

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



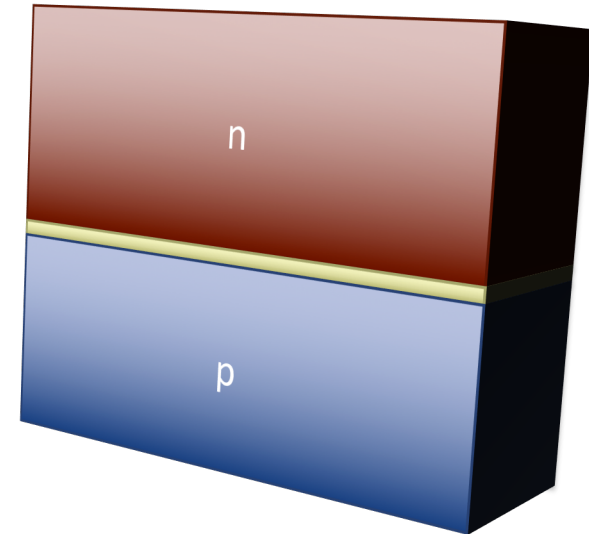
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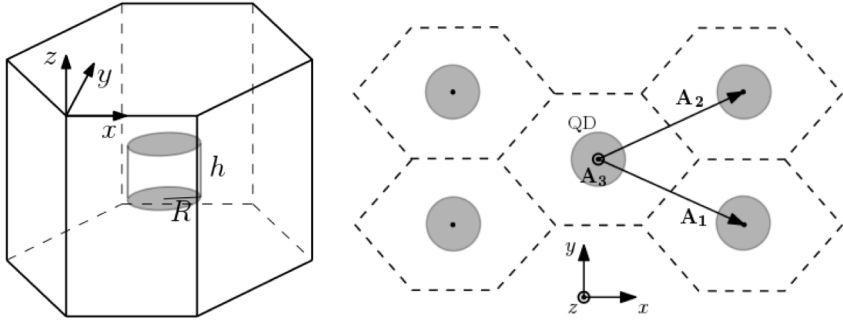
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Jay Mathews

