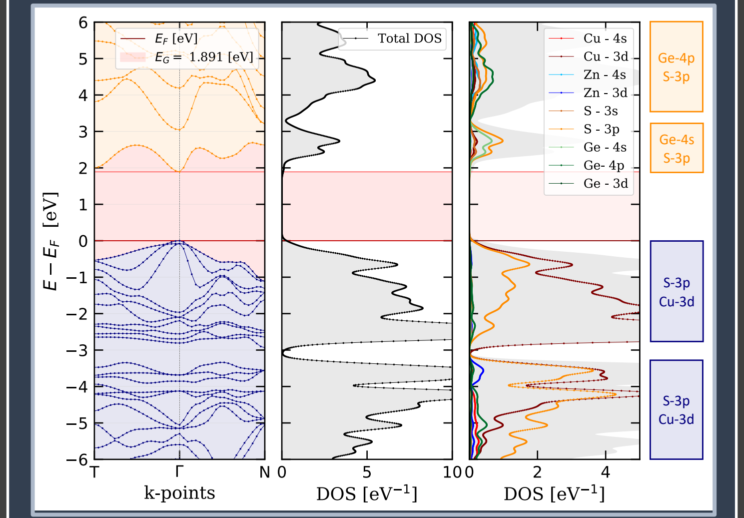
Study of the opto-electronic properties of Cu_2ZnXS_4 (X=Sn,Ge,Si) kesterites as input data for solar cell efficiency modelling

Thomas Ratz[1,2], Jean-Yves Raty[1,3], Guy Brammertz[4], Bart Vermang[2,4,5], Ngoc Duy Nguyen[1]

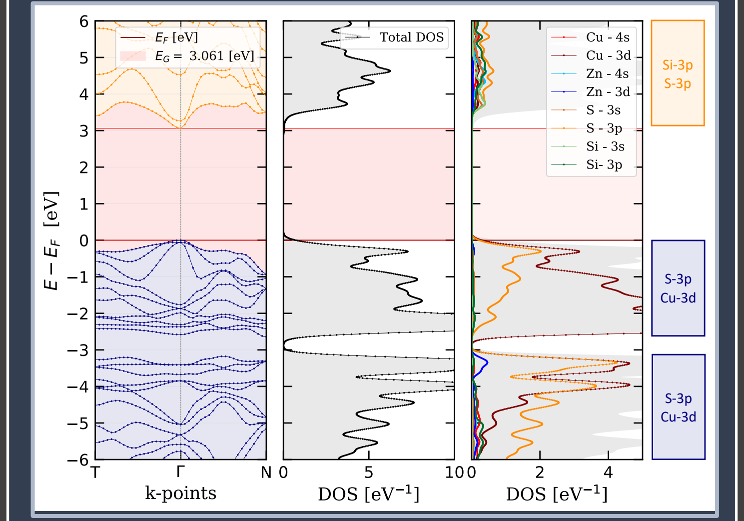
1. *CESAM | Q-MAT | Solid State Physics, Interfaces and Nanostructures, Physics Institute B5a, Allée du Six Août 19, B-4000 Liège, Belgium*
2. *Institute for Material Research (IMO), Hasselt University, Agoralaan gebouw H, B-3590 Diepenbeek, Belgium*
3. *University of Grenoble Alpes | CEA-LETI | MINATEC Campus | Rue des Martyrs 17, F-38054 Cedex 9 Grenobles, France*
4. *IMEC division IMOMEC | partner in Solliance, Wetenschapspark 1, B-3590 Diepenbeek, Belgium*
5. *Energyville, Thor Park 8320, B-3600 Genk, Belgium*



Cu_2ZnSnS_4



Cu_2ZnGeS_4



Cu_2ZnSiS_4

Insights of Sn substitution by Ge and Si in S-kesterite compounds using DFT approach

→ Structural properties:

Kesterite lattice contraction

→ Electronic properties:

Significant bandgap increase and slight increase of m^*

→ Optical properties:

Absorption coefficients of the order of 10^4 cm^{-1}

Improved Shockley-Queisser model[1]

DFT input data: $\alpha(E), n(E), R(E)$

Model param.: $T = 300K, d$

$$A(E) = (1-R)\exp(-2\alpha d)$$

$$R_{rad}(n),\ R_{nrad}(Q_i, R_{rad})$$

$$\eta, J_{SC}, V_{OC}, FF$$

[1] Blank et al., *Phys. Rev. App.*, 8(2), 024032 (2017)

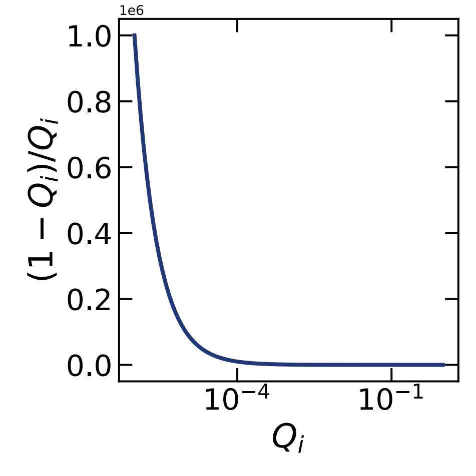
Solar cell modelling

Modelling of the non-radiative recombination rate via an external parameter: Q_i

$$R_{nrad} = R_{rad}\frac{(1-Q_i)}{Q_i}$$

Methodology:

$\eta(d, Q_i)$ (Fig.1) → $d_{opt}(Q_i)$ → $\eta(Q_i)\big|_{d_{opt}}$ (Fig.2)



