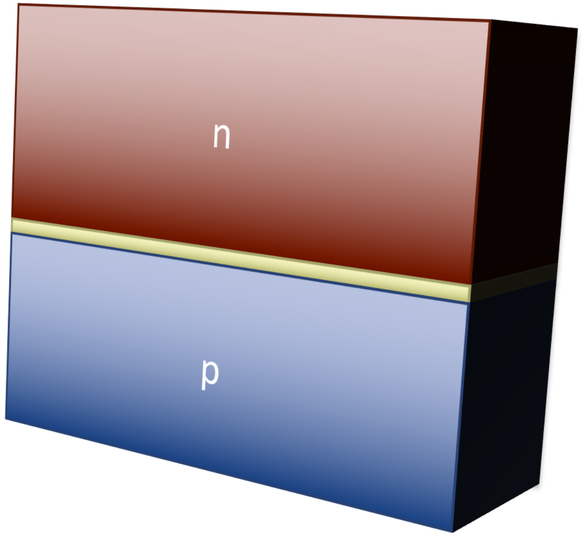
Intermediate band materials for high efficiency solar cells: overview and future directions

uOttawa



Jacob J Krich

Department of Physics
&
School of Electrical Engineering
and Computer Science

University of Ottawa

Collaborators

uOttawa

Eduard Dumitrescu
Akshay Krishna
Kyle Robertson
Luc Robichaud
Peter Rose
Anna Trojnar
Josh Wheeler
Matt Wilkins
Daixi Xia
Emily Zhang

Karin Hinzer
- **Ross Cheriton**
- Alex Walker

US Army Research

Jeff Warrender
- Quentin Hudspeth
- Philippe Chow

McGill/Michigan

Zetian Mi
- Ashfiqua Connie
- Hieu Nguyen

Stanford

Aaron Lindenberg

Middlebury

Renee Sher

Australian National University

Jim Williams
- Shao Qi Lim
- Wenjie Yang

Harvard

Bertrand Halperin
Michael Aziz
- Dan Recht

Eric Mazur

Toronto

Alán Aspuru-Guzik

MIT

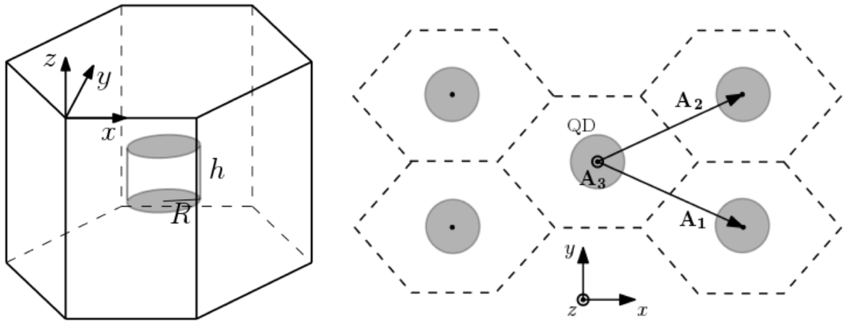
Tonio Buonassisi
- Austin Akey
- Christie Simmons
- **Joe Sullivan**
- Mark Winkler

University of Dayton

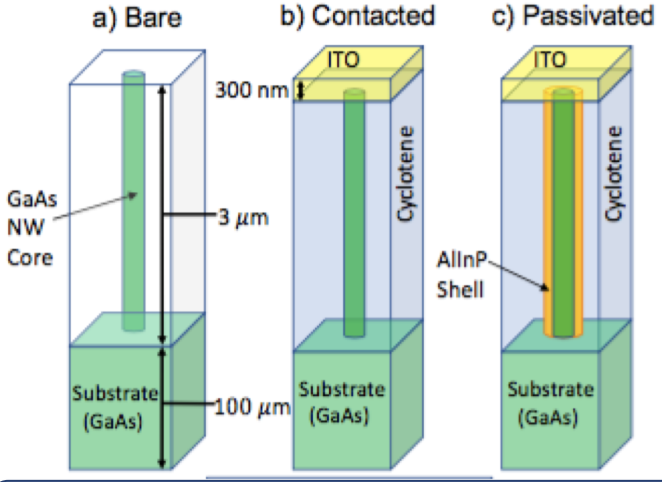
Jay Mathews
- Yining Liu

Present topics in the group

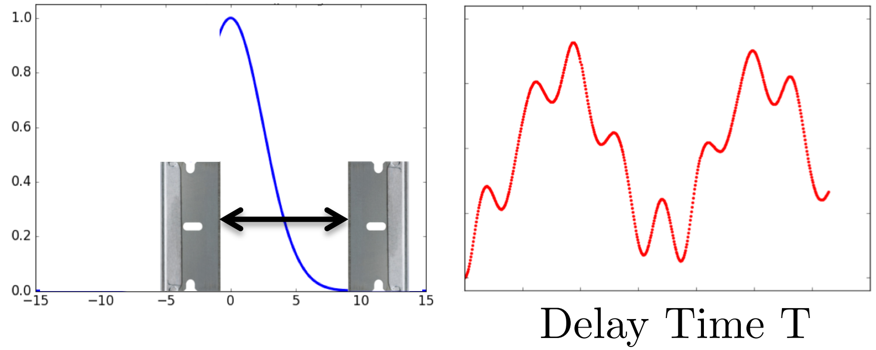
Intermediate band materials



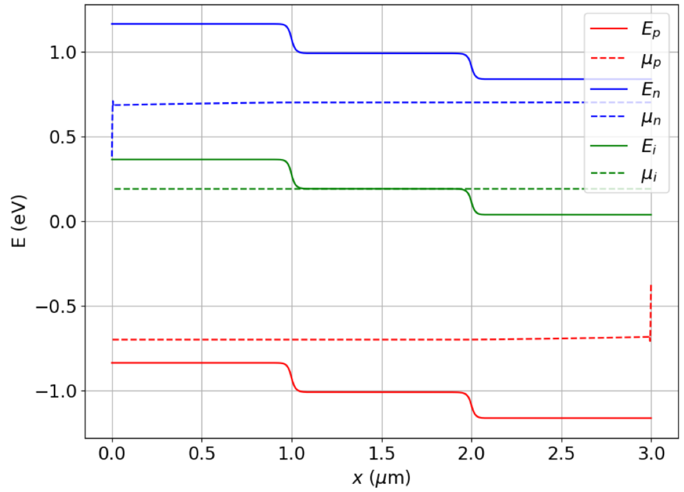
Nanowire PV



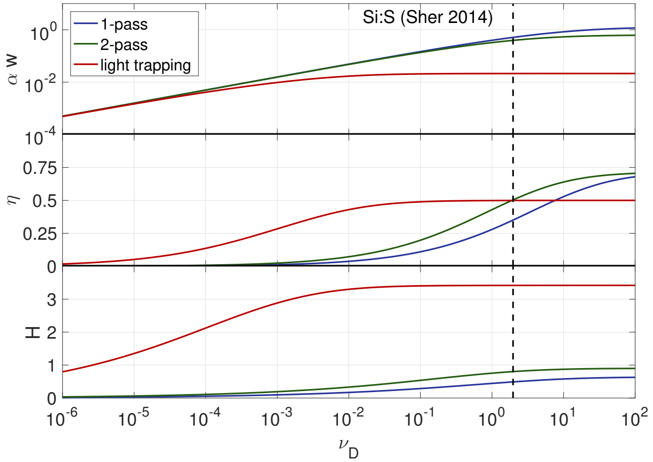
Quantum biology/ nonlinear spectroscopy



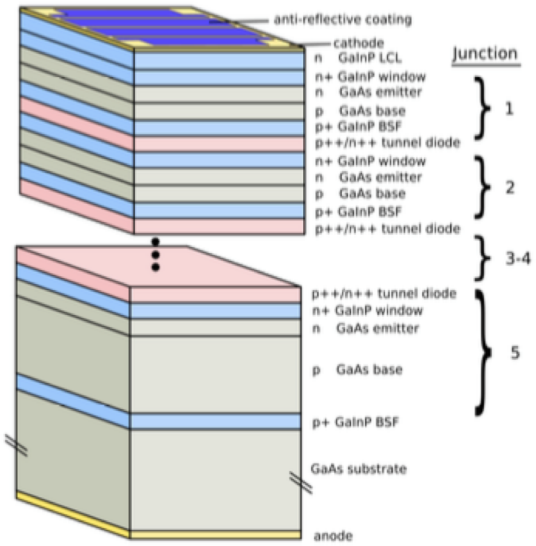
IB device modeling



IB IR photodetectors



Monochromatic PV

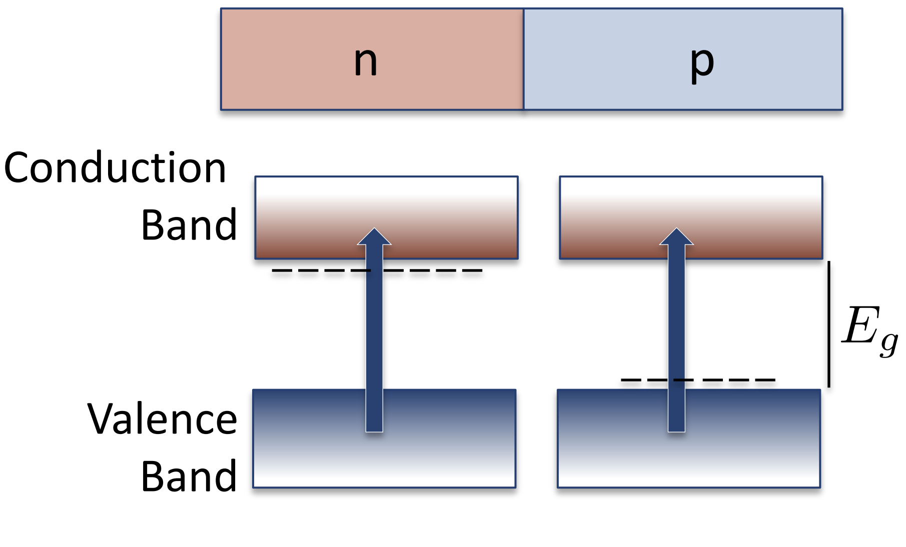


Jacob J. Krich

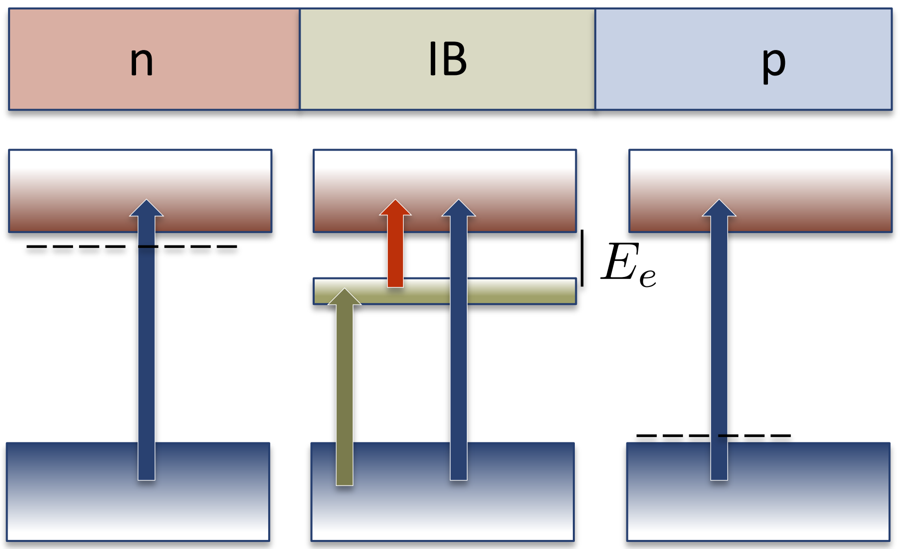
Outline

- Intermediate band solar cells
  - 3 material classes
- Figure of merit
  - Measurements
  - Predictions
- New developments
  - InGaN quantum dots in nanowires
  - Device model

