Band Tails in Cd(Se,Te) Device Models

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Presented at: CdTe PV Workshop, Oct. 20, 2022, Toledo, Ohio

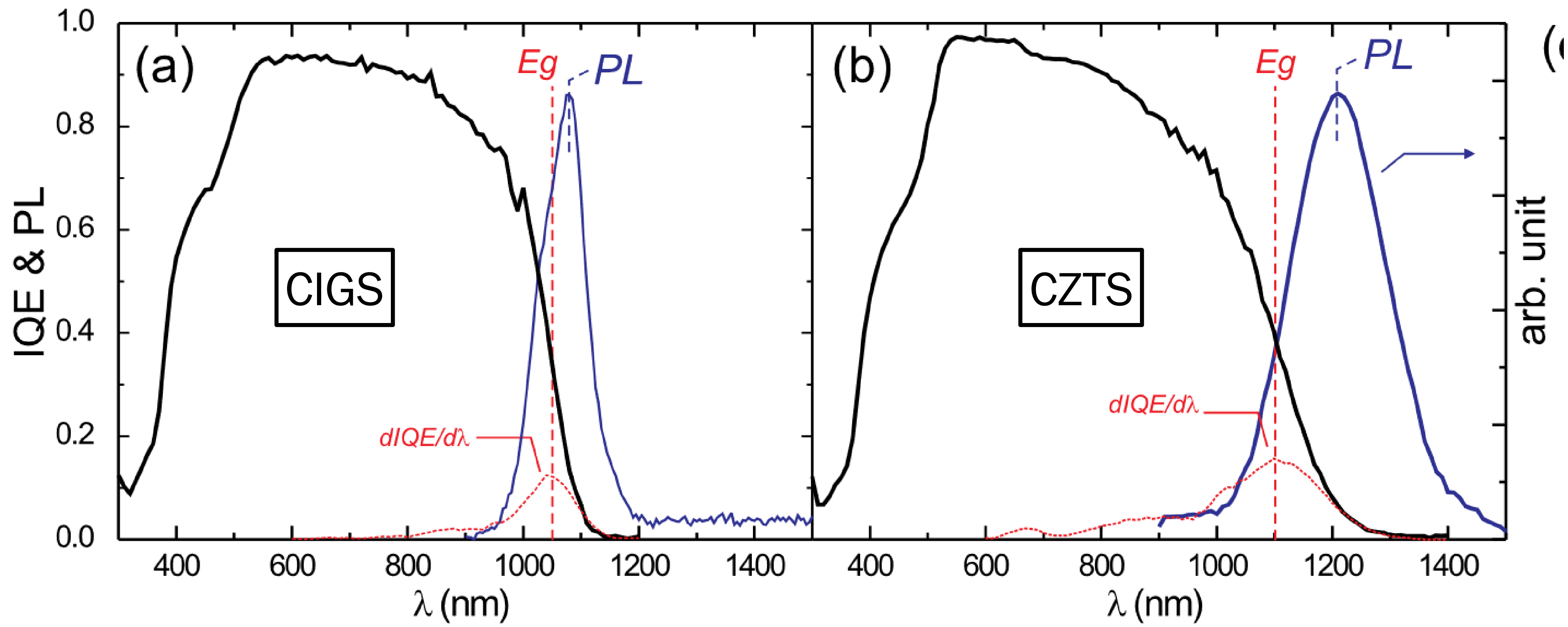
Overview

Incorporating band tail physics in Cd(Se,Te) device models

- Origin and observations of band tails
- Impacts on device performance from analytical calculations
- Band tail models – generalized model
- Inputs to device simulations – abs coefficient (α) and luminescence band gap (E_{PL}) from theory or measurement
- Initial device simulation results

Band Tails – Origin and Observation

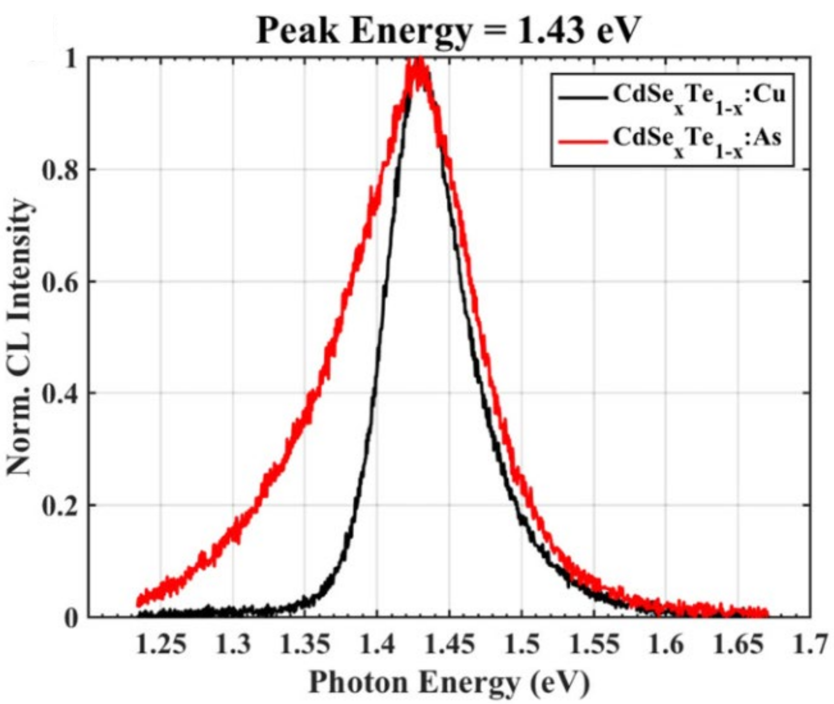
- caused by disorder – thermal or structural
- band gap fluctuations – elemental inhomogeneity [Cd(Se,Te)]
- electrostatic potential fluctuations – charged defect/dopant inhomogeneity, strong compensation, grain boundaries
- observations of sub-band gap absorption [1]
- luminescence peak red-shifted from absorption band gap in PV devices [2]



[1] F. Urbach, “The long-wavelength edge of photographic sensitivity and of the electronic absorption of solids,” *Physical Review*, vol. 92, no. 5, p. 1324, 1953.
[2] T. Gokmen, O. Gunawan, T. K. Todorov, and D. B. Mitzi, “Band tailing and efficiency limitation in kesterite solar cells,” *Applied Physics Letters*, vol. 103, no. 10, p. 103506, 2013.