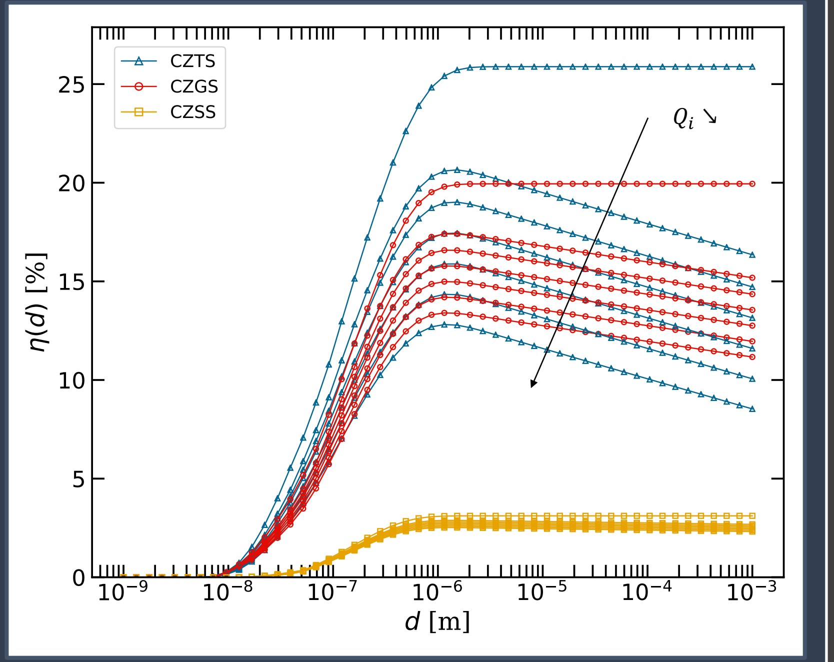


Fig. 1: Cell efficiency with respect to the absorber layer thickness

- Optimal absorber layer thicknesses between 1.15 and 2.68 μm
- Disparity between the Si and the two other compounds in the reported cell efficiencies due to J_{SC} limitations
- Distinguishable behaviour between $R_{nrad} = 0$ ($Q_i = 1$) and $R_{nrad} > 0$ ($Q_i < 1$) with respect to the absorber thickness d

Correlation between non-radiative recombination rate and solar cell characteristics

- Decrease of the cell efficiency taking into account the materials reflectivity
- The kesterite absorptance fixes the absolute efficiency loss with respect to Q_i (Fig. 2)
- **From Sn to Si kesterite,** η decreases explained by the J_{SC} drop not compensated by the increase of V_{OC} (Fig. 3)

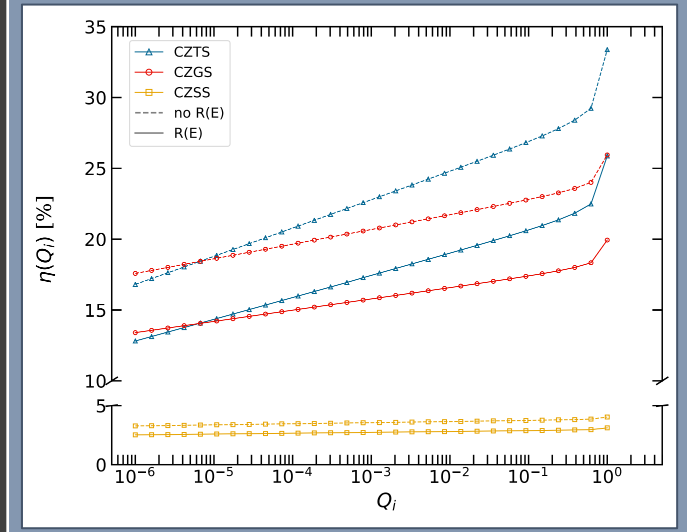


Fig. 2: Cell efficiency with respect to Q_i for an optimal absorber thickness value

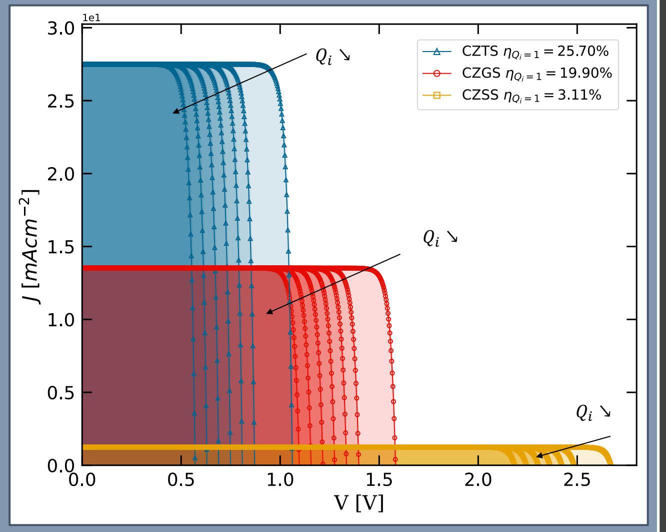


Fig. 3: JV cruves for $d = 1.5\ \mu m$ with respect to Q_i

Materials	E_G [eV]	Q_i	J_{SC} [$mAcm^{-2}$]	V_{OC} [V]	η [%]
CZTS	1.32	1	27.68	1.06	25.88
		10^{-4}	27.19	0.70	15.88
CZGS	1.89	1	13.54	1.58	19.94
		10^{-4}	13.45	1.22	14.98
CZSS	3.06	1	1.24	2.67	3.11
		10^{-4}	1.23	2.31	2.66

In a nutshell

- Possible efficiency imrpovement of 10% (CZTS) and 4.96% (CZGS) via the reduction of R_{nrad}
- With higher bandgap and interesting efficiencies, CZGS could be used in tandem approach
- CZSS might be implemented for PW windows