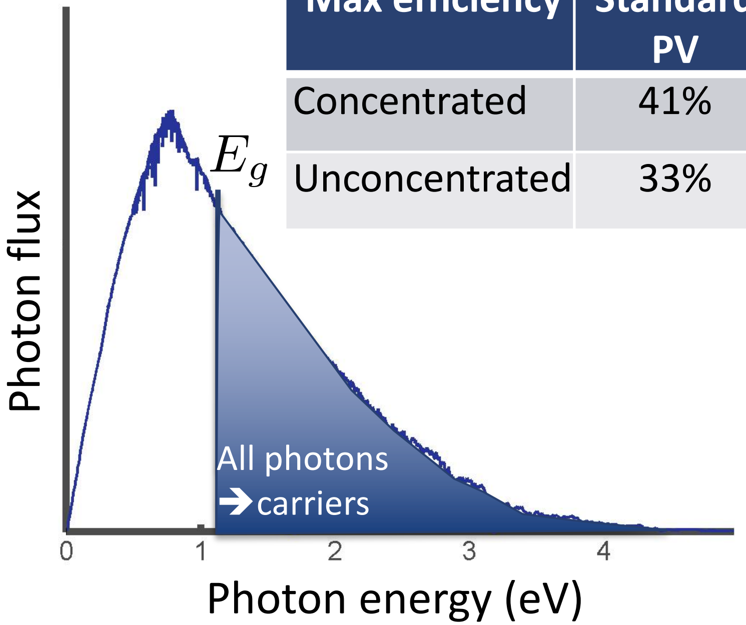
Standard PV

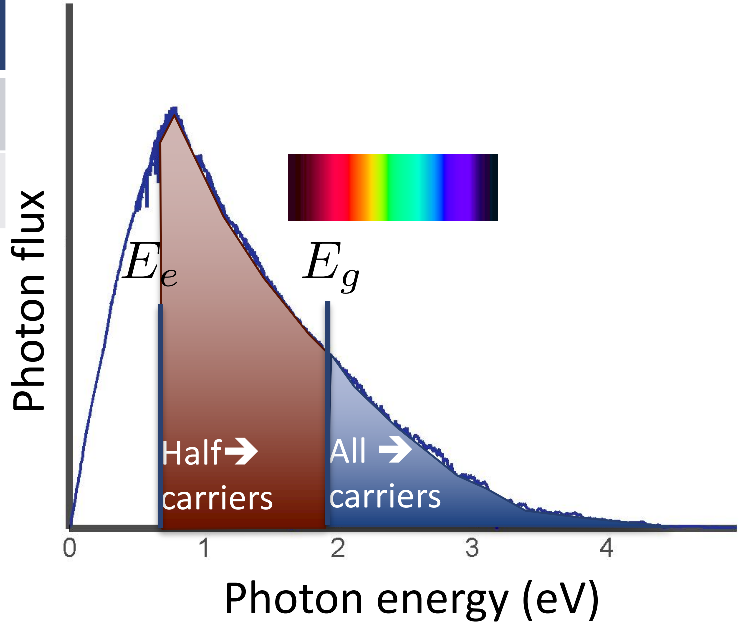


Intermediate band PV

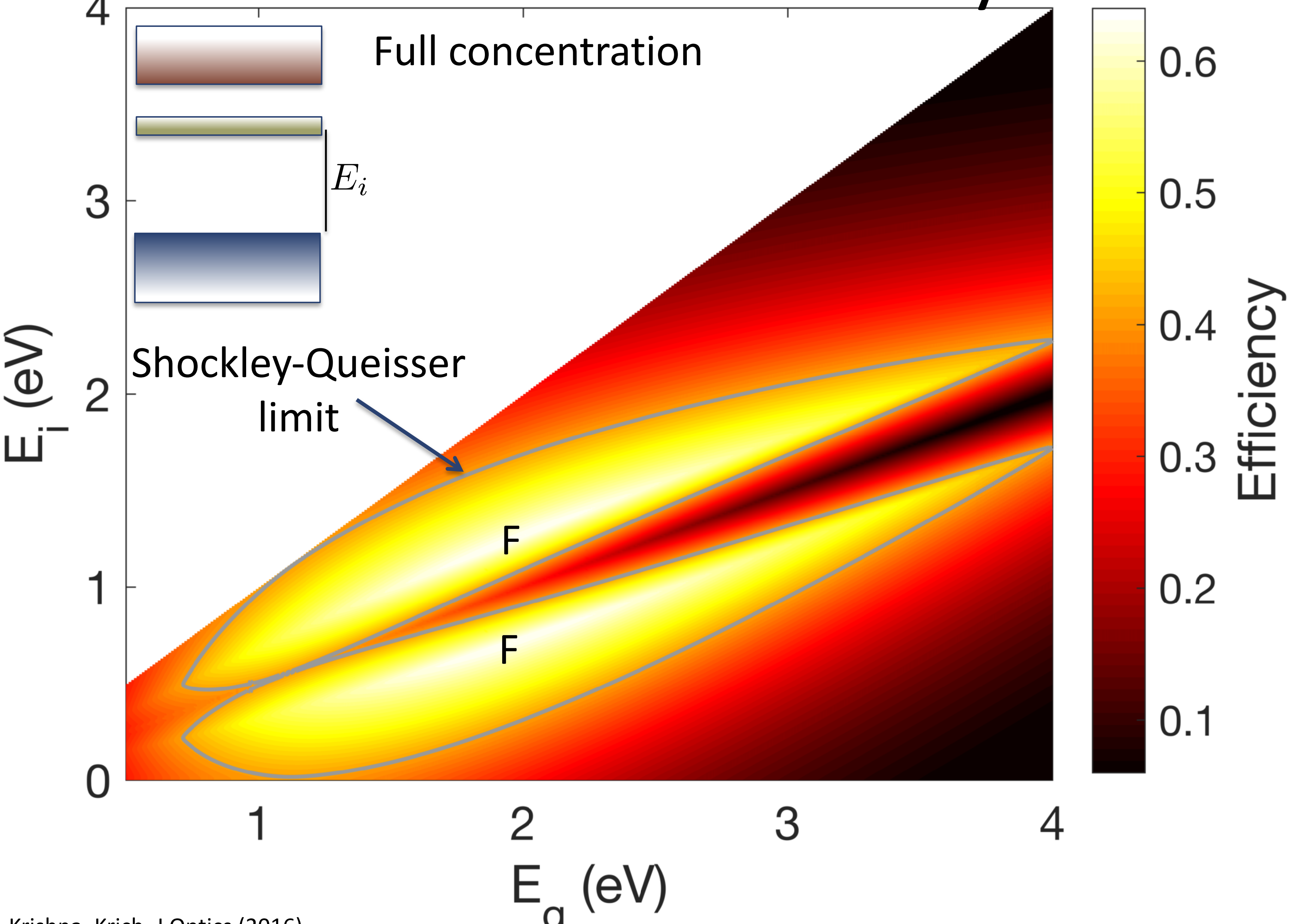


Max efficiency	Standard PV	IBPV
Concentrated	41%	63%
Unconcentrated	33%	47%



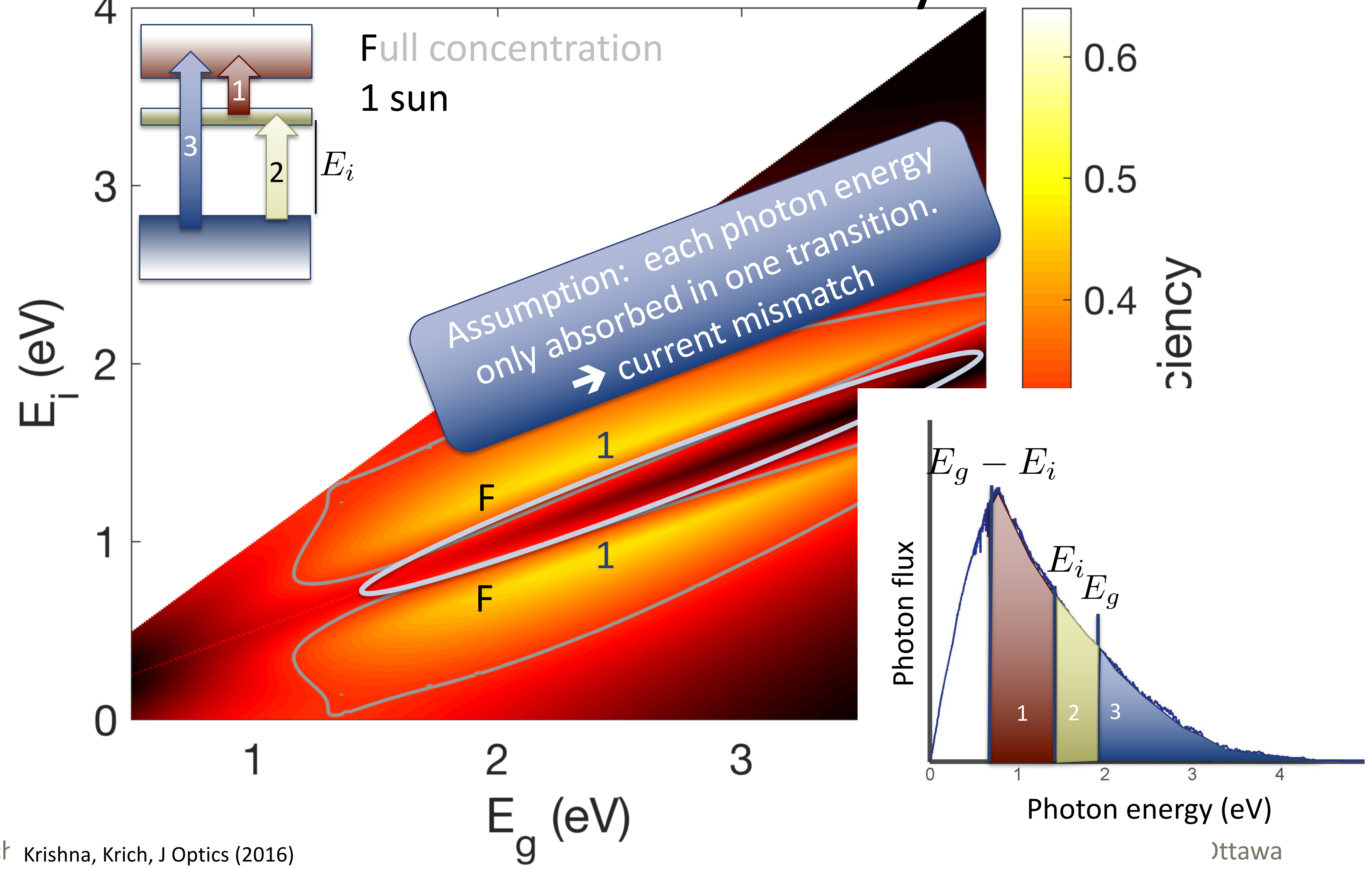


Detailed balance efficiency limits



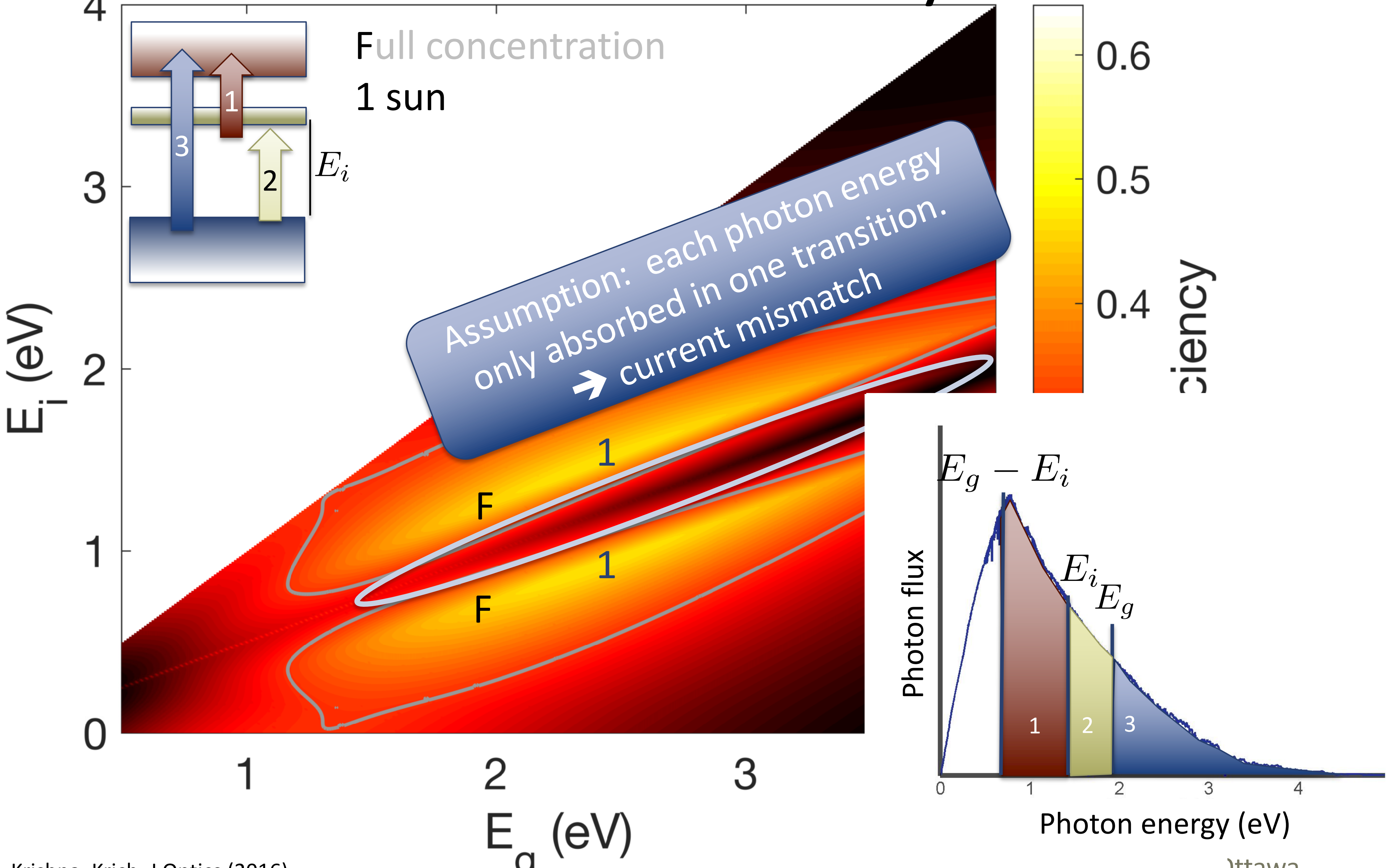
Krishna, Krich, J Optics (2016)

Detailed balance efficiency limits



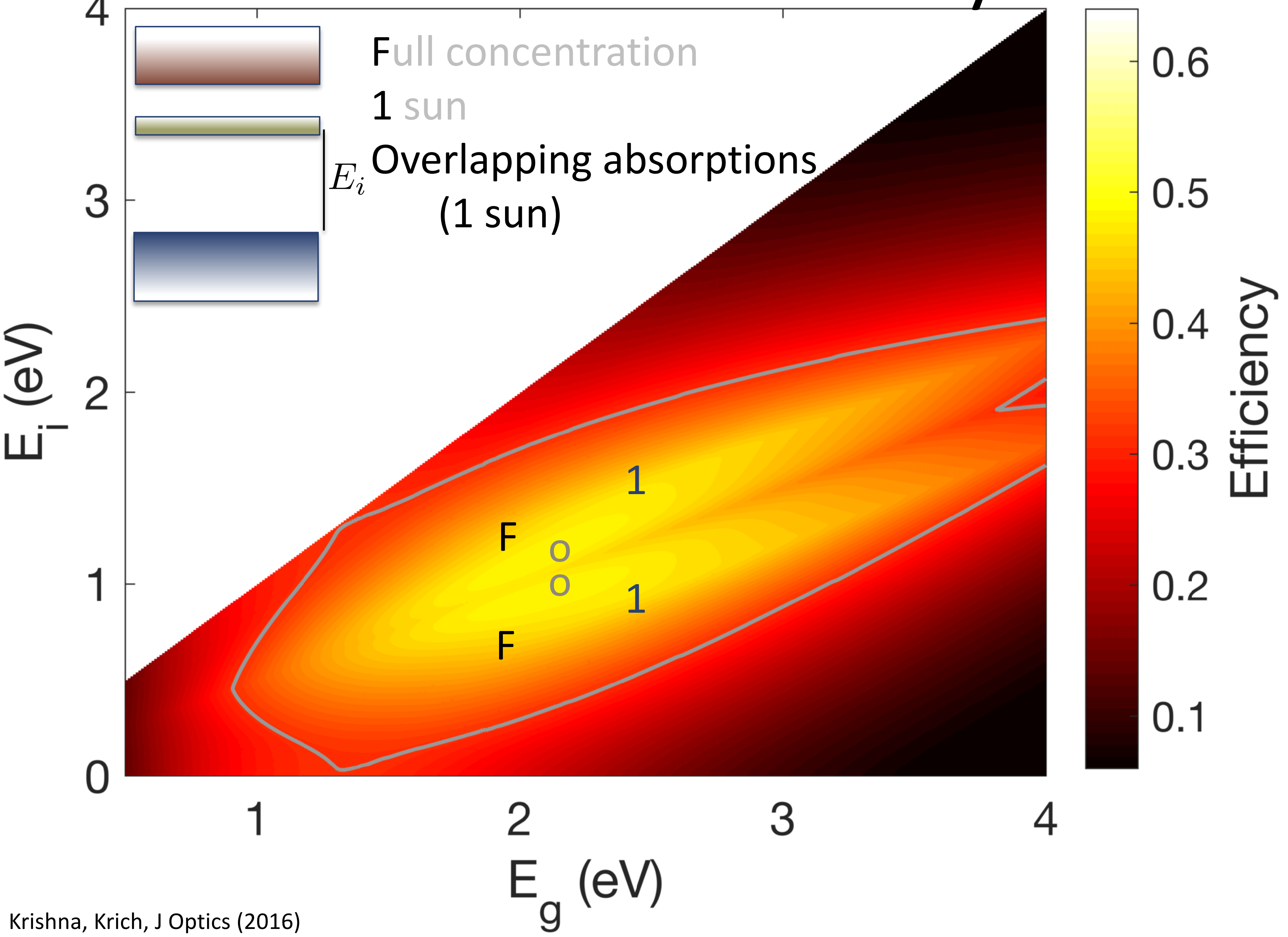
 Krishna, Krich, J Optics (2016)

Detailed balance efficiency limits



 Krishna, Krich, J Optics (2016)

Detailed balance efficiency limits

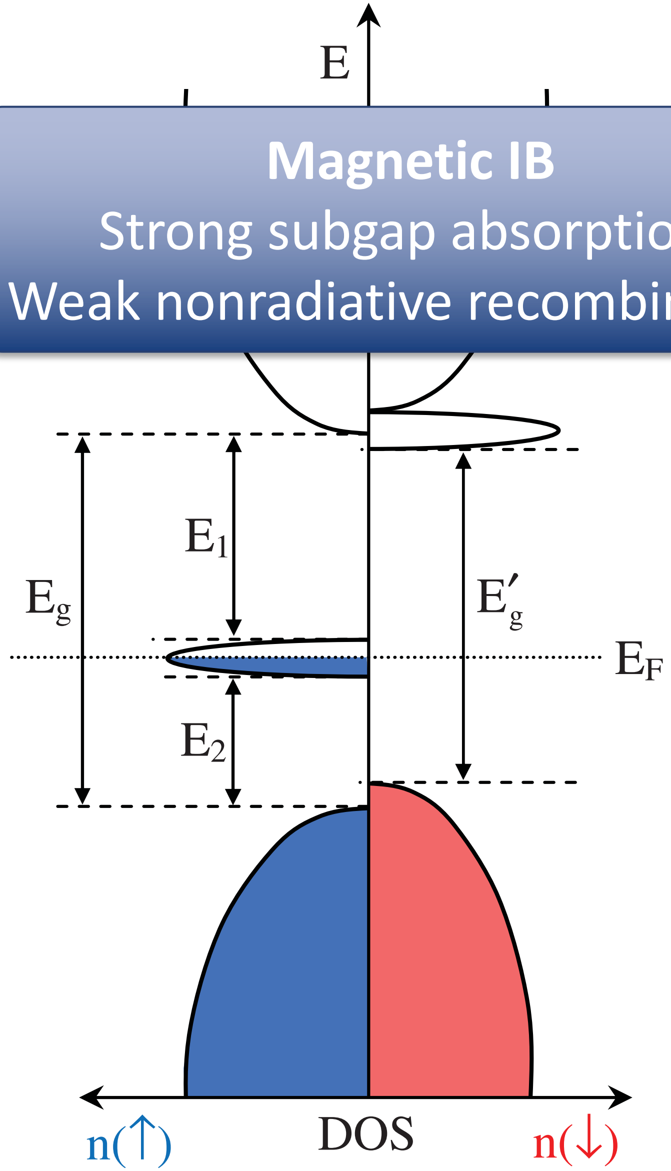


Krishna, Krich, J Optics (2016)