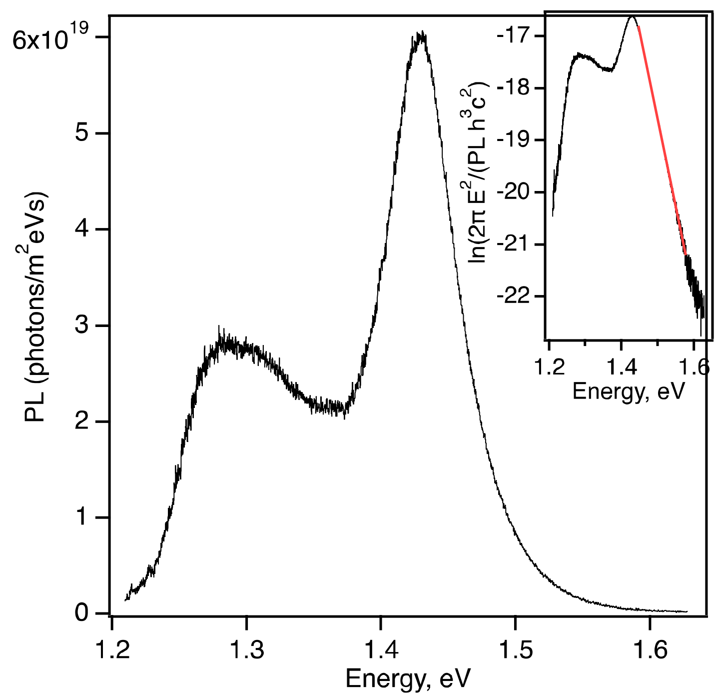
Band Tails - Observations

Due to difficulties with measuring band tails, they might have been missed in the past, e.g.:



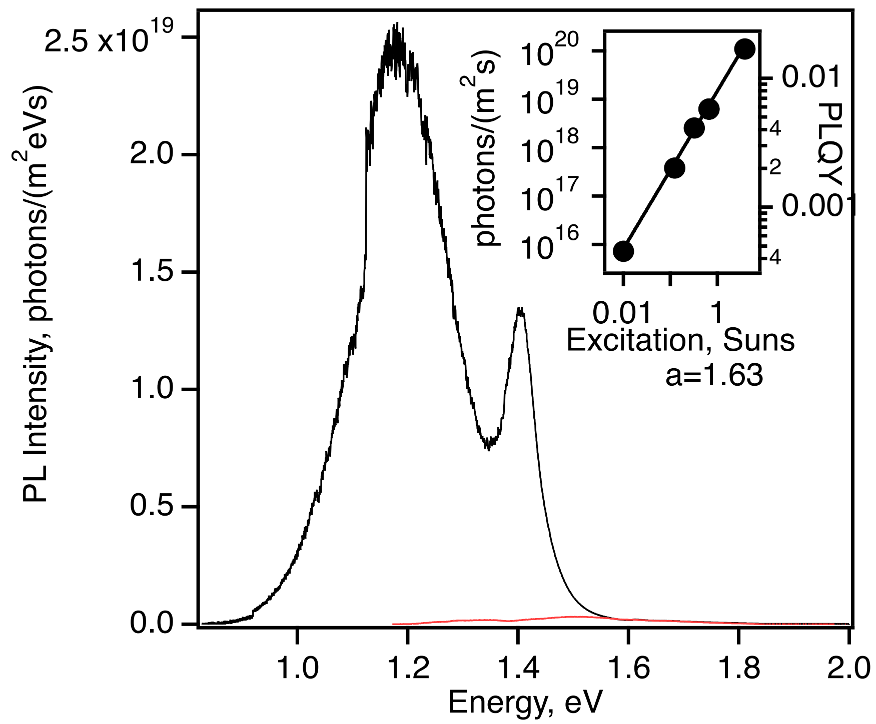
- Spectrally not-corrected data (underestimate tails at <1.3eV)
- CL shows increasing sub-band gap features with As incorporation compared to Cu.
- Connections to electric potential fluctuations

J. Moseley et al., “Impact of dopant-induced optoelectronic tails on open-circuit voltage in arsenic-doped Cd (Se) Te solar cells,” Journal of Applied Physics, vol. 128, no. 10, p. 103105, 2020.



- Si, detector, intensity calibration with claimed “traceable” method, still likely incorrect <1.3 eV.
- PL tails in undoped CdSeTe, radiative voltage 1.13 V

Kuciauskas et al, IEEE JPV (2022)

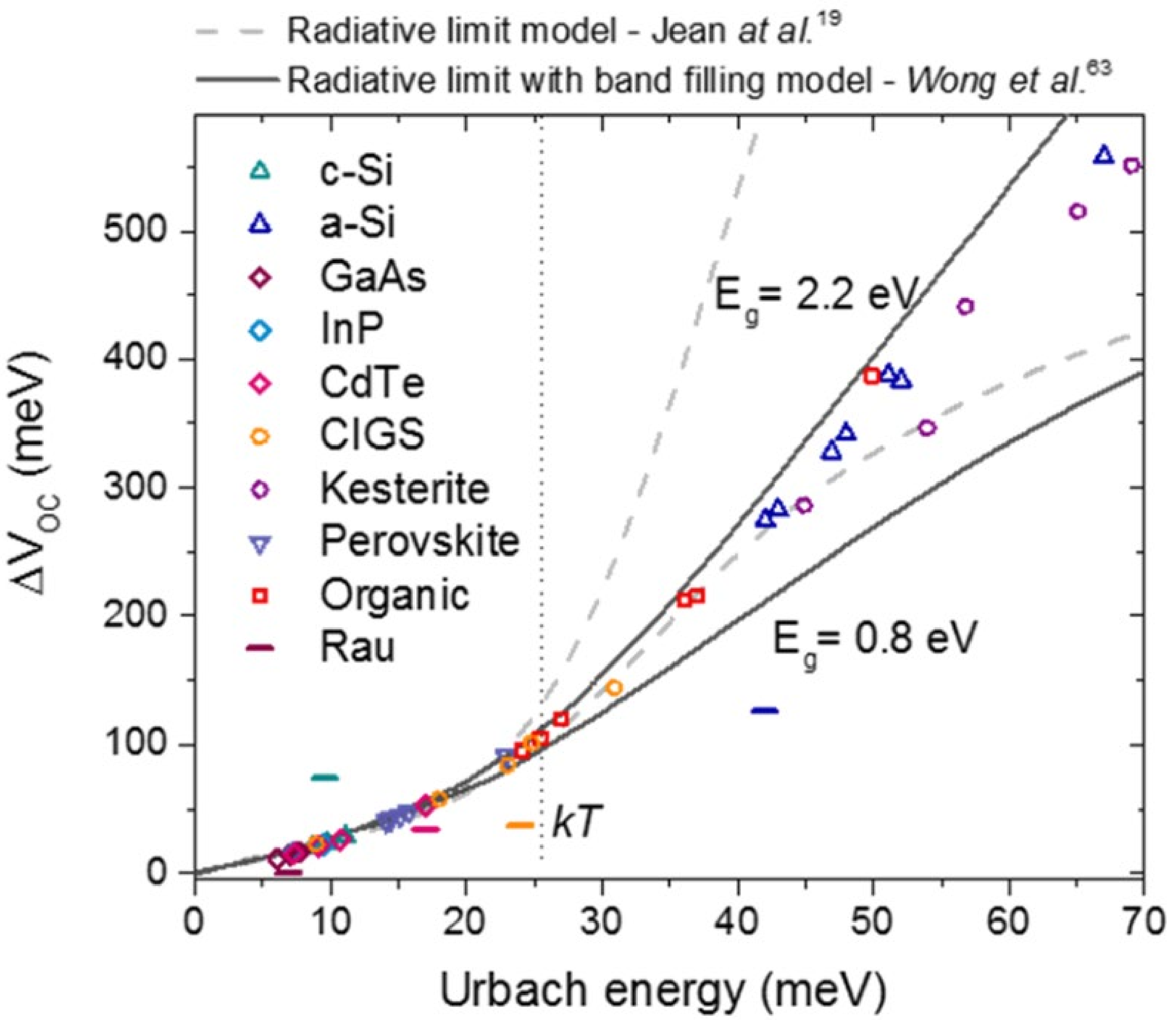


- Combined calibrated InGaAs and Si detectors;
- Large tails in high lifetime CST
- Radiative volage 1.03 V