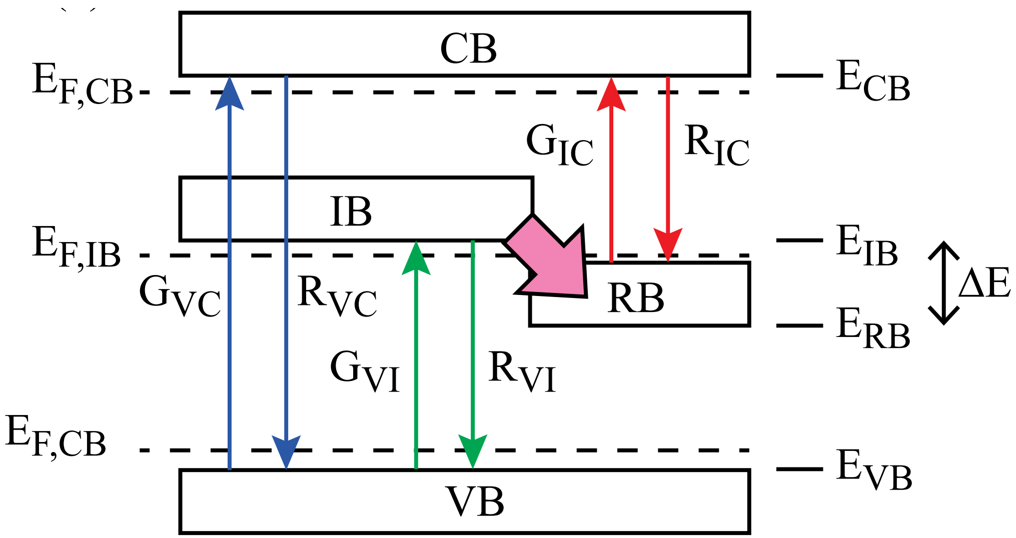
IBPV variants

Magnetic IB
Strong subgap absorption,
Weak nonradiative recombination

Ratchet band
Turn off recombination pathways
Better voltage matching



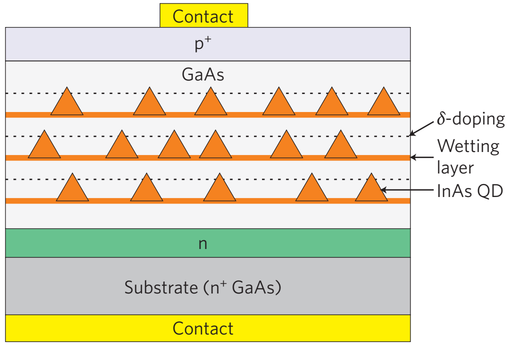
Olsson, Domain, Guillemoles, PRL 2009



Yoshida, Ekins-Daukes, Farrell, Phillips, APL 2012

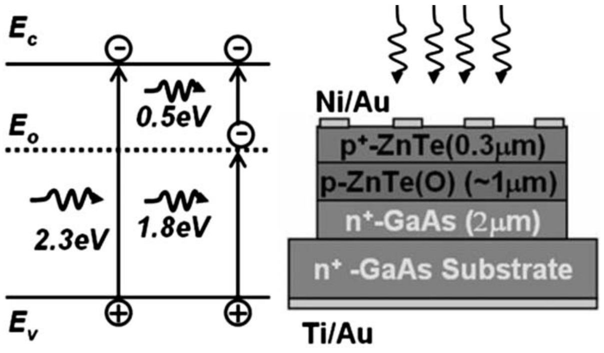
3 Candidate Materials Classes

1 Quantum dots



Luque et al., Nat Photon 2012

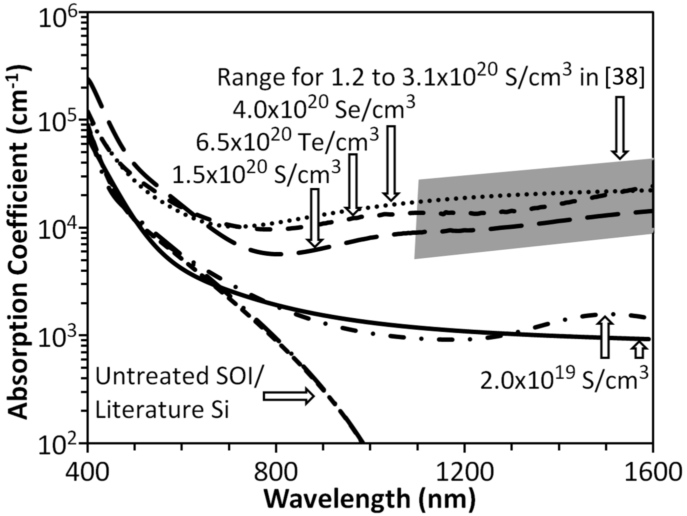
2 Highly-mismatched alloys



ZnTeO

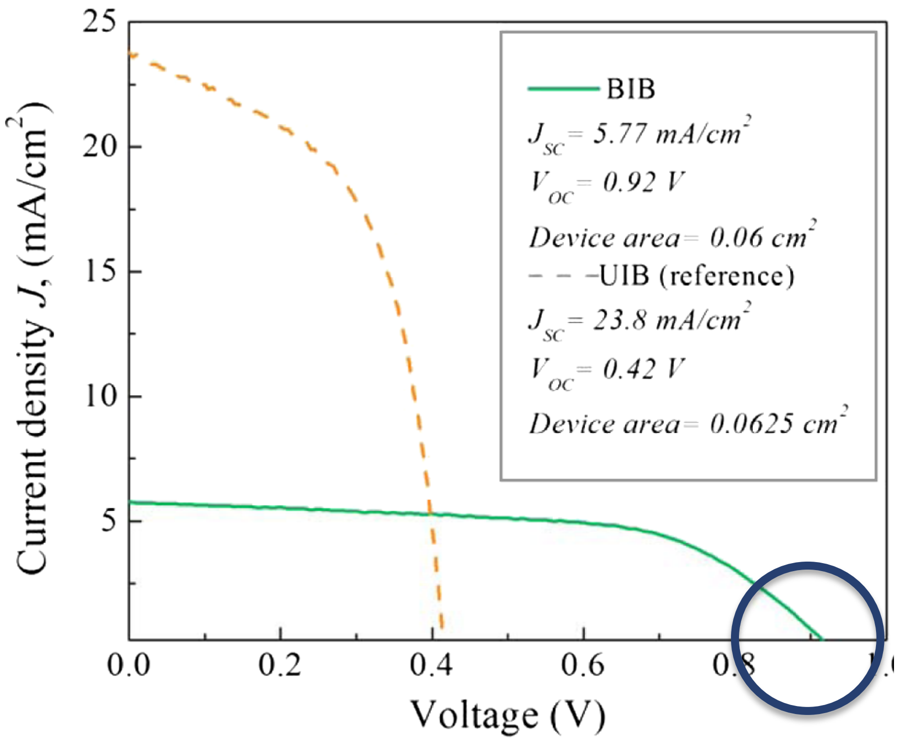
Wang et al., APL 2009

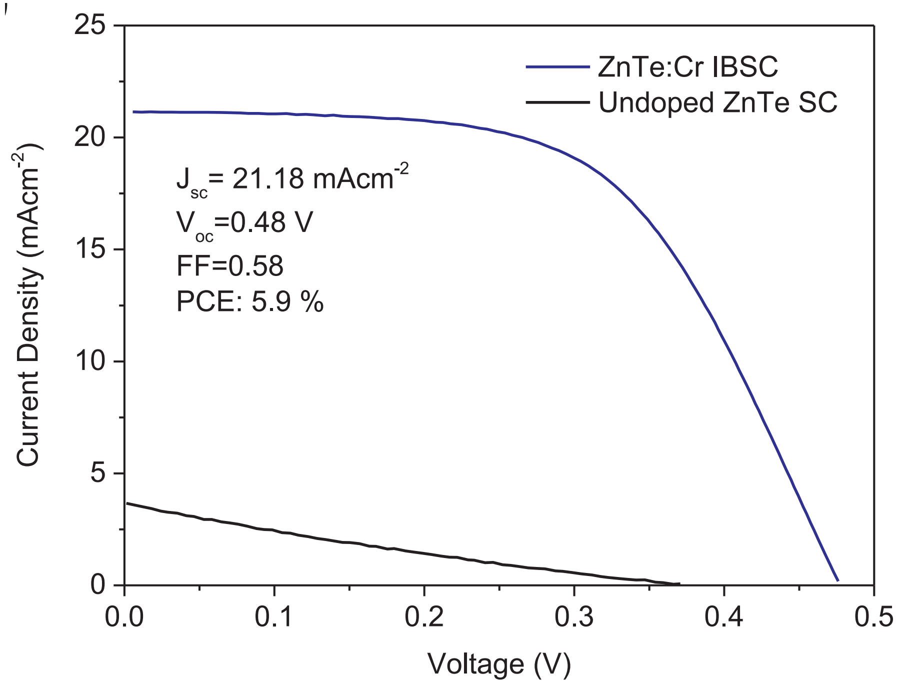
3 Hyperdoped silicon



Pan et al, APL (2011)

Best bulk IBPV devices so far



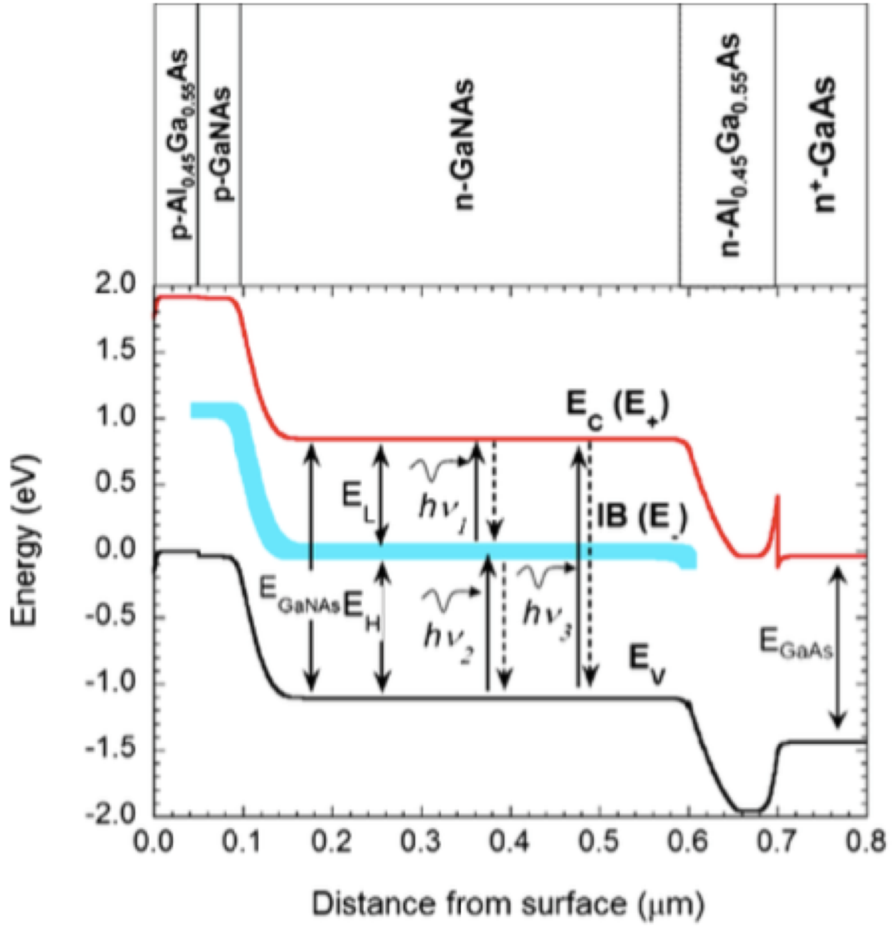


GaAs/GaNAs
<1% efficient
López et al., PRL 2011

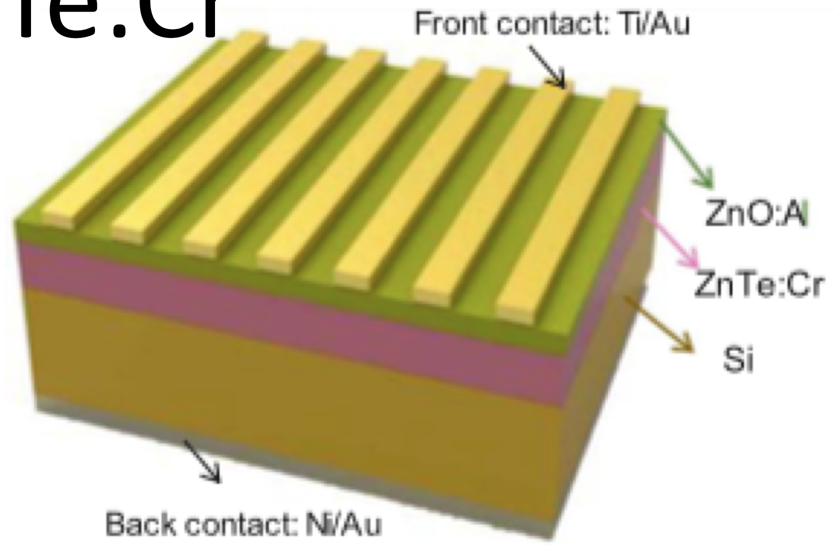
Devices not optimized, but clear lifetime problem.

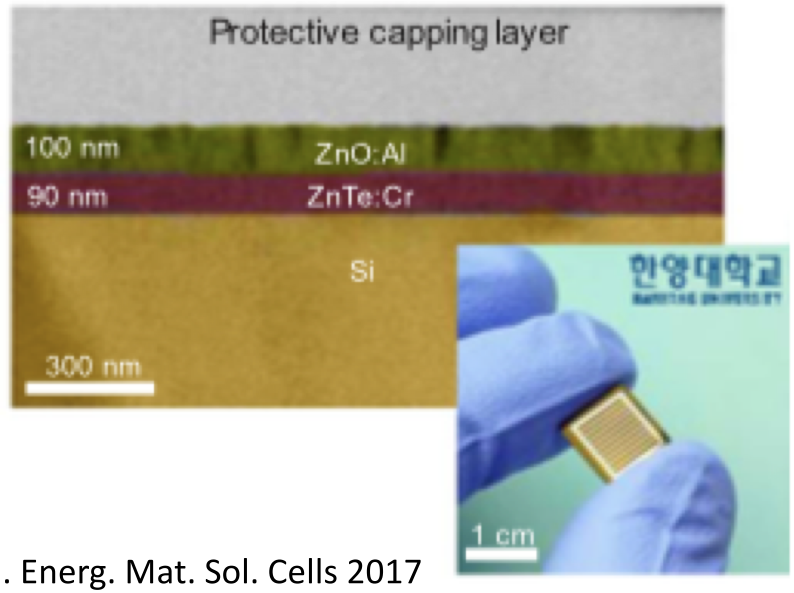
ZnTe:Cr
5.9% efficient
Lee et al., Sol. Energ. Mat. Sol. Cells 2017

GaNAs and ZnTe:Cr



López et al., PRL 2011

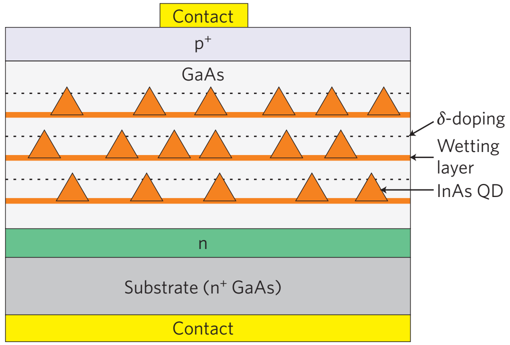




Lee et al., Sol. Energ. Mat. Sol. Cells 2017

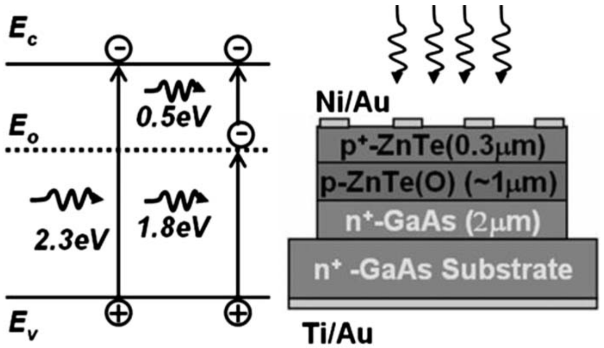
3 Candidate Materials Classes

1 Quantum dots



Luque et al., Nat Photon 2012

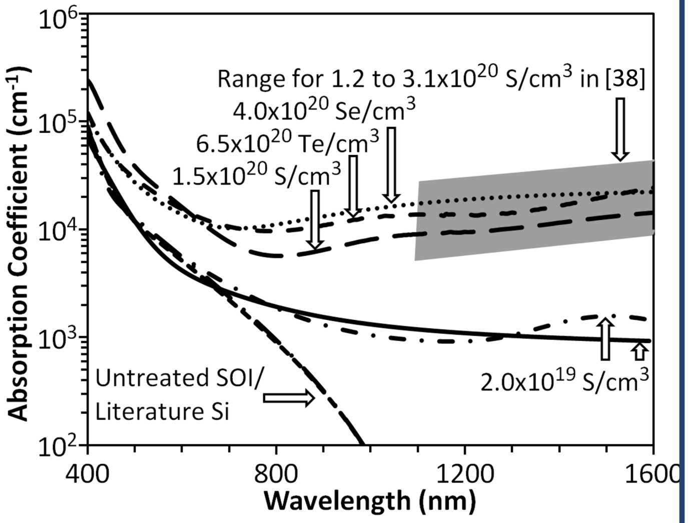
2 Highly-mismatched alloys



ZnTeO

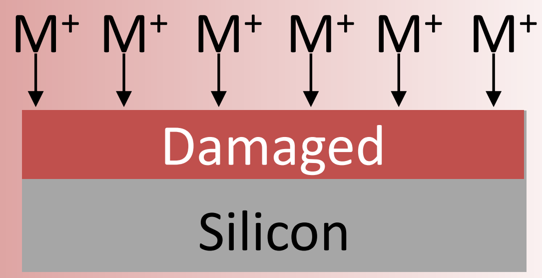
Wang et al., APL 2009

3 Hyperdoped silicon



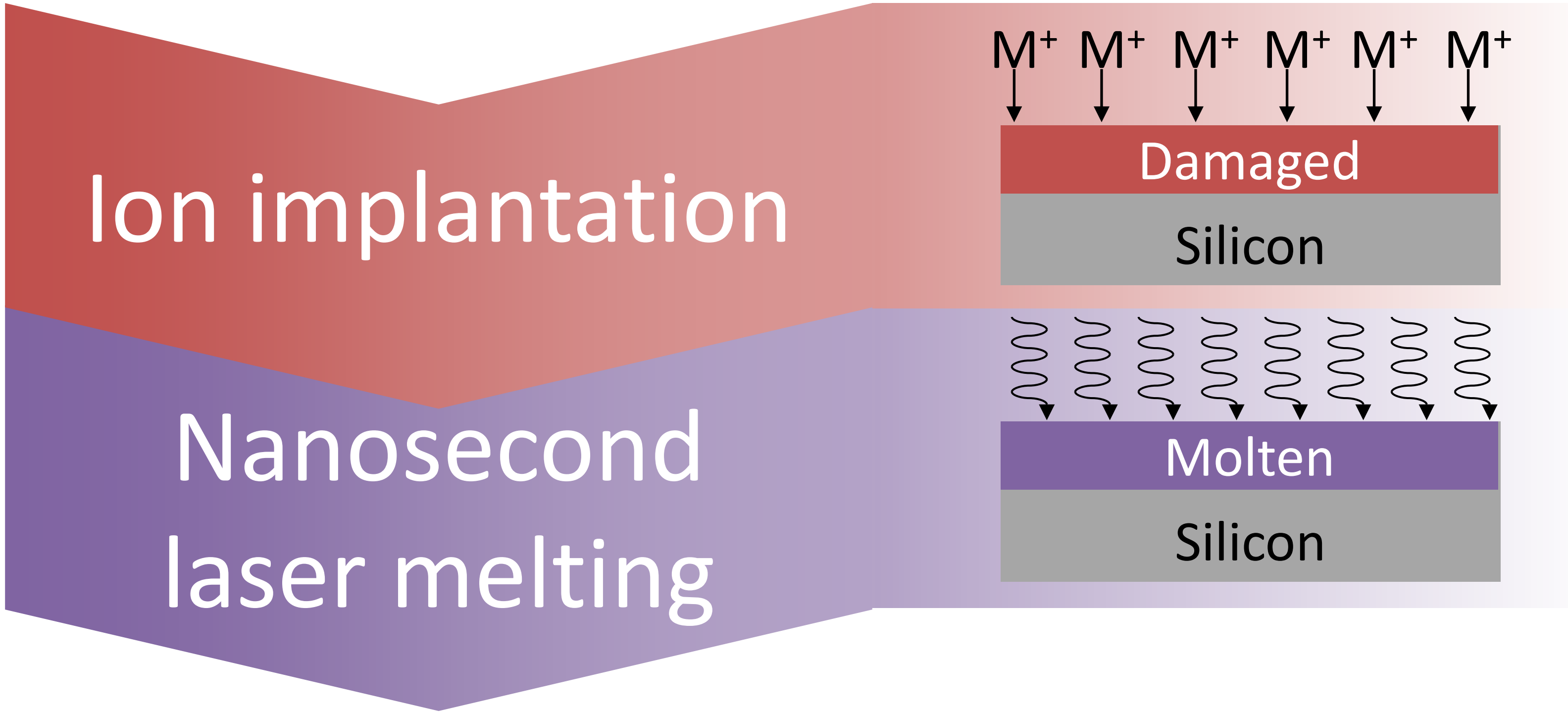
Pan et al, APL (2011)

Ion implantation



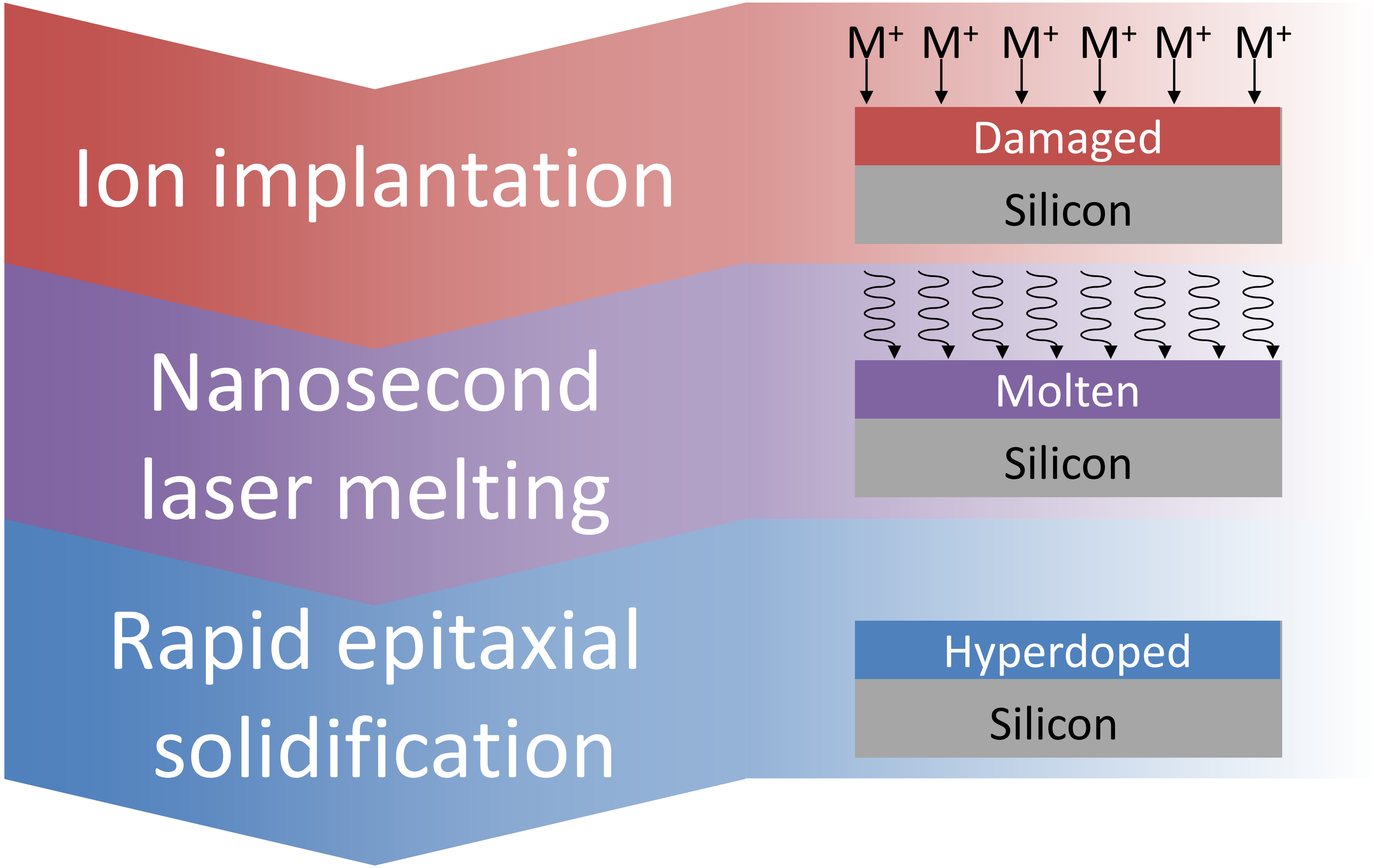
ANU

Slide from Dan Recht



ANU

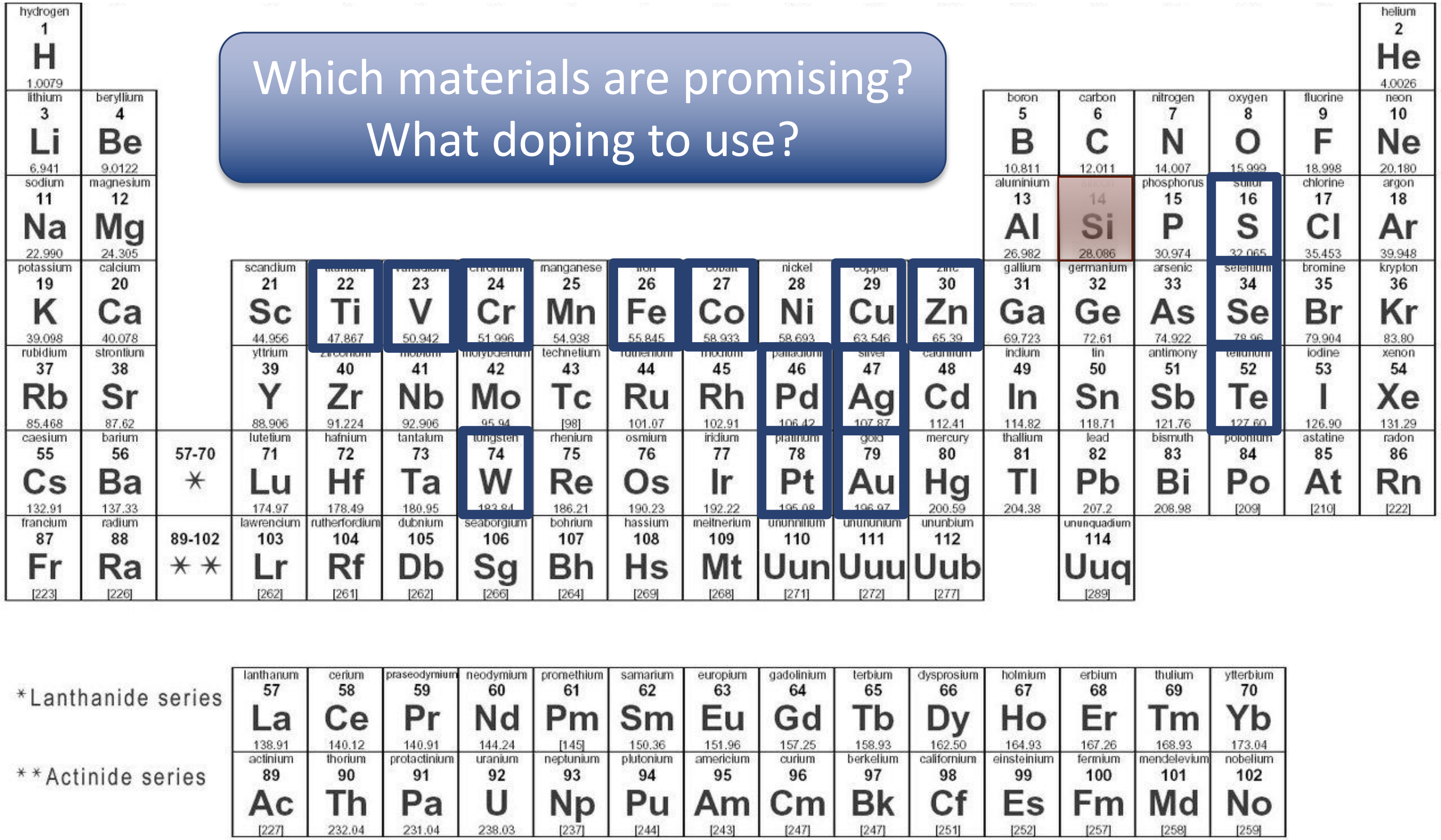
Benét Labs
New York



ANU

Benét Labs
New York

Hyperdoping in Silicon



https://commons.wikimedia.org/wiki/File:Modern_Periodic_Table.jpg

Figures of merit

Absorber materials

- Band gaps
- Absorptivity α
- Lifetime τ
- Mobility μ

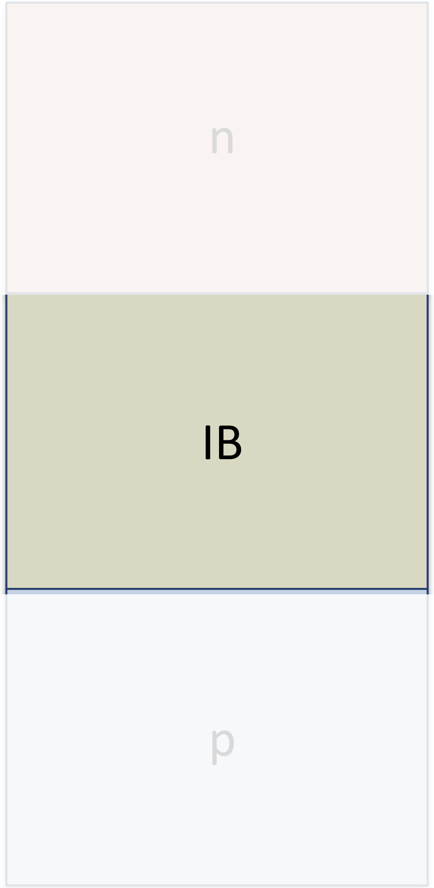
Devices

- Efficiency
- V_{oc}
- J_{sc}
- FF

Want:

- Absorber only
- High predictive value

Indicate when to work on devices



Motivating a fig

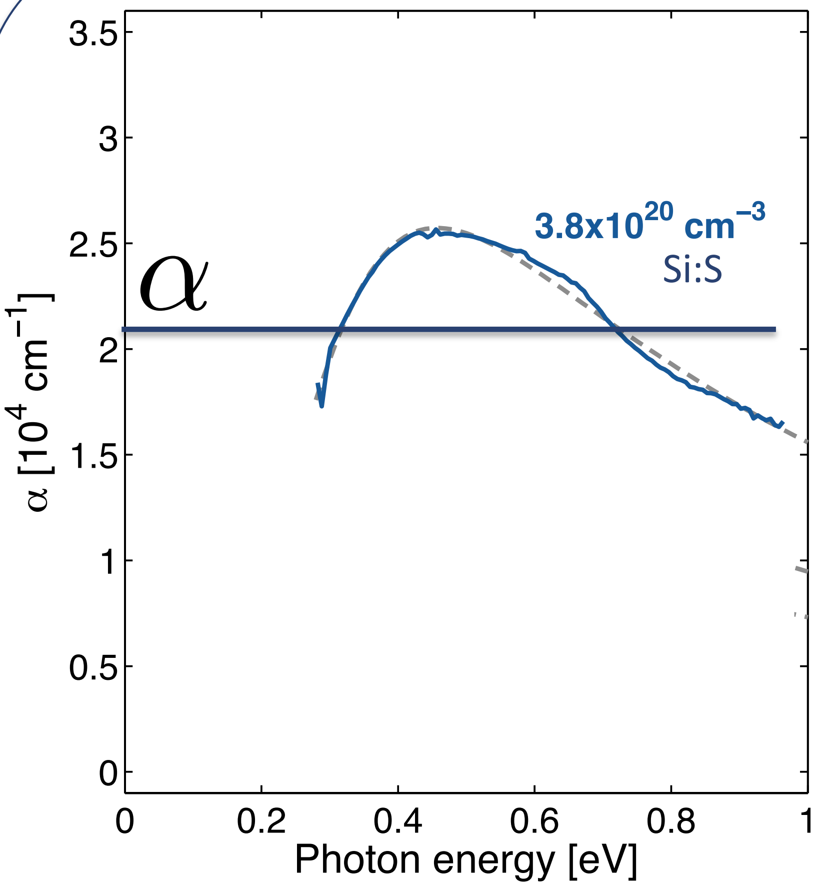
A good device has

carrier **lifetime** in IB region

$$\frac{\tau}{t} \gg 1$$

ar

transit time through IB region



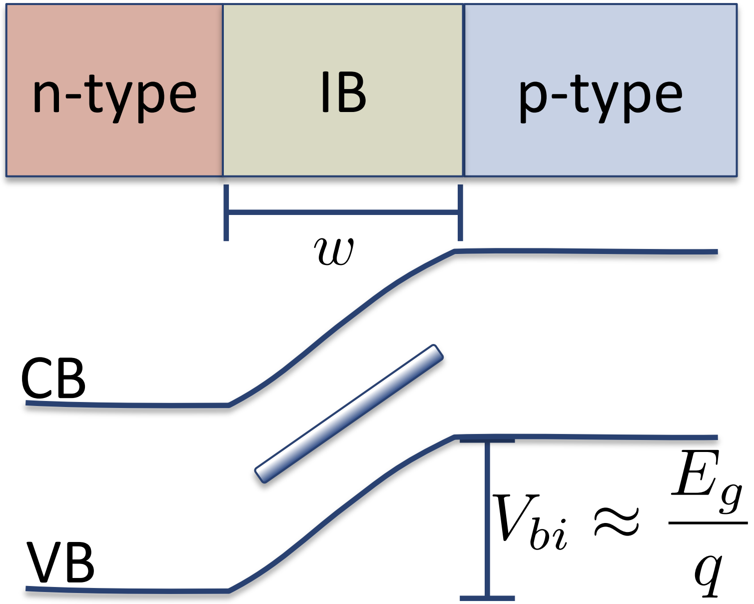
Sullivan et al., JAP 2013

Krich, Halperin, and Aspuru-Guzik, J App Phys 2012

Drift Device

$$E = \frac{V_{bi}}{w} \approx \frac{E_g}{qw}$$

$$t = \frac{w}{v_{\mathrm{drift}}} = \frac{w}{\mu E} \approx \frac{w^2 q}{\mu E_g} \approx \frac{q}{\mu E_g \alpha^2}$$



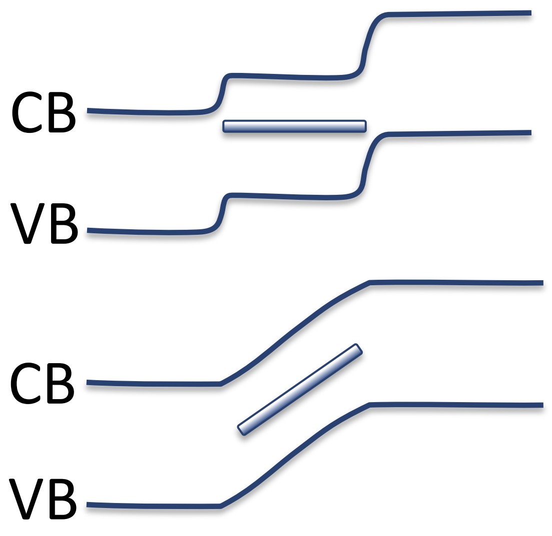
$$\frac{\tau}{t} \approx \boxed{\nu_{\mathrm{drift}} = \frac{E_g}{q}\mu\alpha^2\tau}$$

Krich, Halperin, and Aspuru-Guzik, J App Phys 2012

Comparison of figures of merit

$$\nu_{diff} = \frac{k_b T}{q}\mu\alpha^2\tau$$

$$\nu_{drift} = \frac{E_g}{q}\mu\alpha^2\tau$$

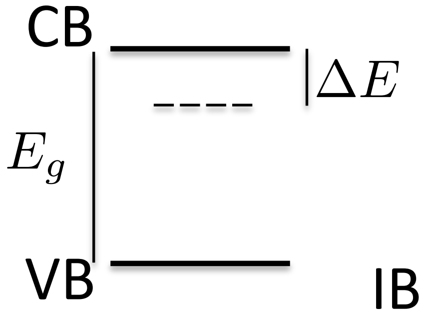


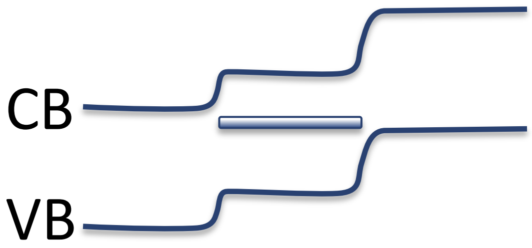
Measurable parameters of IB material alone.

Good devices: large ν for both electrons and holes.