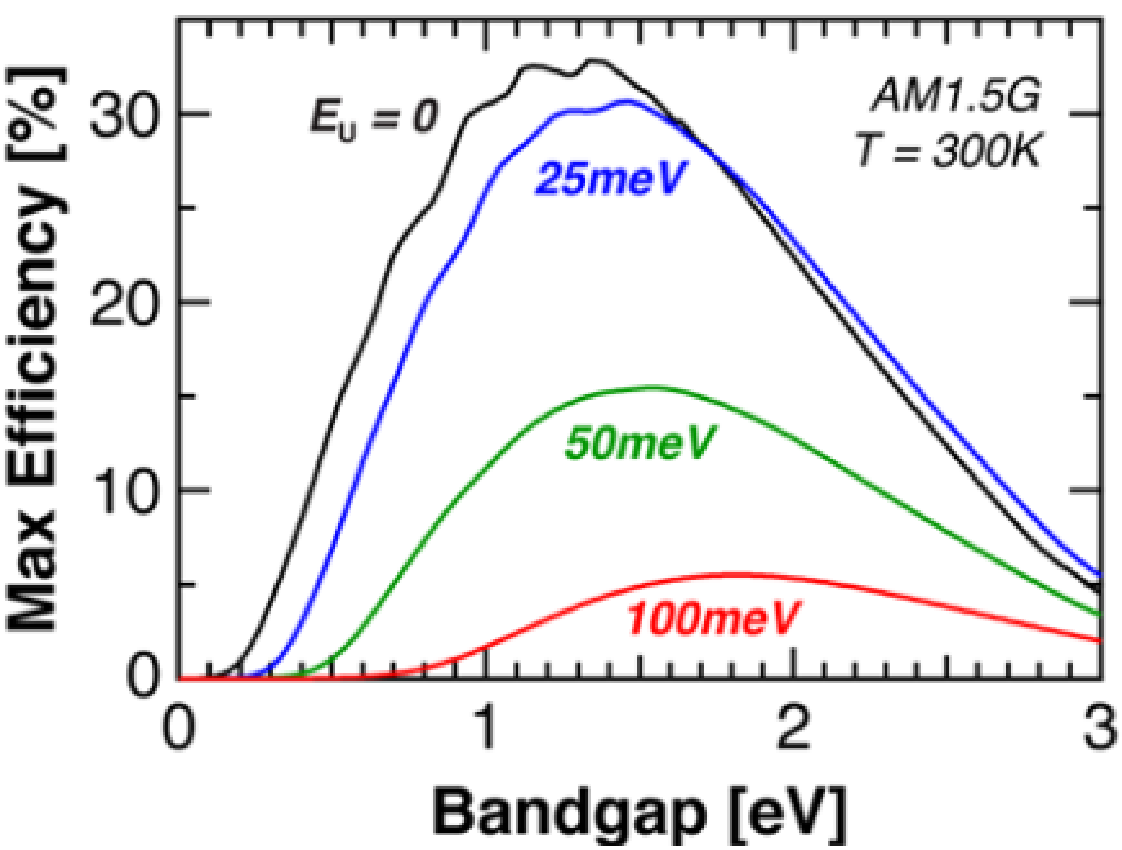
C. Reich, Ph.D. thesis, CSU (2022)

Impact on Performance

V_{oc} variation with Urbach energy [1], [2]



Max. efficiency with different Urbach energies [3]



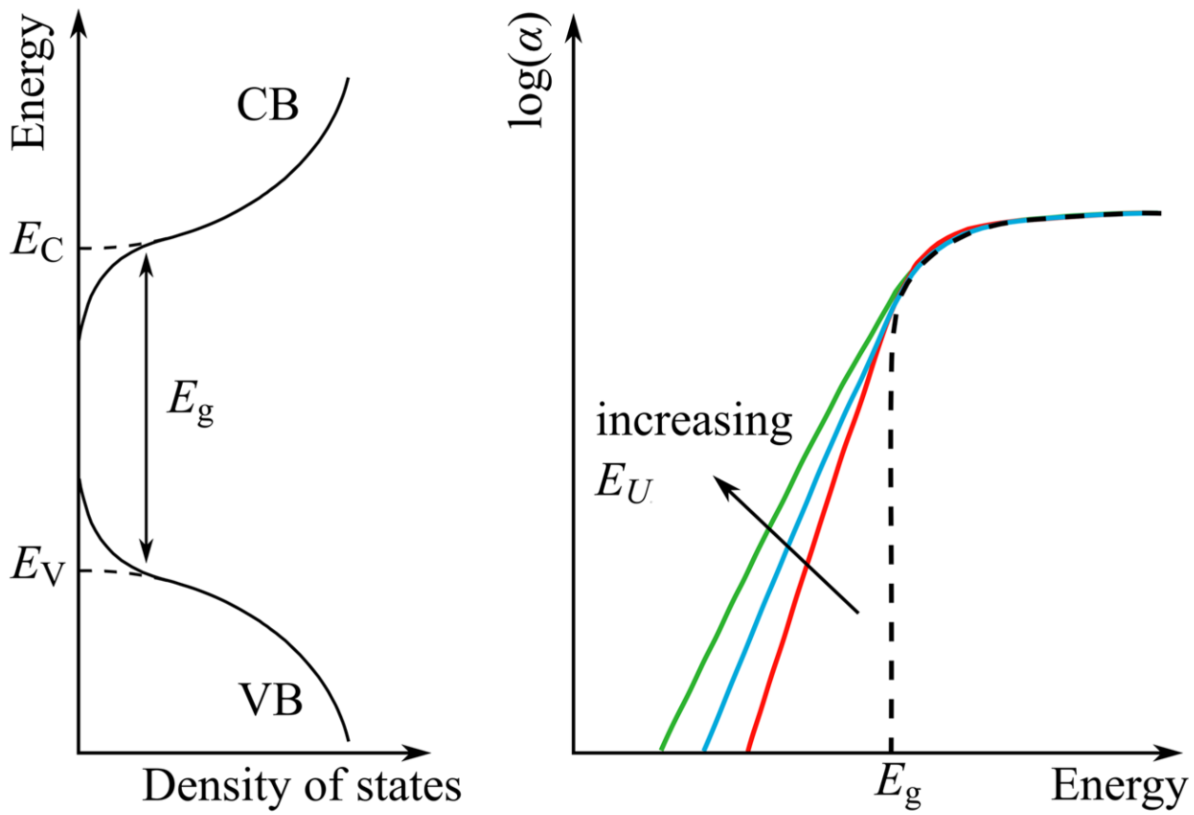
[1] E. Ugur, M. Ledinský, T. G. Allen, J. Holovský, A. Vlk, and S. De Wolf, "Life on the Urbach Edge," *J. Phys. Chem. Lett.*, vol. 13, no. 33, pp. 7702–7711, Aug. 2022.