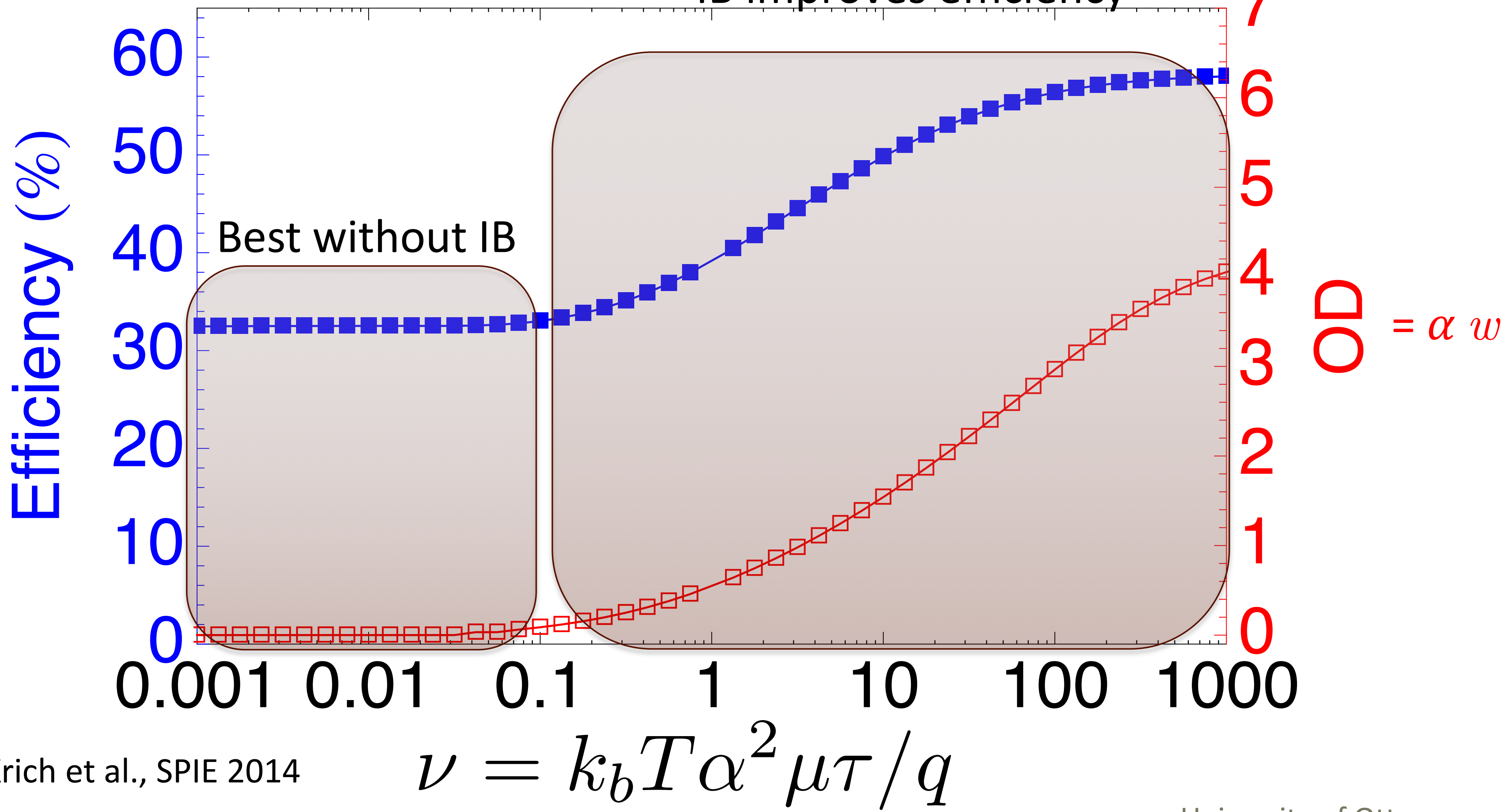
Krich, Halperin, and Aspuru-Guzik, J App Phys 2012

E_g = 1.9 eV
ΔE = 0.7 eV
full concentration





IB improves efficiency



Krich et al., SPIE 2014

Light trapping

Effectively increase *α* by $4n^2 \approx 47$

Increases ν by $(4n^2)^2 \approx 2000$

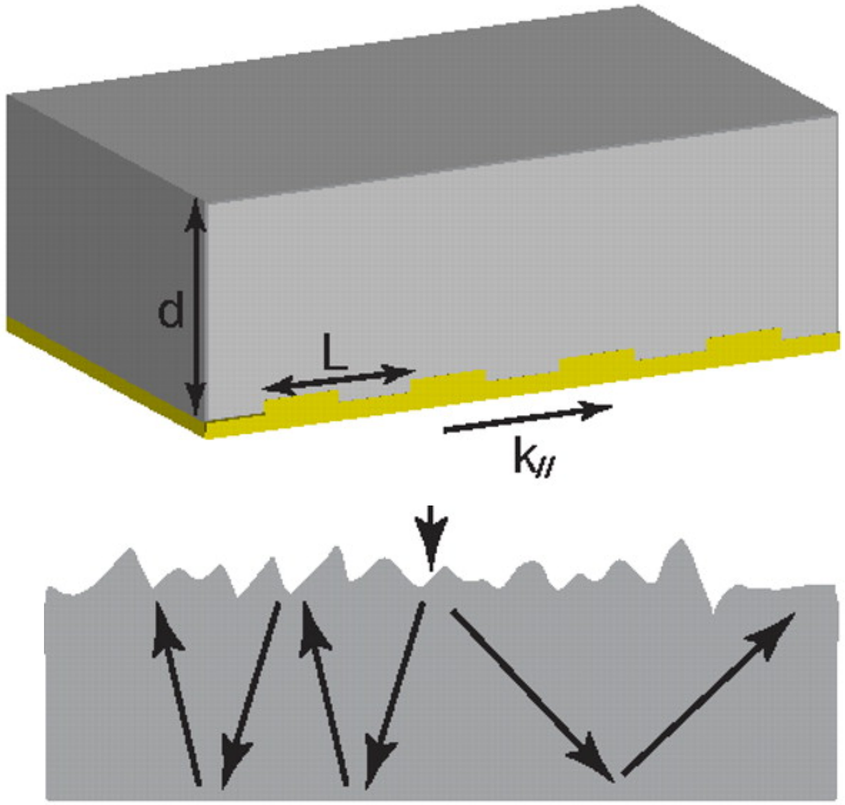


Figure from Yu et al, PNAS 2010

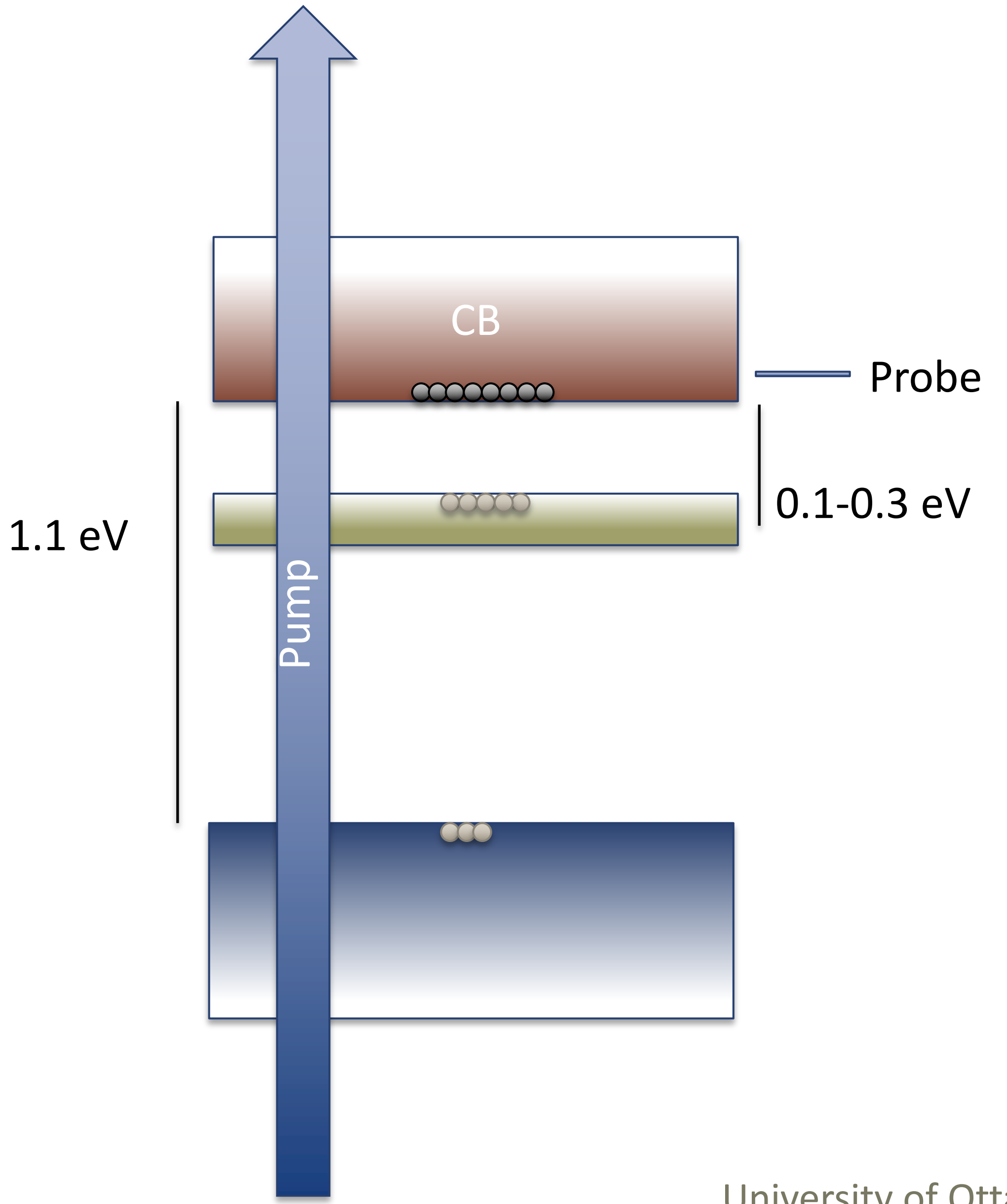
Outline

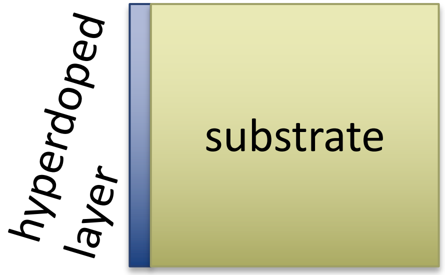
- Intermediate band solar cells
  - 3 material classes
- Figure of merit
  - **Measurements**
  - Predictions
- New developments
  - InGaN quantum dots in nanowires
  - Device model

THz measurements of carrier lifetime

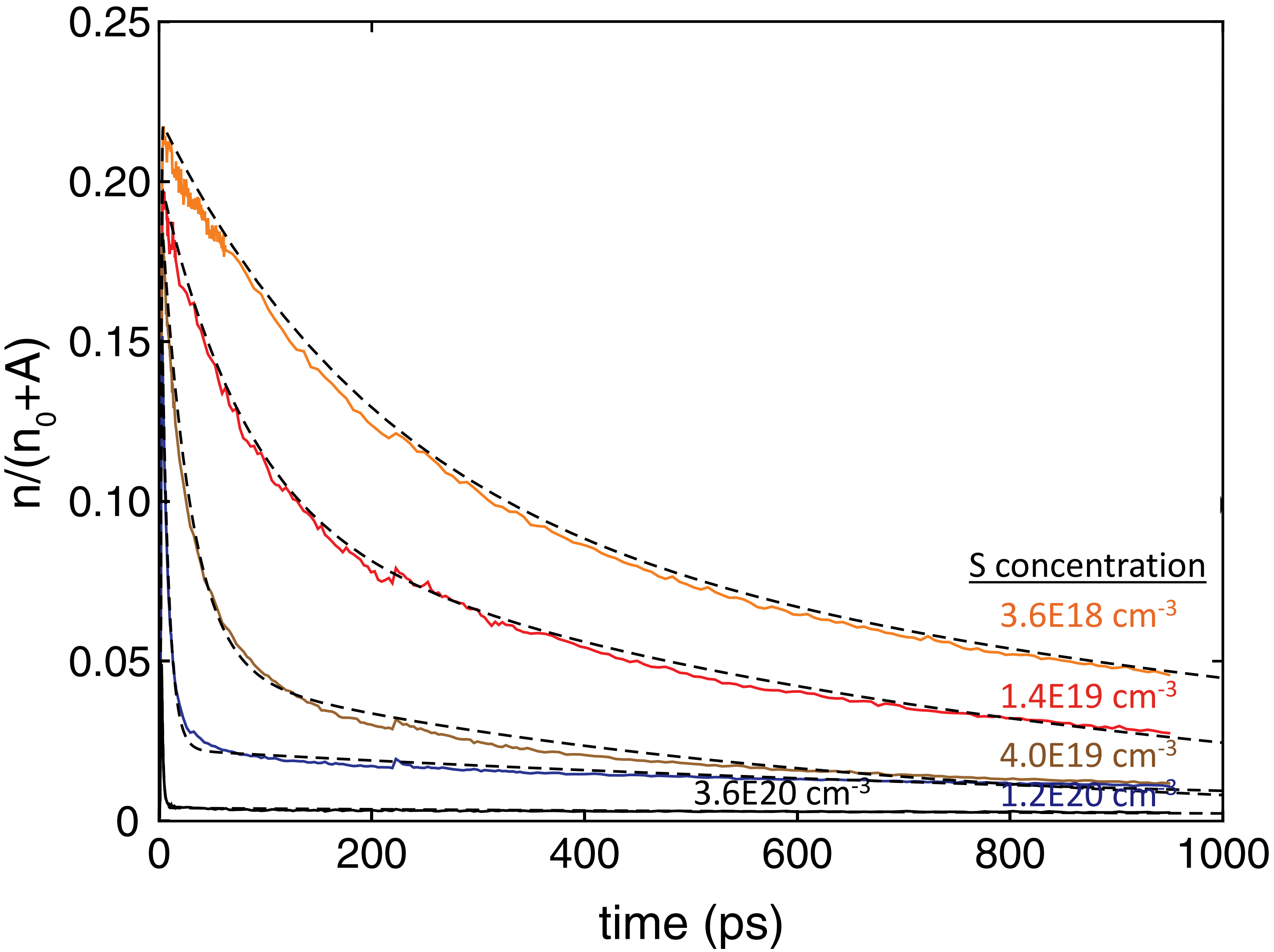
Pump

- 50 fs, 400 nm
- Absorbed mostly in hyperdoped region



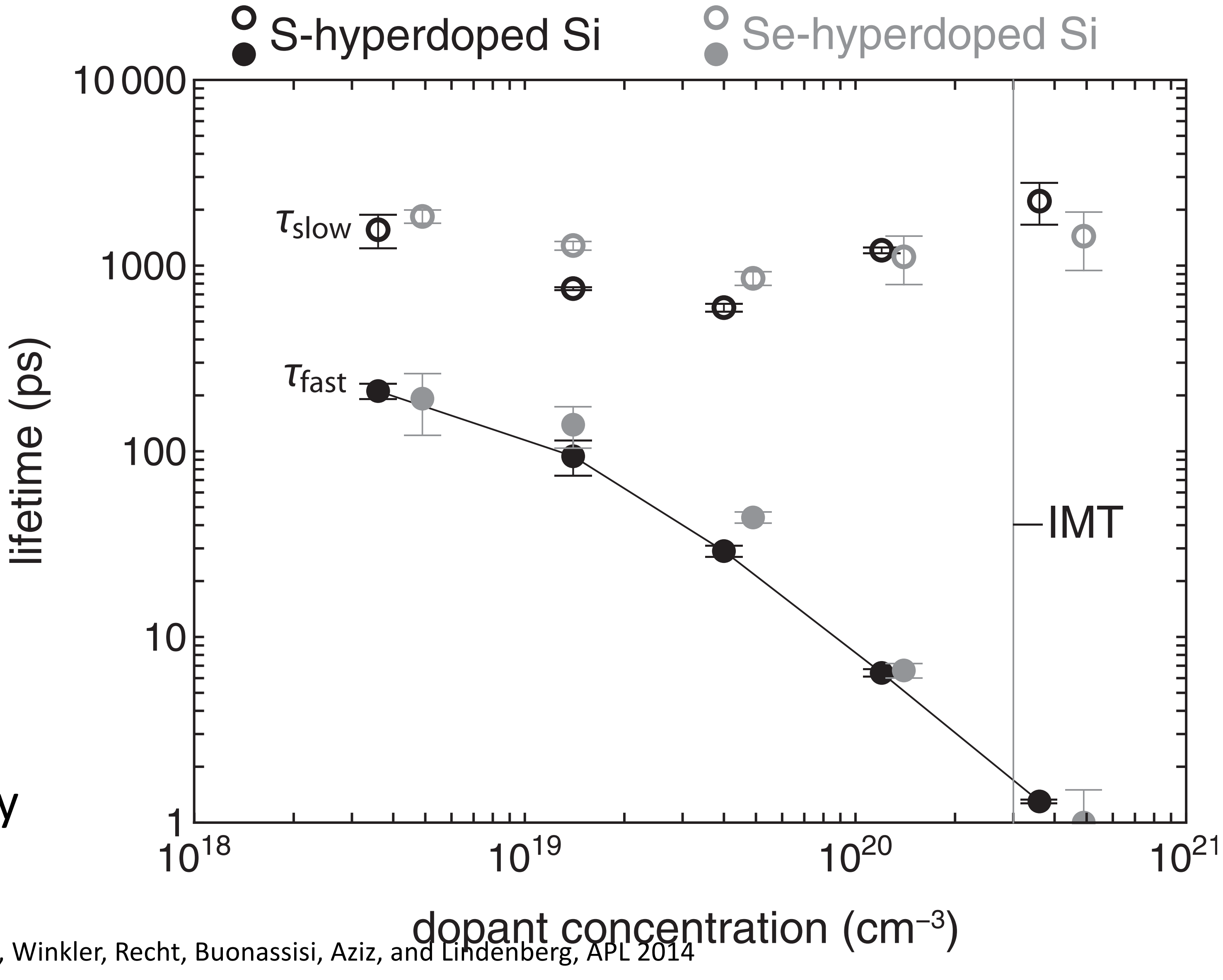


fs THz study of trapping times in Si:S and Si:Se



Sher, Simmons, Krich, Akey, Winkler, Recht, Buonassisi, Aziz, and Lindenberg, APL 2014