[2] J. Wong, S. T. Omelchenko, and H. A. Atwater, "Impact of Semiconductor Band Tails and Band Filling on Photovoltaic Efficiency Limits," ACS Energy Lett., vol. 6, no. 1, pp. 52–57, Jan. 2021, doi: 10.1021/acsenergylett.0c02362.

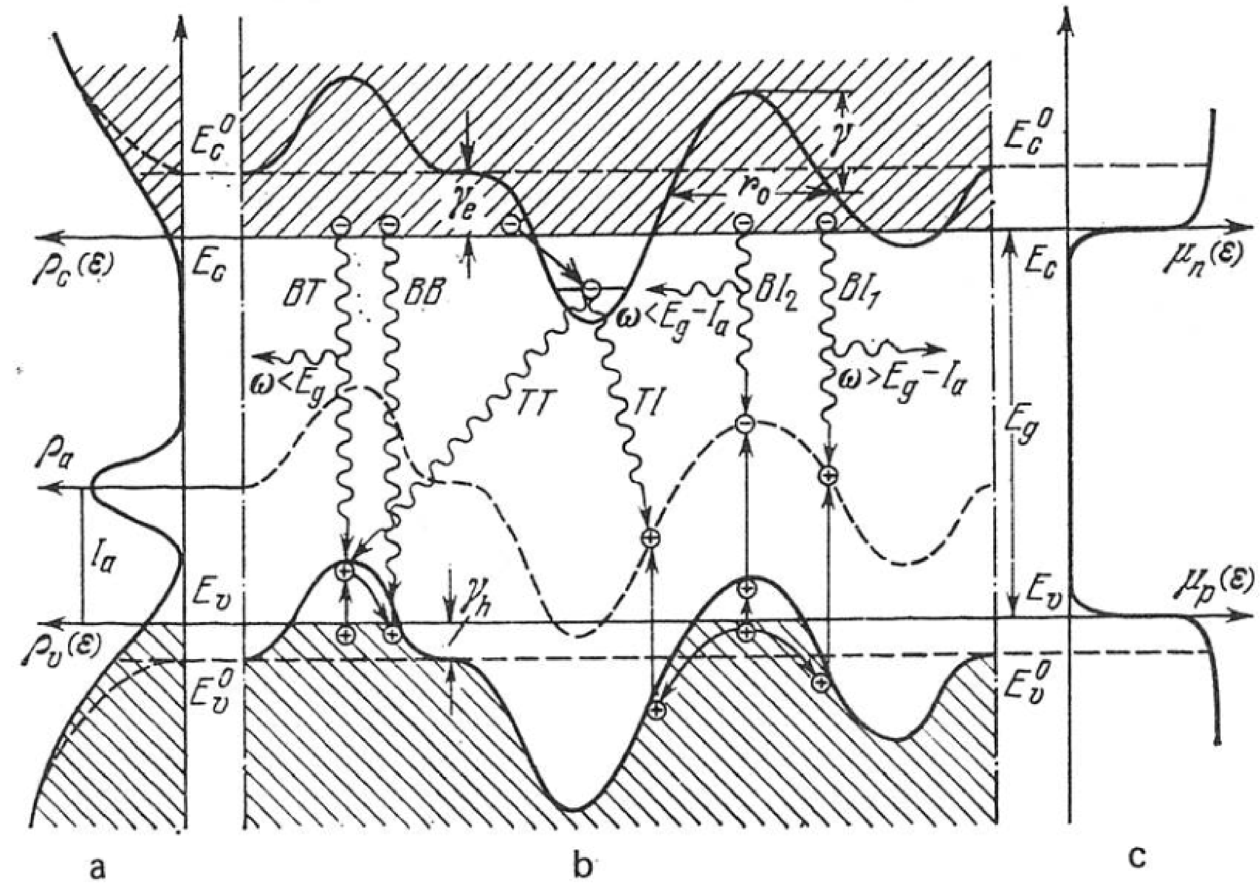
[3] J. Jean et al., "Radiative efficiency limit with band tailing exceeds 30% for quantum dot solar cells," ACS Energy Letters, vol. 2, no. 11, pp. 2616–2624, 2017.

Band Tails Models

simple exponential (Urbach) tail [1]



electrostatic fluctuations in a strongly compensated (nondegenerate) heavily doped semiconductor [2]



[1] M. H. Wolter et al., “How band tail recombination influences the open-circuit voltage of solar cells,” Progress in Photovoltaics: Research and Applications, 2021.
[2] A. P. Levanyuk and V. V. Osipov, “Edge luminescence of direct-gap semiconductors,” Soviet Physics Uspekhi, vol. 24, no. 3, p. 187, 1981.

Band Tails Models

- Sub-band gap absorption models:

$\alpha \propto \exp\left(\frac{-E}{\gamma}\right)$ Urbach [1], $\gamma \sim 5 - 10$ meV for GaAs, $\gamma \sim 50$ meV for a-Si.

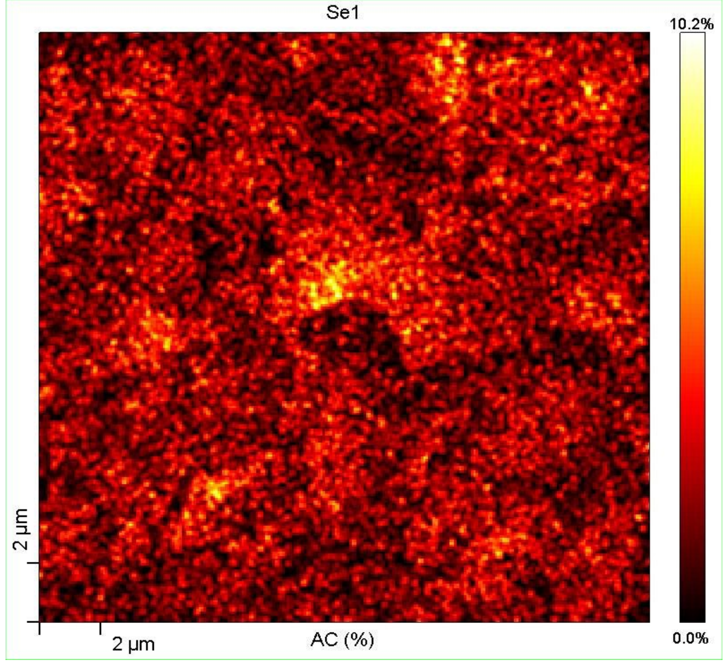
$\alpha \propto \exp\left(\frac{-E}{\gamma}\right)^2$ Thomas-Fermi [2], electrostatic potential fluctuations.

$\alpha \propto \exp\left(\frac{-E}{\gamma}\right)^{5/4}$ screened Thomas-Fermi [3], high density of charged impurity.

$\alpha \propto \exp\left(\frac{-E}{\gamma}\right)^{3/2}$ Franz-Keldysh, photon assisted tunneling [4].