fs THz study of trapping times in Si:S and Si:Se



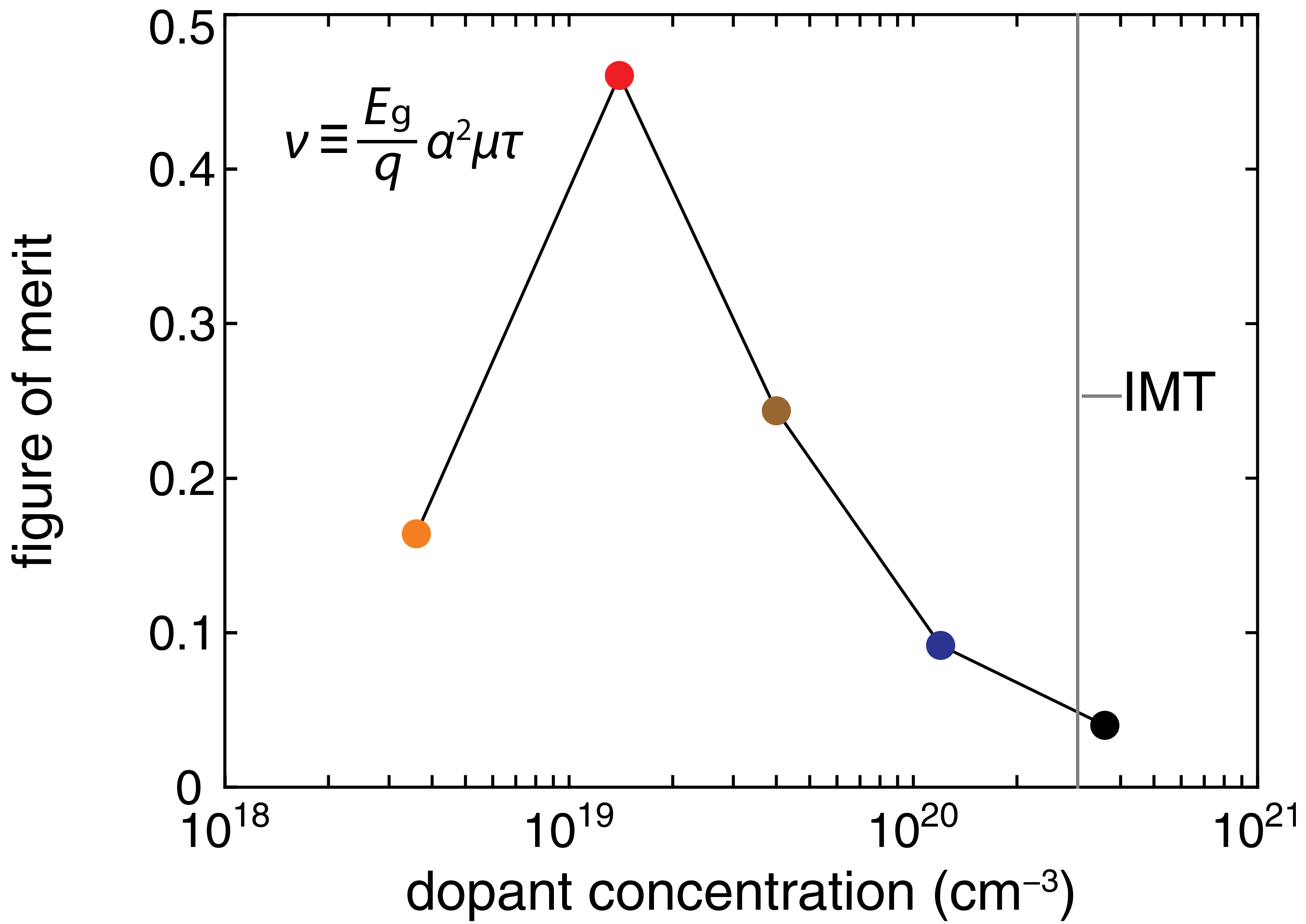
No evidence of lifetime recovery

Sher, Simmons, Krich, Akey, Winkler, Recht, Buonassisi, Aziz, and Lindenberg, APL 2014

ν peaks at lower concentration.

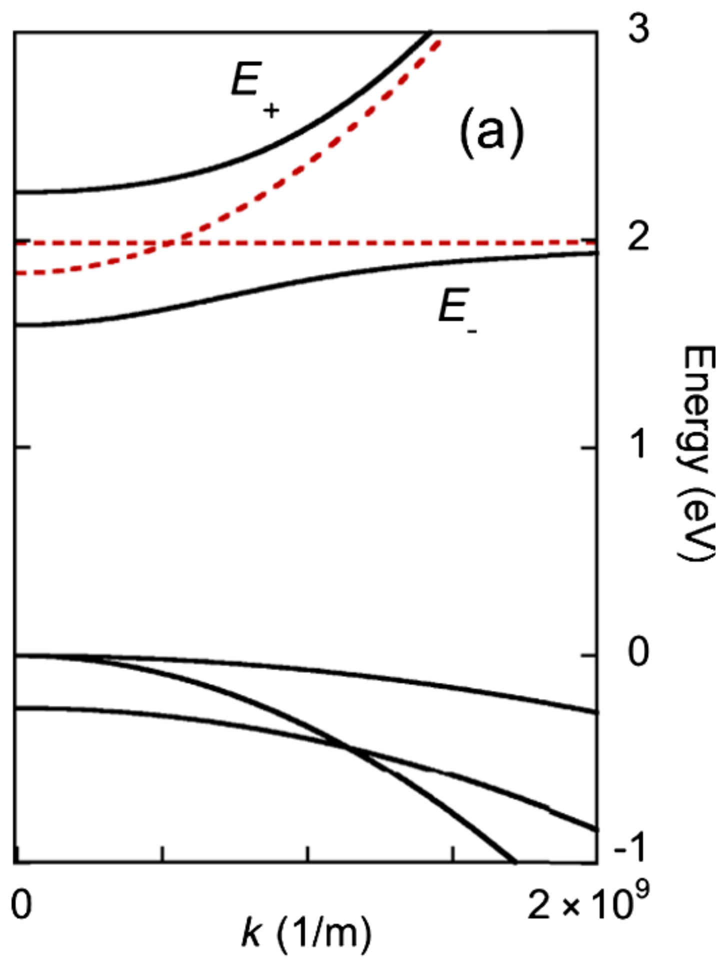
Still hyperdoped.

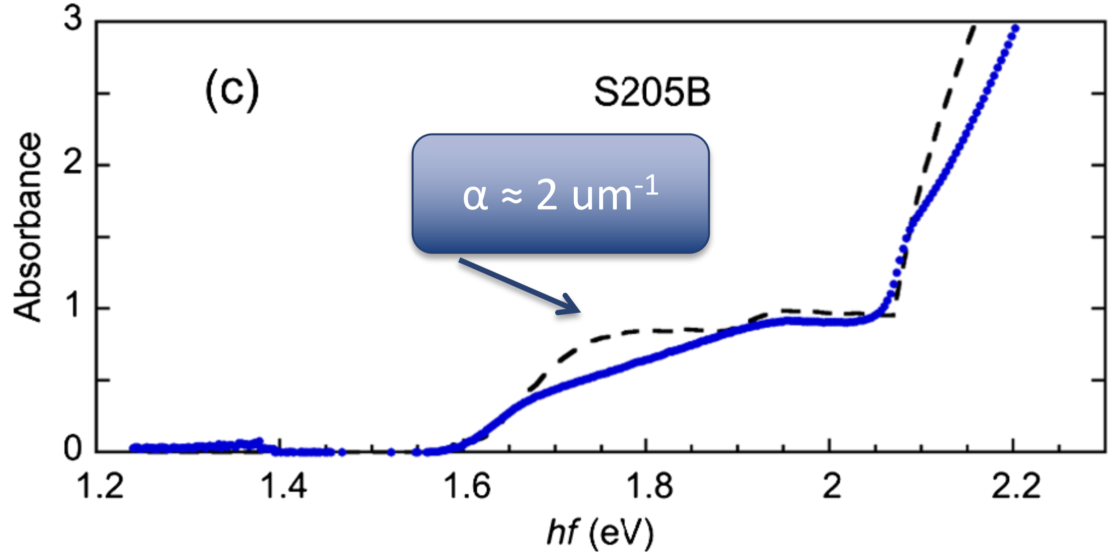
Hole figure of merit not measured.



Sher, Simmons, Krich, Akey, Winkler, Recht, Buonassisi, Aziz, and Lindenberg, APL 2014

$GaP_yAs_{1-x-y}N_x$





$\tau = 23 \text{ ps} \qquad E_g = 2.1 \text{ eV}$

Estimate $\mu = 1000 \text{ cm}^2/\text{Vs}$

$$\nu_{\text{drift}} = 19$$

Heyman et al, PR Applied (2017)

SCIENTIFIC REPORTS

OPEN

Multicolor emission from intermediate band semiconductor $ZnO_{1-x}Se_x$

Received: 06 December 2016
Accepted: 03 February 2017
Published: 13 March 2017

M. Welna[1], M. Baranowski[1,2], W. M. Linhart[1], R. Kudrawiec[1], K. M. Yu[3,4], M. Mayer[3] & W. Walukiewicz[3]

Photoluminescence and photomodulated reflectivity measurements of ZnOSe alloys are used to demonstrate a splitting of the valence band due to the band anticrossing interaction between localized Se states and the extended valence band states of the host ZnO matrix. A strong multiband emission associated with optical transitions from the conduction band to lower E_- and upper E_+ valence subbands has been observed at room temperature. The composition dependence of the optical transition energies is well explained by the electronic band structure calculated using the *kp* method combined with the band anticrossing model. The observation of the multiband emission is possible because of relatively long recombination lifetimes. Longer than 1 ns lifetimes for holes photoexcited to the lower valence subband offer a potential of using the alloy as an intermediate band semiconductor for solar power conversion applications.

Outline

- Intermediate band solar cells
  - 3 material classes
- Figure of merit
  - Measurements
  - **Predictions**
- New developments
  - InGaN quantum dots in nanowires
  - Device model

Predicting ν

$$\nu_{drift} = \frac{E_g}{q}\mu\tau\alpha^2$$

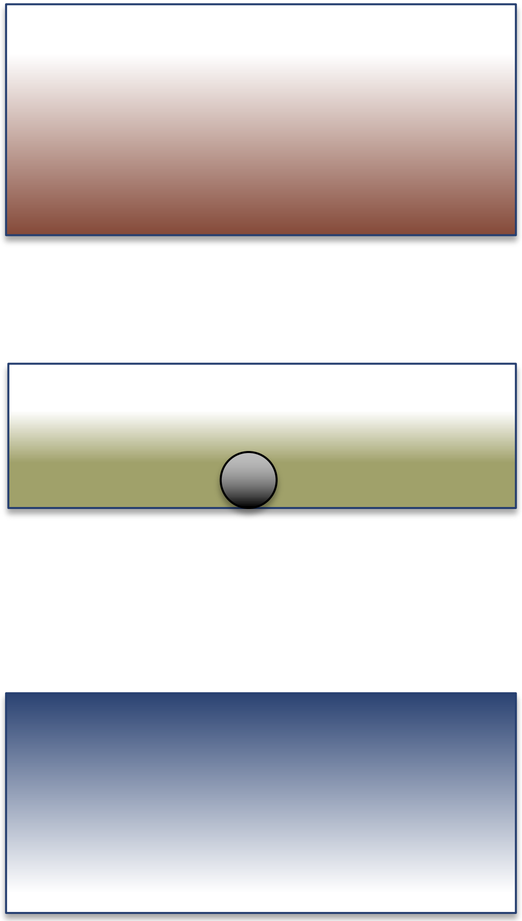
$$\alpha \propto N_I$$

$$\frac{1}{\mu} = \frac{1}{\mu_{\text{latt}}} + \frac{1}{\mu_{ni}}$$

constant

$$\mu_{ni} \propto \frac{1}{N_I}$$

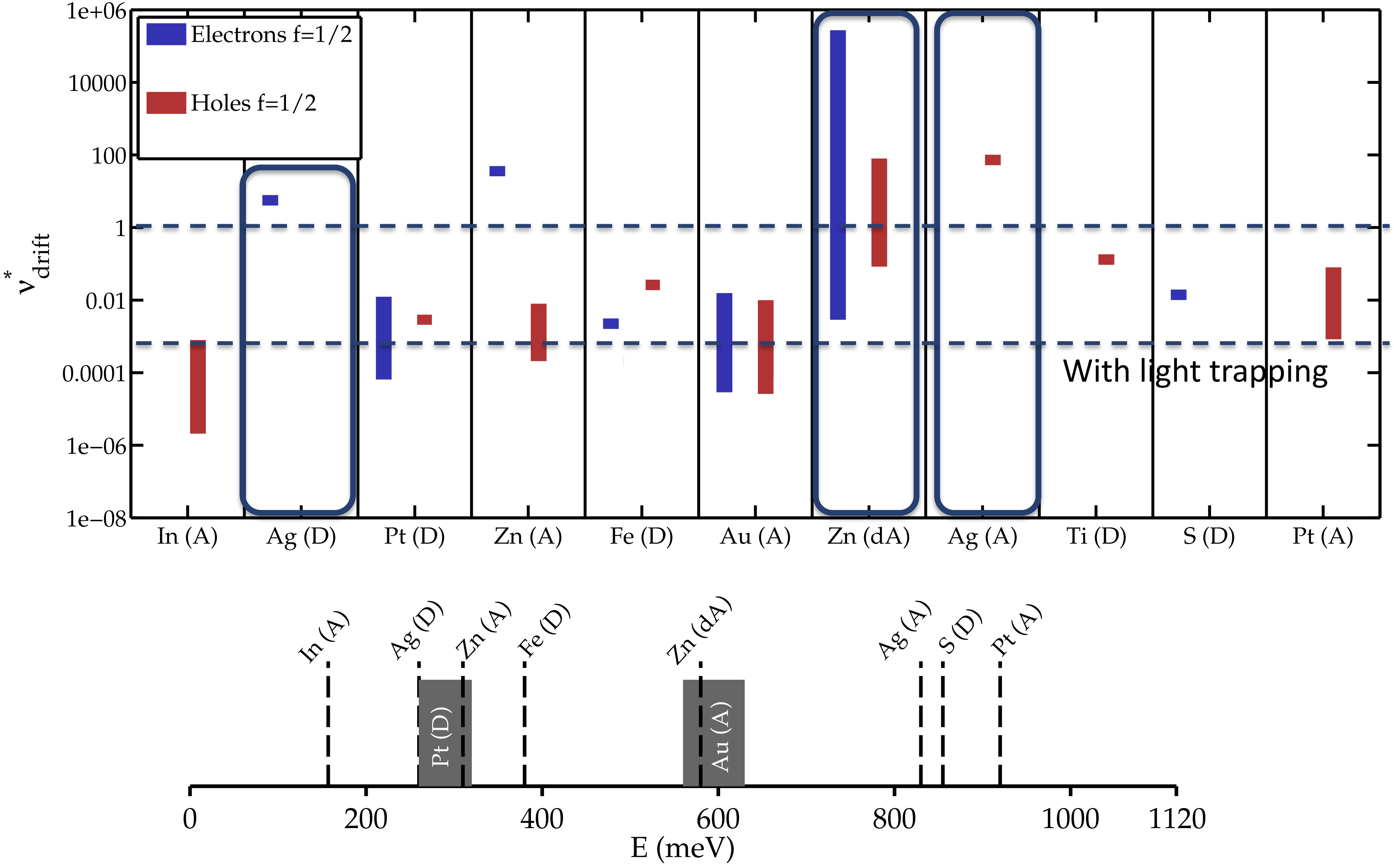
$$\tau \propto \frac{1}{N_I}$$



Small N_I: $\nu \propto N_I$

Large N_I: $\nu \to \nu^*$

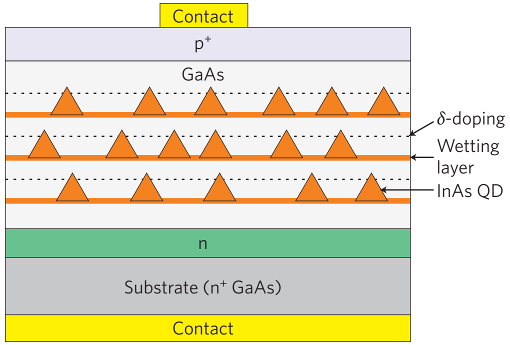
S. Li and W. Thurber, *Solid State Electronics*, ***20***, *609 (1977)*