- Band gap fluctuations model [5]:

$$\alpha \propto \int_0^\infty \frac{1}{\sigma_g\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{E_g - \bar{E}_g}{\sigma_g}\right)^2\right] \sqrt{E - E_g} dE_g$$



courtesy C. Perkins, NREL

- Se inhomogeneity suggests band gap distribution.

[1]] F. Urbach, "The long-wavelength edge of photographic sensitivity and of the electronic absorption of solids," *Physical Review*, vol. 92, no. 5, p. 1324, 1953.
[2] E. O. Kane, "Thomas-Fermi approach to impure semiconductor band structure," Physical Review, vol. 131, no. 1, p. 79, 1963.
[3] B. I. Shklovskii and A. L. Efros, Electronic properties of doped semiconductors, vol. 45. Springer Science & Business Media, 2013.
[4] M. Fox, "Optical properties of solids." American Association of Physics Teachers, 2002.
[5] J. Mattheis, U. Rau, and J. H. Werner, "Light absorption and emission in semiconductors with band gap fluctuations—A study on Cu(In,Ga)Se_2 thin films," Journal of applied physics, vol. 101, no. 11, p. 113519, 2007.

Band Tails Models

BGSU

- Katahara [1] fit PL data starting from generalized model, inspired by Kane [2]:

$$\alpha = \alpha_0 \sqrt{\gamma} G\left(\frac{E - E_g}{\gamma}\right)(f_v - f_c)$$

- $\alpha_0 \sim 10^5$ cm^{-1}eV$^{-1/2}$, E is photon energy, E_g is unperturbed band gap.
- $G(x)$ is the convolution of the square root DOS for extended states and sub-gap DOS to form a continuous function:

$$G(x) = \frac{1}{2\Gamma(1 + \frac{1}{\theta})} \int_{-\infty}^{\infty} \exp(-|x|^{\theta}) \sqrt{x - x'}\, \mathrm{d}x$$

$\theta = 1$ Urbach
$\theta = 5/4$ screened Thomas-Fermi
$\theta = 3/2$ Franz-Keldysh
$\theta = 2$ Thomas-Fermi.

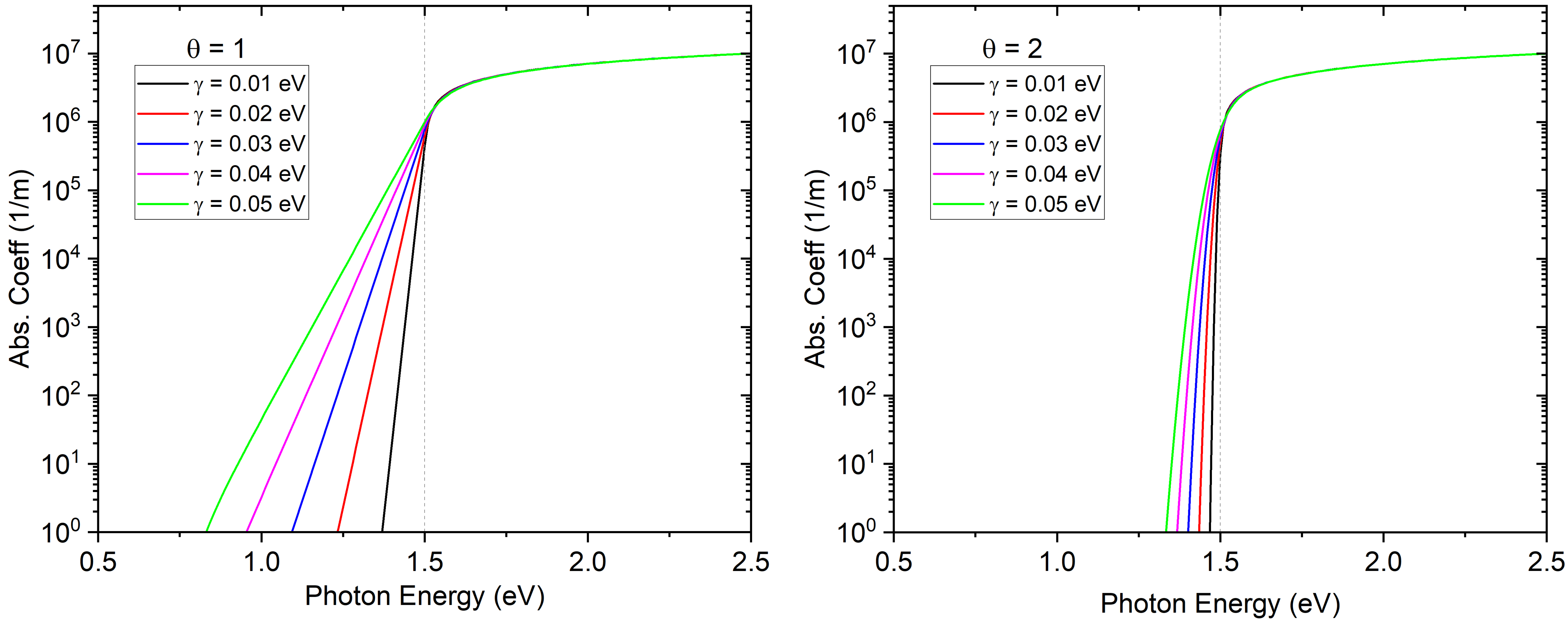
- f_v and f_c are valence and conduction band tail occupancies, and for a given QLFS = $\Delta\mu$, band-filling factor can be approximated:

$$(f_v - f_c) = 1 - \frac{2}{\exp\left(\frac{E - \Delta\mu}{2kT}\right) + 1}$$

[1] J. K. Katahara and H. W. Hillhouse, "Quasi-Fermi level splitting and sub-bandgap absorptivity from semiconductor photoluminescence," Journal of Applied Physics, vol. 116, no. 17, p. 173504, 2014.
[2] E. O. Kane, "Thomas-Fermi approach to impure semiconductor band structure," Physical Review, vol. 131, no. 1, p. 79, 1963.

Inputs for Device Simulation

- Calculate α for input to device models – shown below.
- Can also obtain α from measurement.

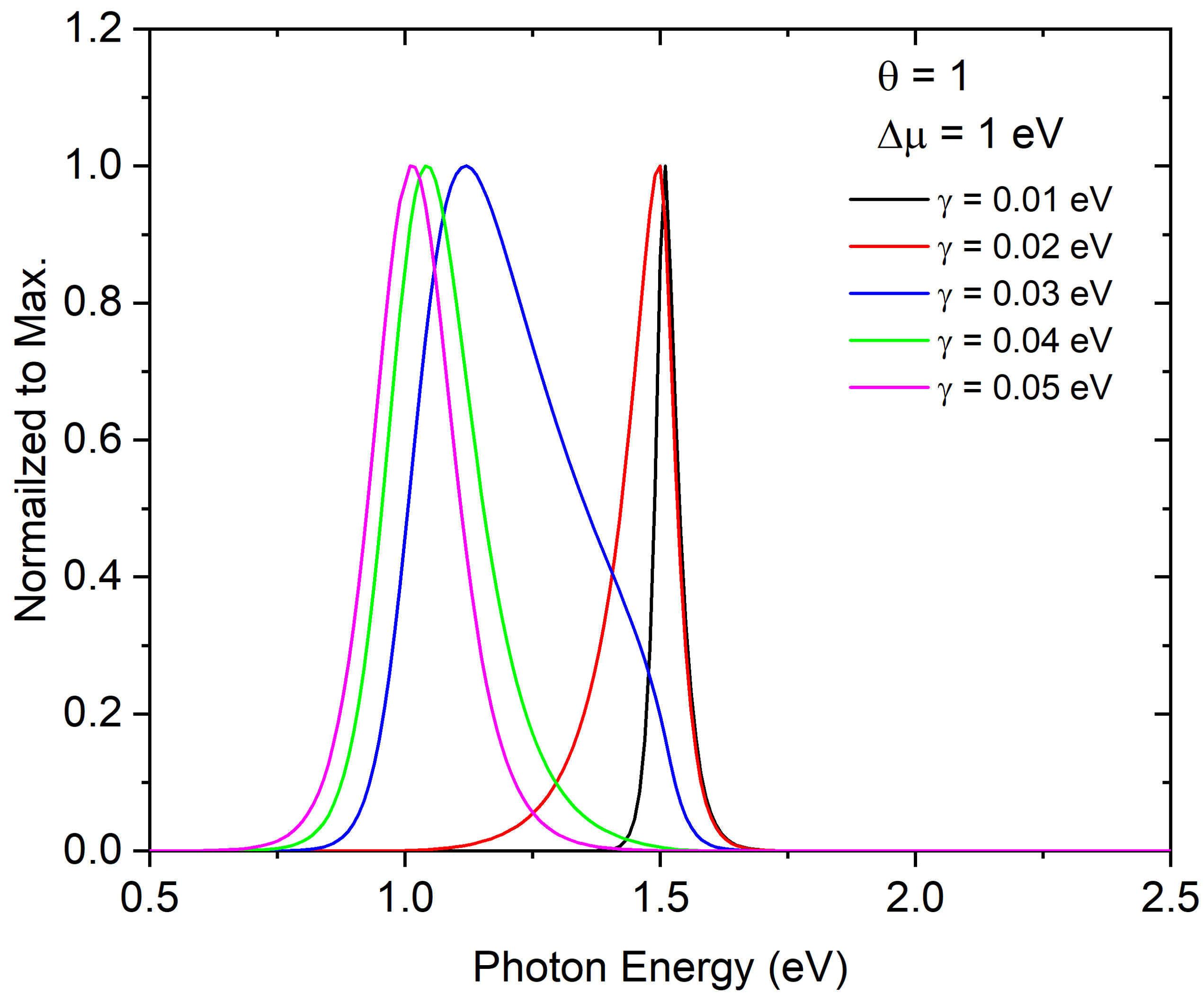


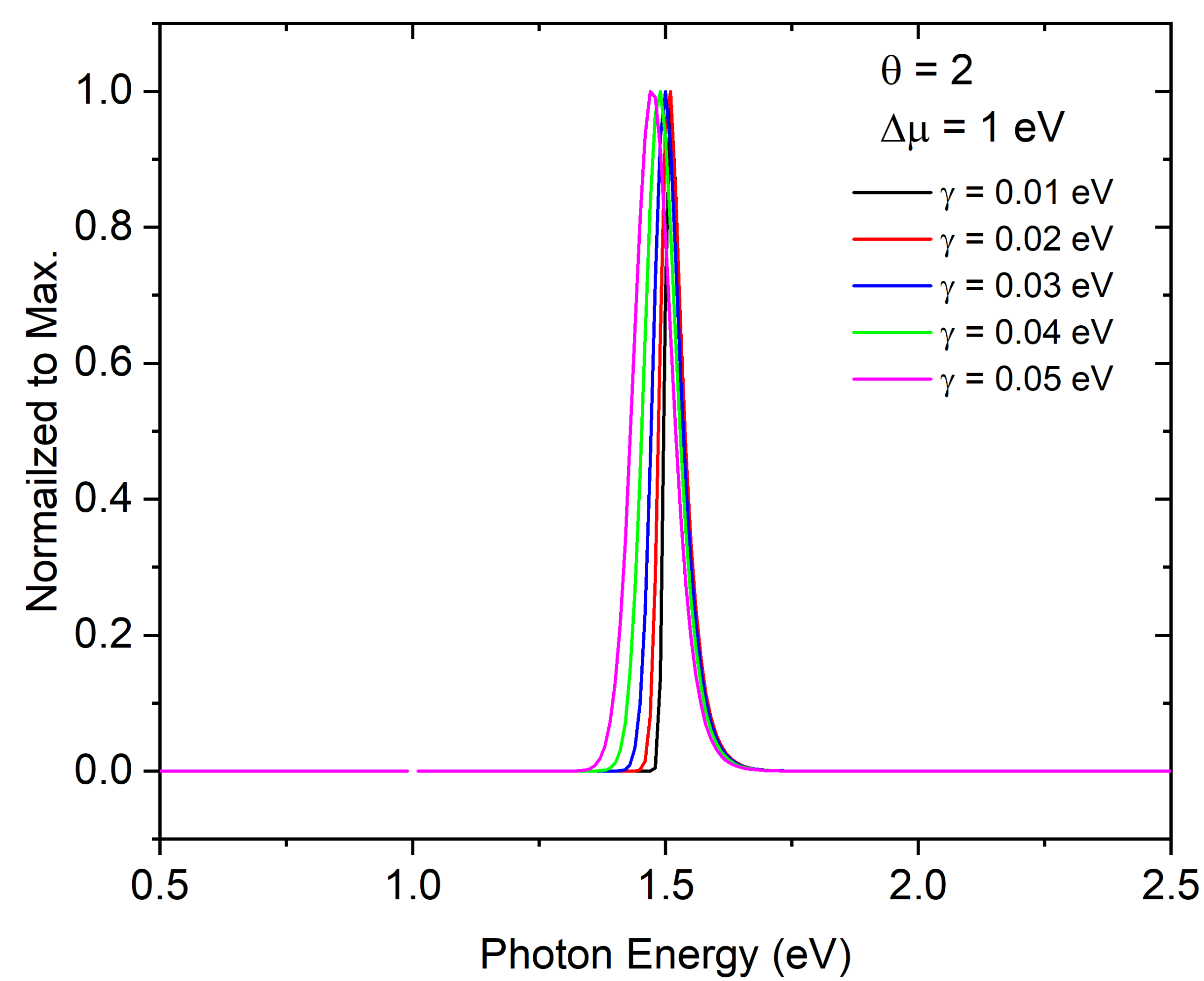
Inputs for Device Simulation

- PL gap, E_{PL}, is taken as the peak PL energy, calculated from:

$$I_{PL}(E) = \frac{2\pi a(E)}{\hbar^3 c^2} \frac{E^2}{\exp\left(\frac{E-\Delta\mu}{kT}\right) - 1}$$