Sullivan, Simmons, Buonassisi, Krich, JPV 2015

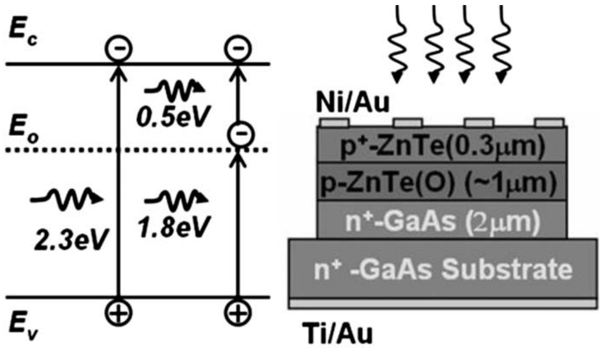
3 Candidate Materials Classes

1 Quantum dots



Luque et al., Nat Photon 2012

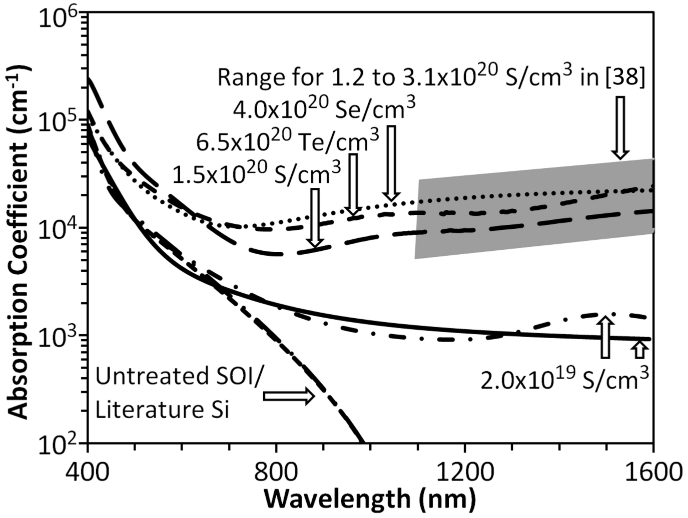
2 Highly-mismatched alloys



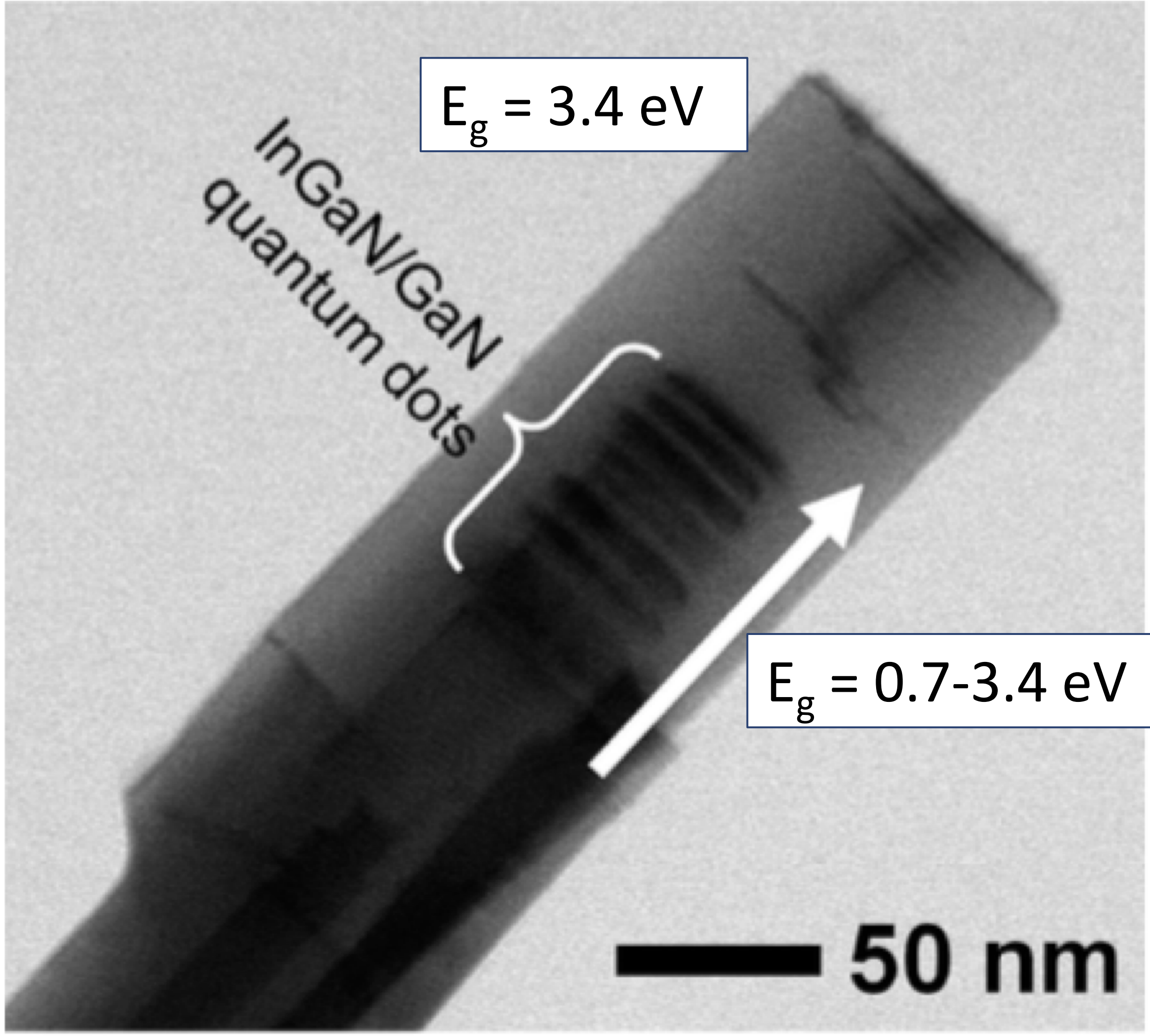
ZnTeO

Wang et al., APL 2009

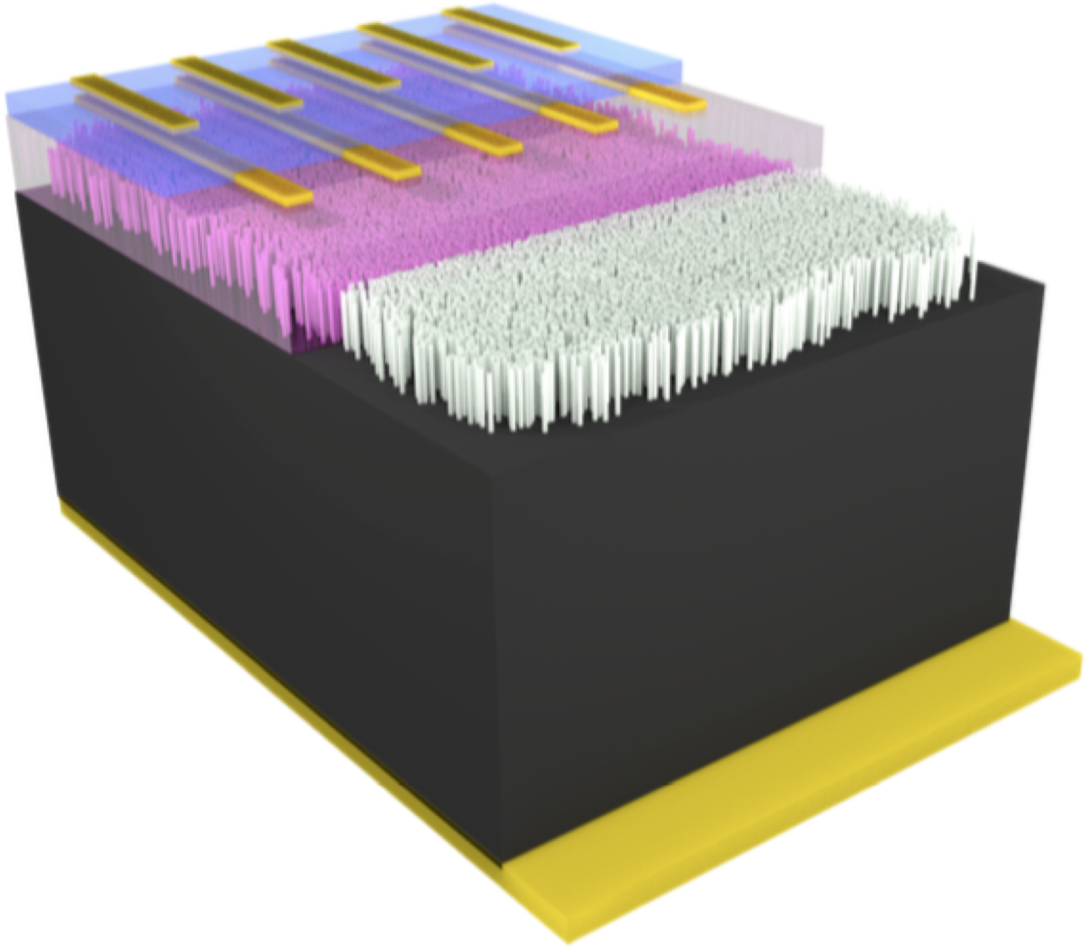
3 Hyperdoped silicon



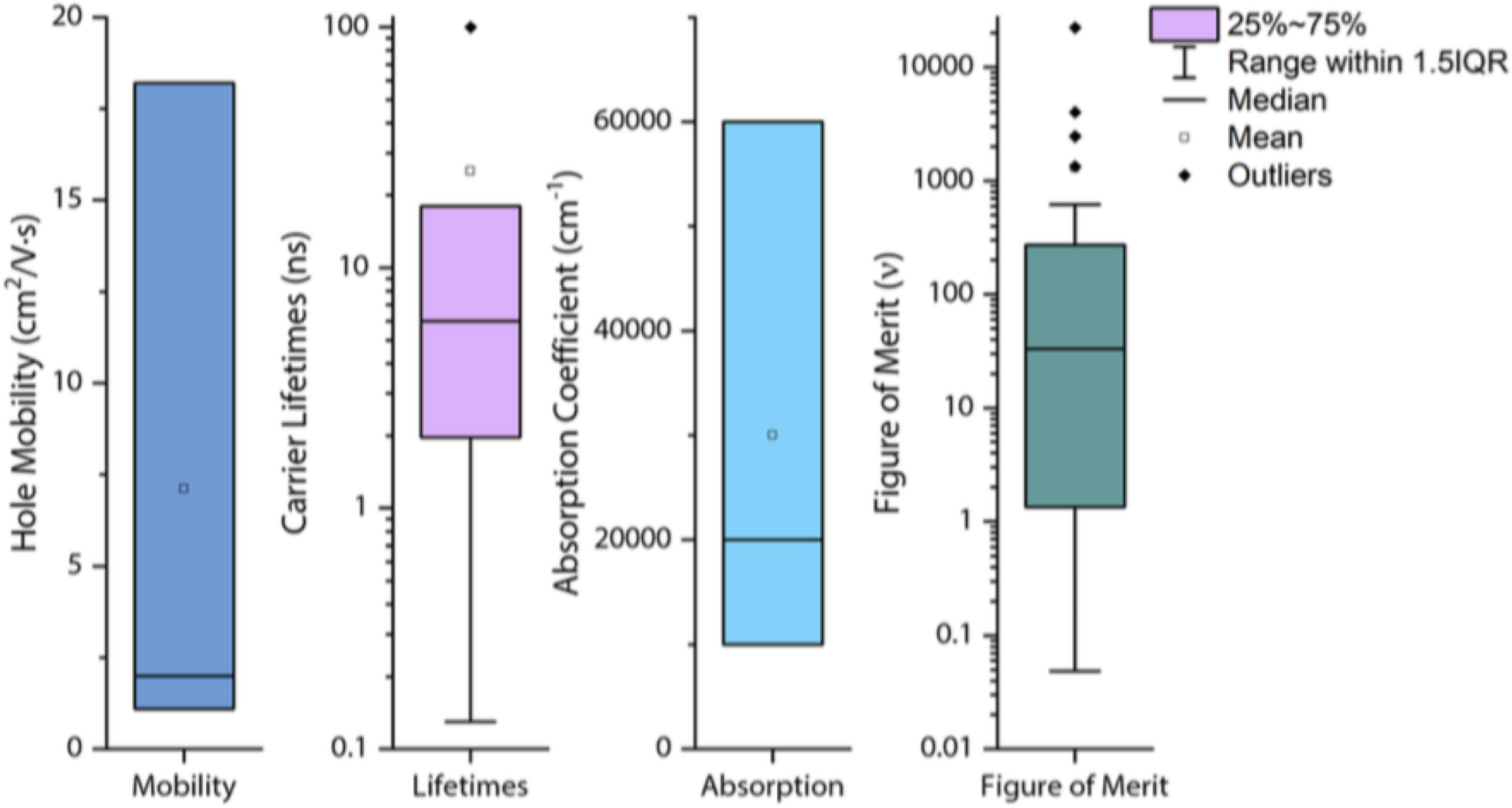
Pan et al, APL (2011)



Nguyen et al., Nano Lett 2011



Ross Cheriton, PhD thesis, 2018



Ross Cheriton, PhD thesis, 2018

Intermediate band device models

Essential to determine requirements for IB absorbers and optimize devices.

Strandberg and Reenaas, PiP 2010

- Radiative recombination only. IB region only, depletion approximation.

Yoshida, Okada, Sano, JAP 2012

- No IB transport.

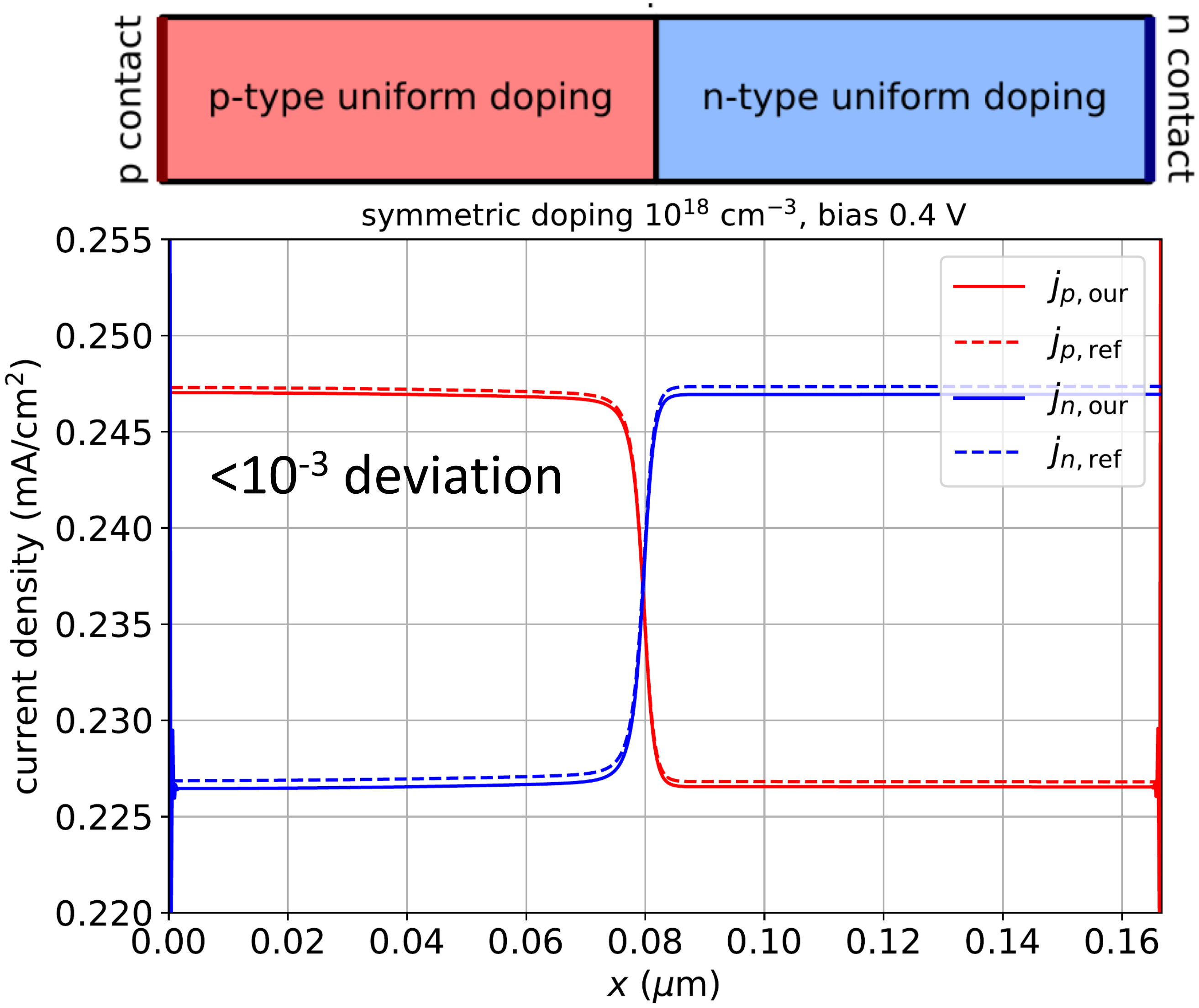
Martí, Cuadra, Luque IEEE TED 2002

- Diffusive only. Radiative recombination only.