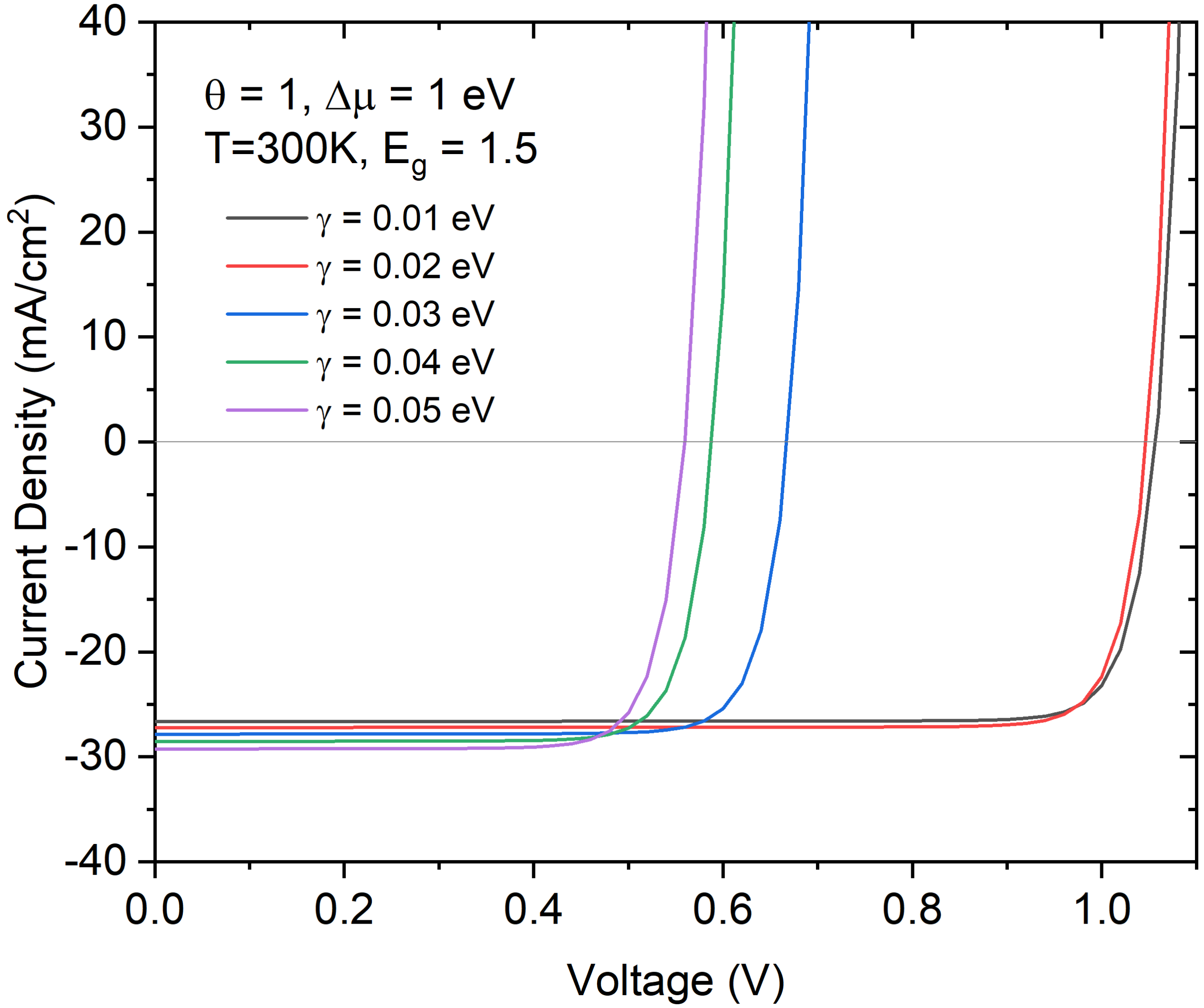
with absorptance: $a = 1 - \exp(-\alpha L)$

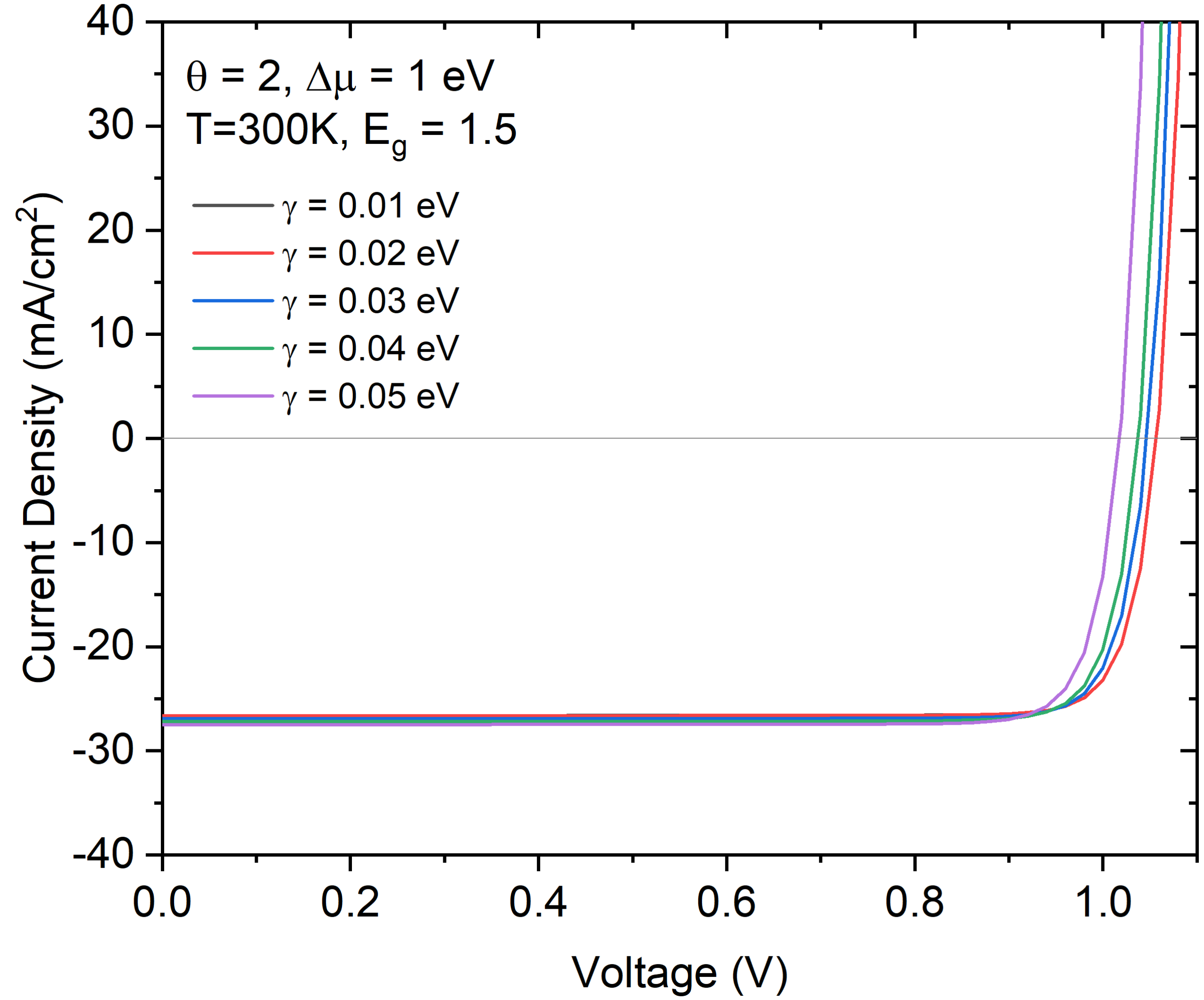




Initial Simulation Results

- initial results for SnO_2/CdTe device model with unperturbed band gap = 1.5 eV
- Significant Voc loss for θ = 1





Summary

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- Generalized band tail model employed in device simulations
  - inputs can be from theory or measurement
- Band tails are observed in PL and CL data
- Result in significant V_{oc} losses
- Simulations useful for predicting band tail effects on device performance and characterization techniques:
  - JVTi, CV, QE
  - e-beam methods - EBIC, CL, and TI
  - TRPL, etc…

Acknowledgements

- DOE-SETO/NREL, “Development and Application of Voltage Loss Analysis for Advanced Thin-Film PV”
  - PI: Darius Kuciauskas.

- DOE-SETO/NREL, “CdTe Core Group”
  - PI: Matthew Reese.

- Students: Sakshi Gupta, Andrew Prostor, Fiona Warner

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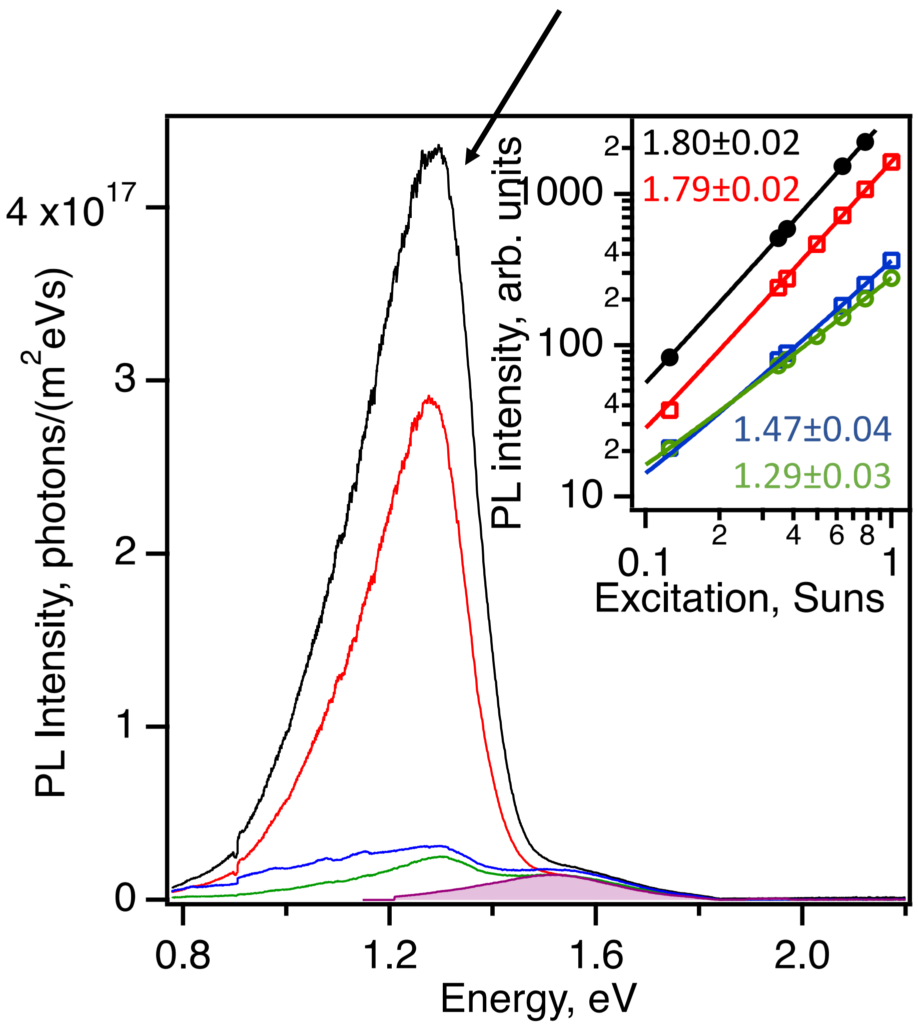
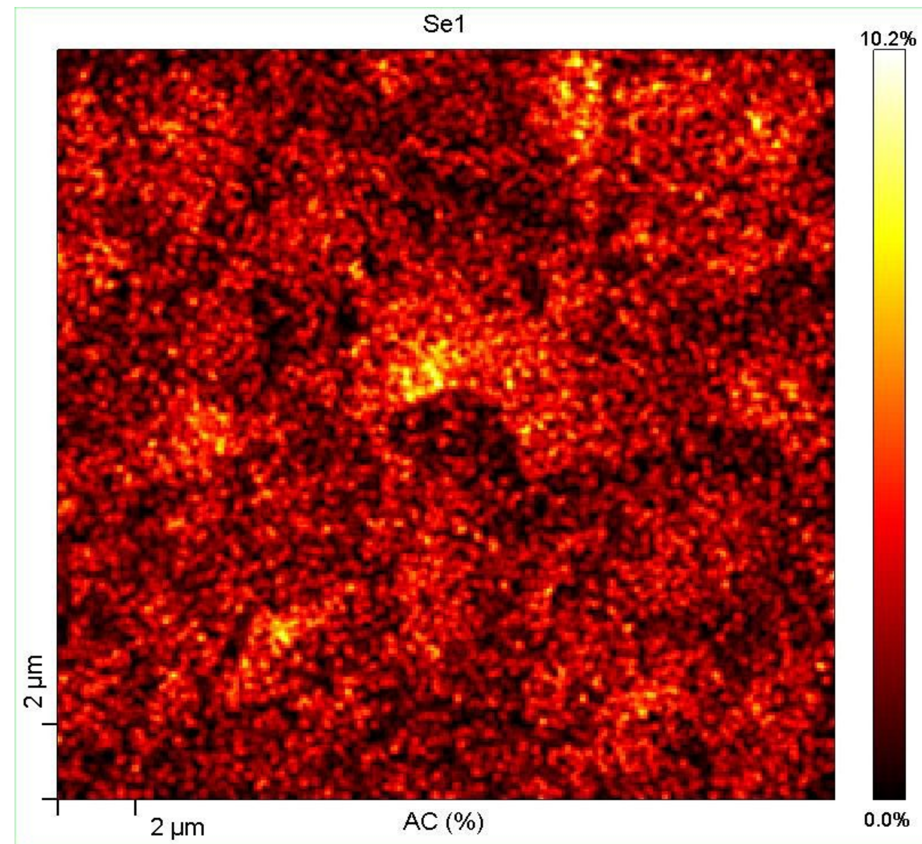
CHANGING LIVES FOR THE WORLD.

Band Tails - Observations

Different tails observed in As-doped absorbers



courtesy D. Kuciauskas, NREL



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- Se inhomogeneity suggests band gap distribution.