Many detailed-balance based models

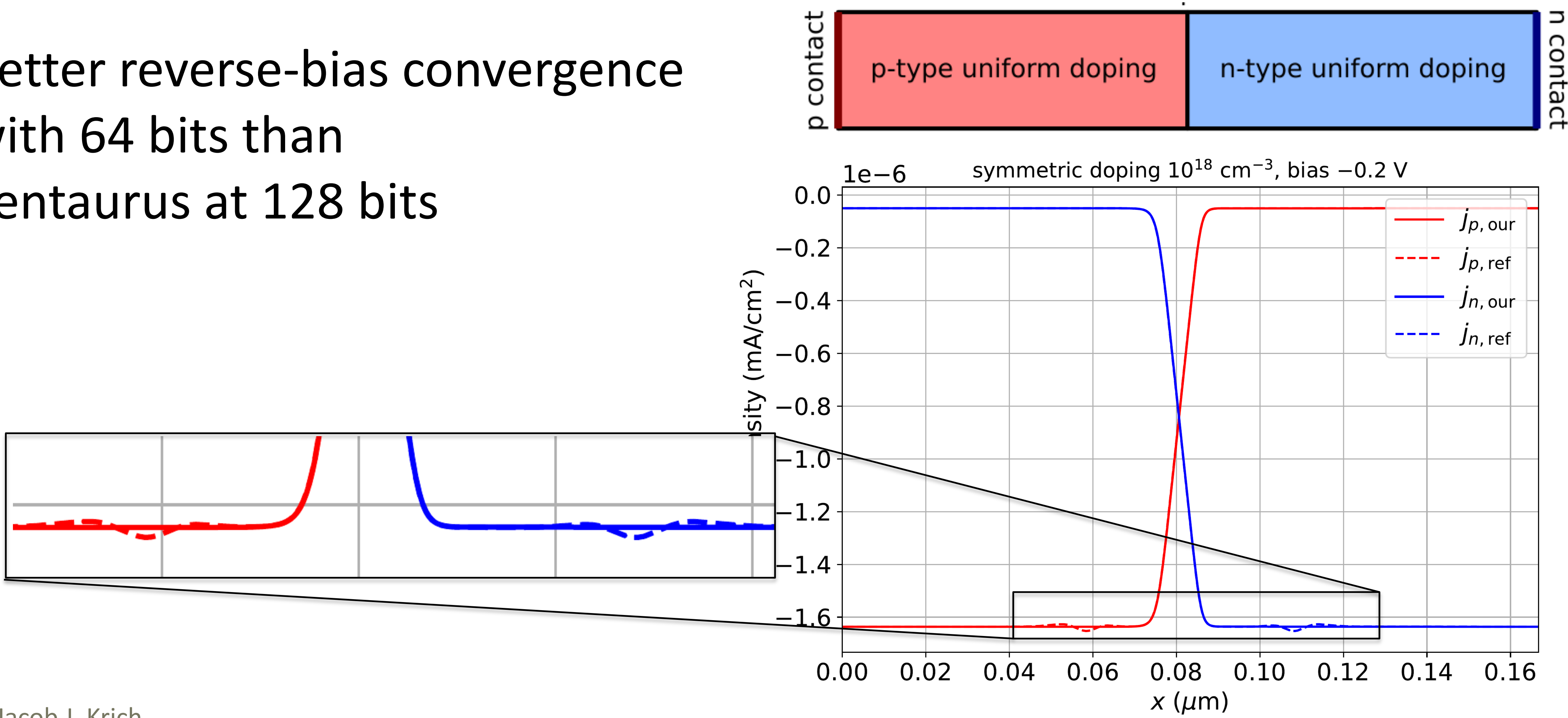
Our device model

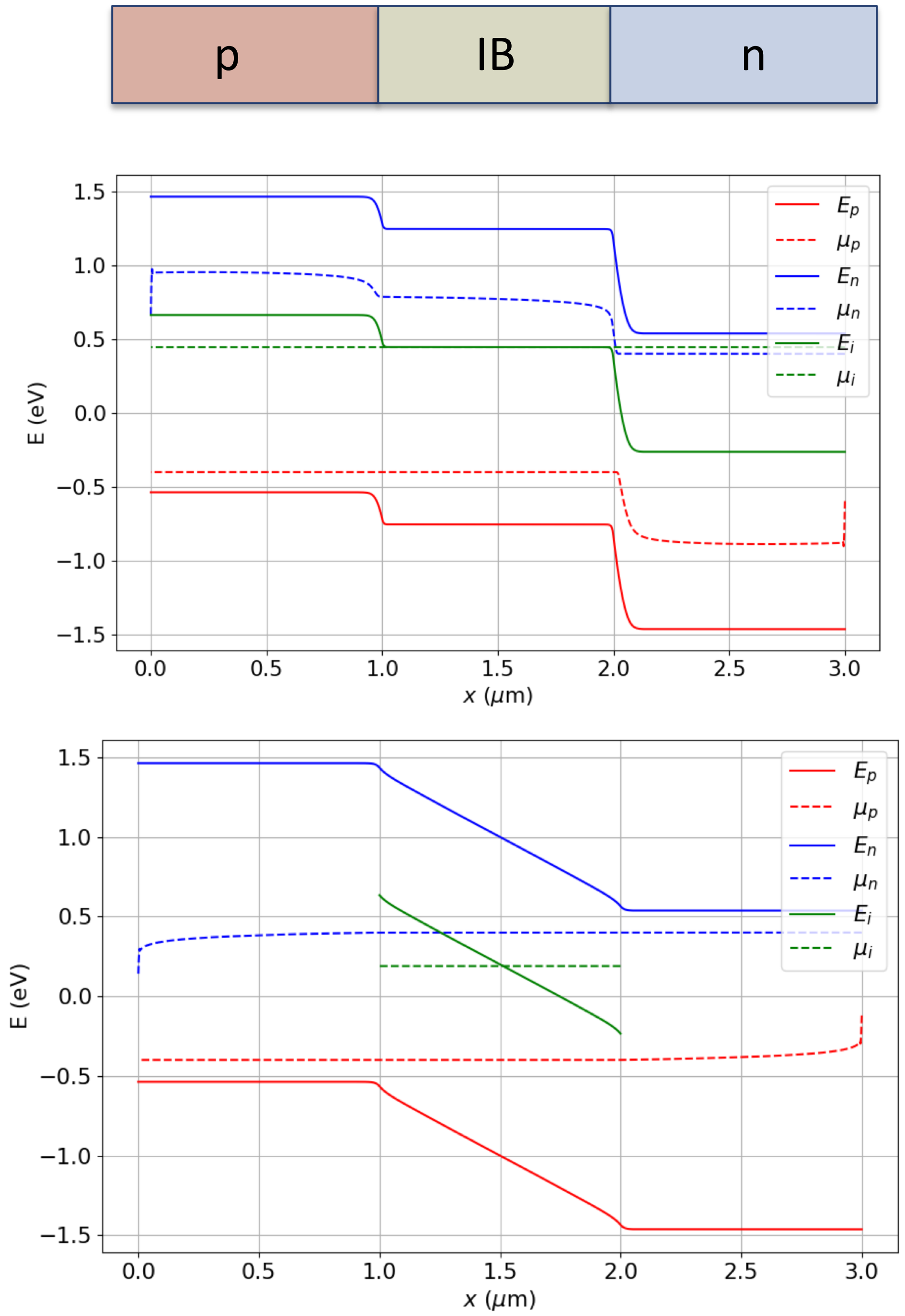
- 2D
- Finite element – built using FEniCS
- Benchmark against Synopsys Sentaurus

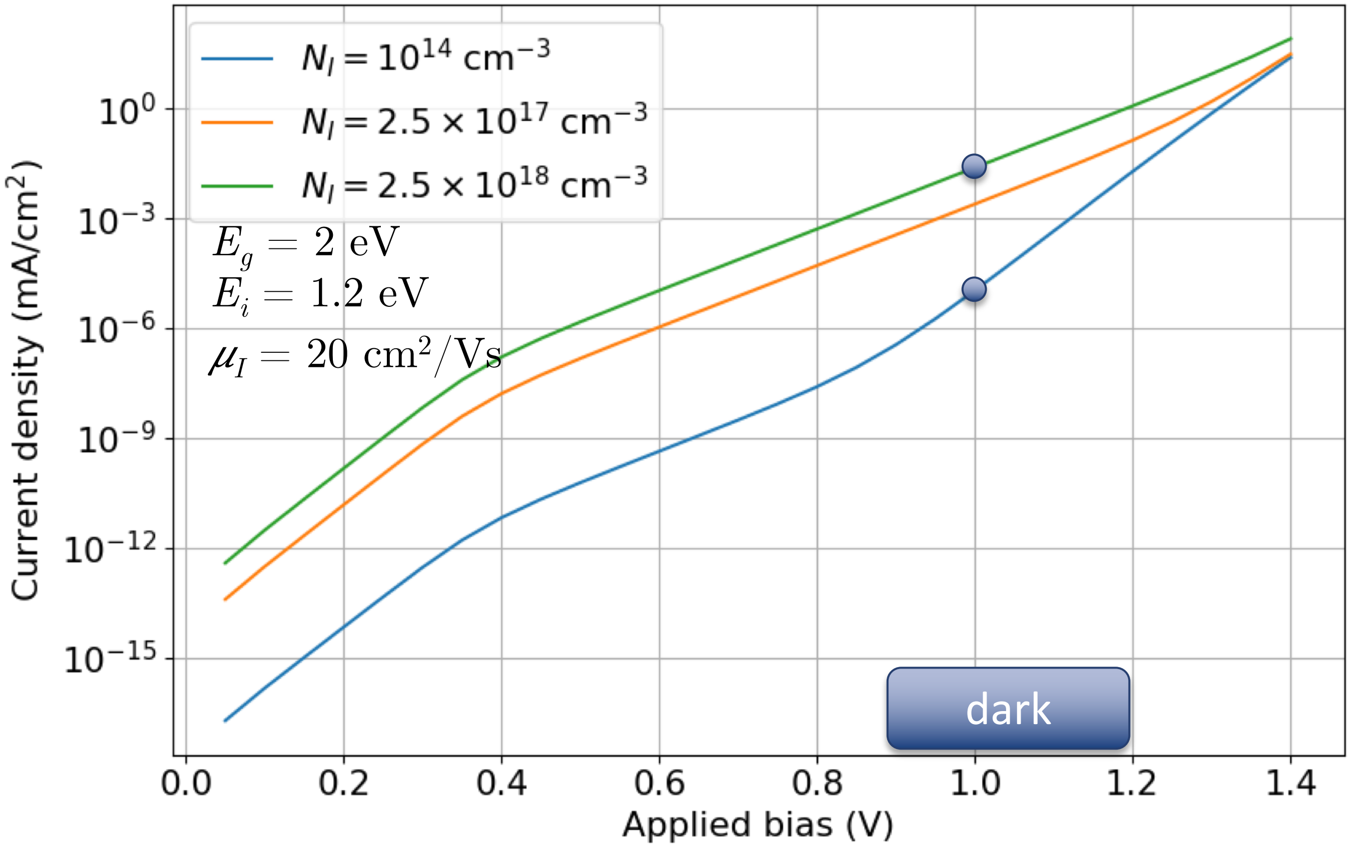


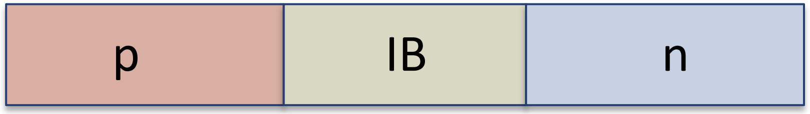
Our device model

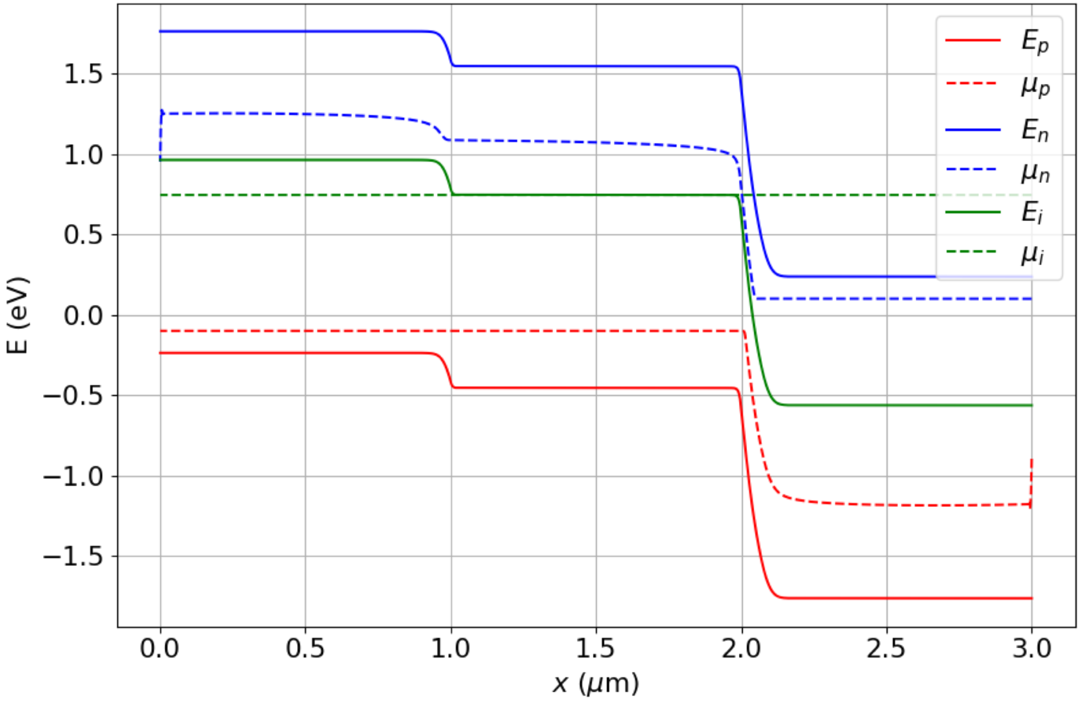
Better reverse-bias convergence with 64 bits than Sentaurus at 128 bits

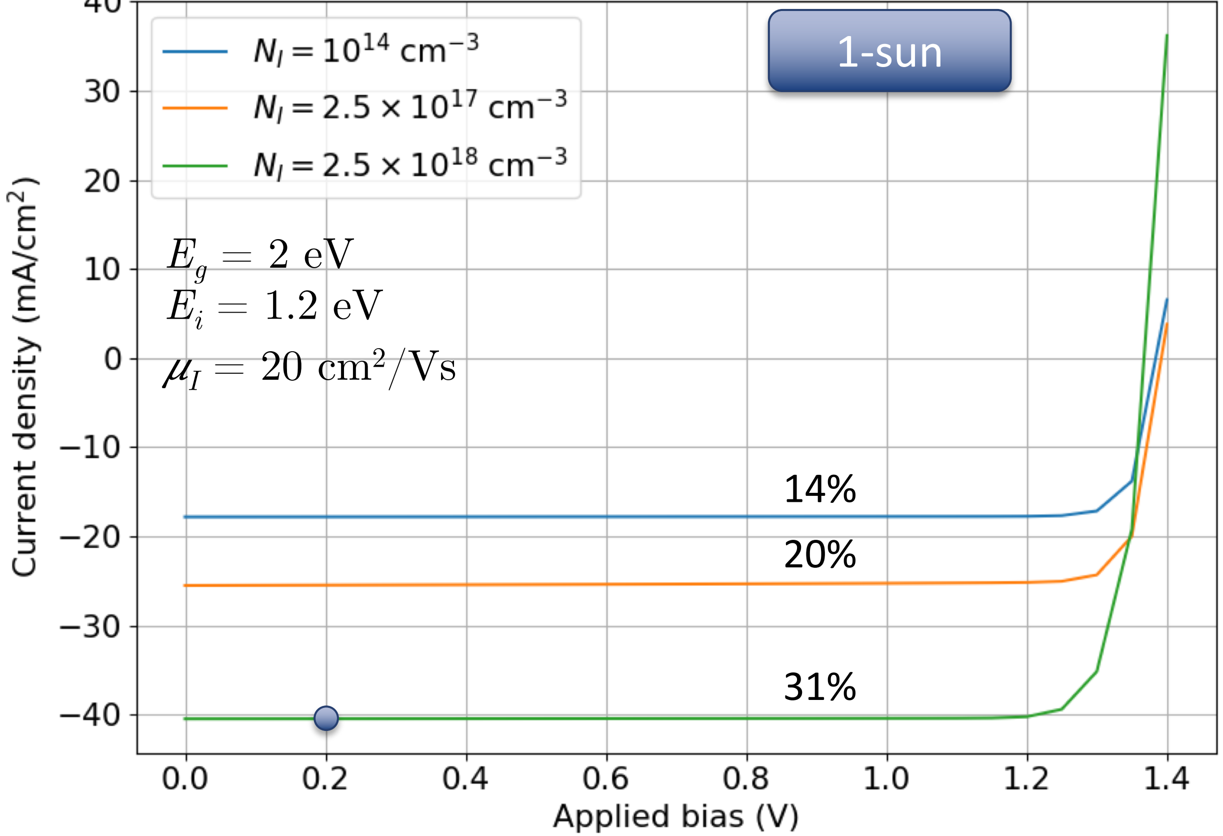



p
IB
n
E (eV)
x (μm)
E_p
μ_p
E_n
μ_n
E_i
μ_i


$N_I = 10^{14}$ cm^{-3}
$N_I = 2.5 \times 10^{17}$ cm^{-3}
$N_I = 2.5 \times 10^{18}$ cm^{-3}
$E_g = 2$ eV
$E_i = 1.2$ eV
$\mu_I = 20$ cm^2/Vs
Current density (mA/cm^2)
Applied bias (V)
dark







- Model released within the year
- Enable better devices and understanding of IB materials

Recap

Intermediate band solar cells

- Great potential
- Need sufficient absorber materials

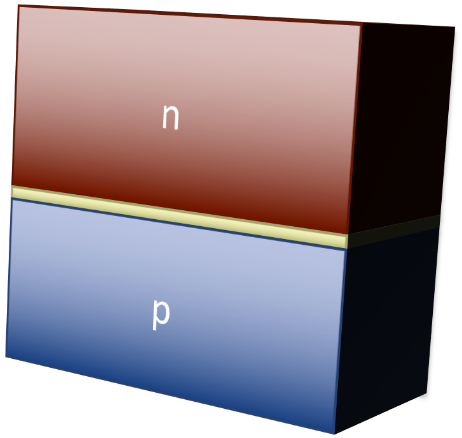


Figure of merit

- guide materials development
- determine when to make a device

Device modeling

- Required to optimize device performance