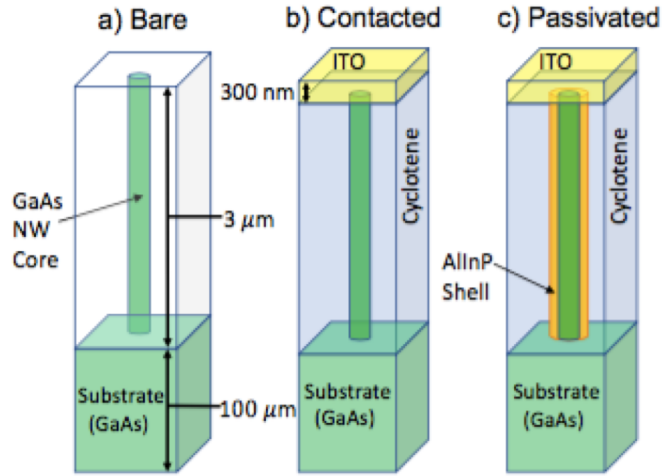
Yining Liu

Present topics in the group

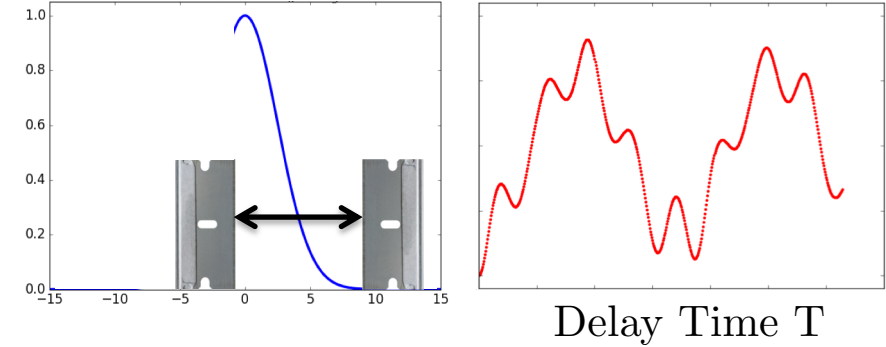
Intermediate band materials



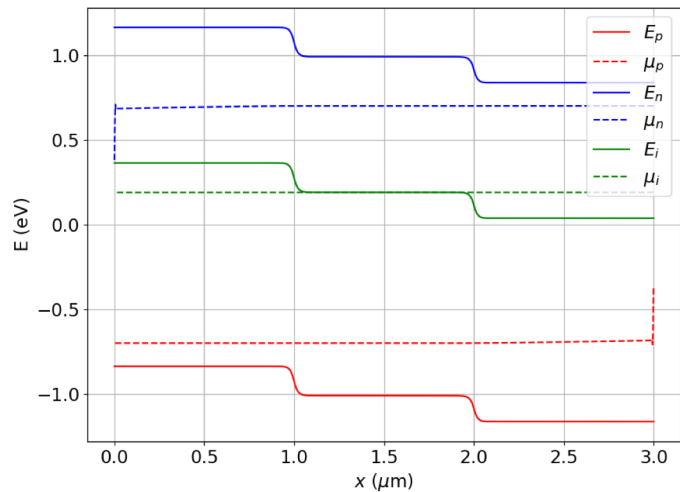
Nanowire PV



Quantum biology/ nonlinear spectroscopy

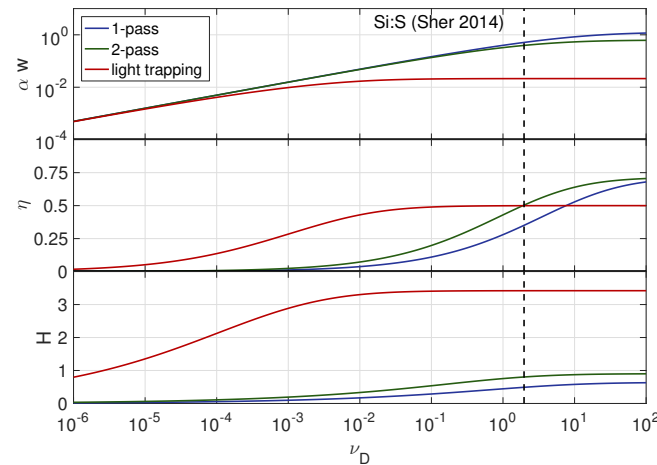


IB device modeling

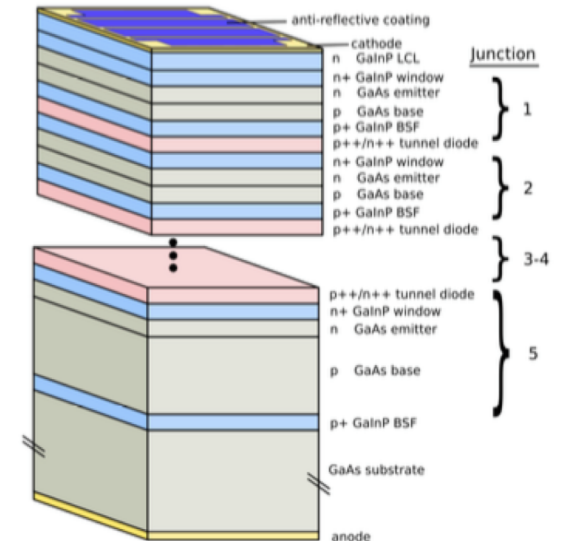


Jacob J. Krich

IB IR photodetectors



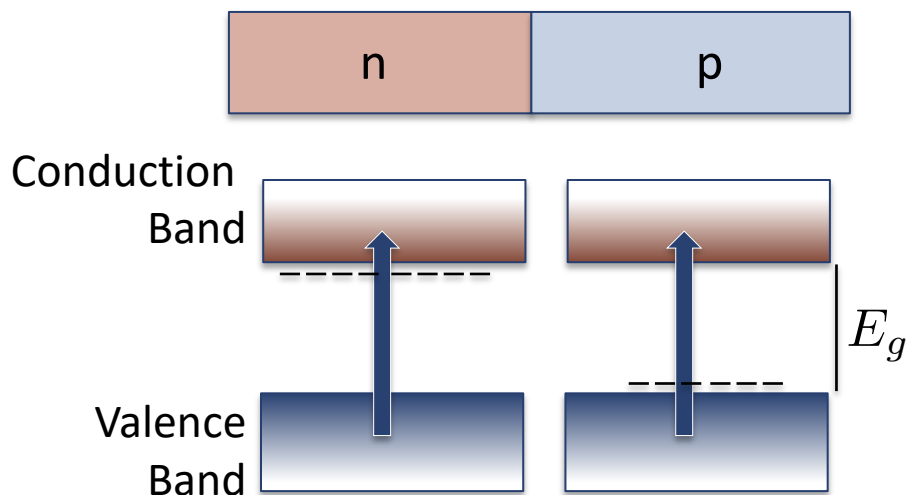
Monochromatic PV



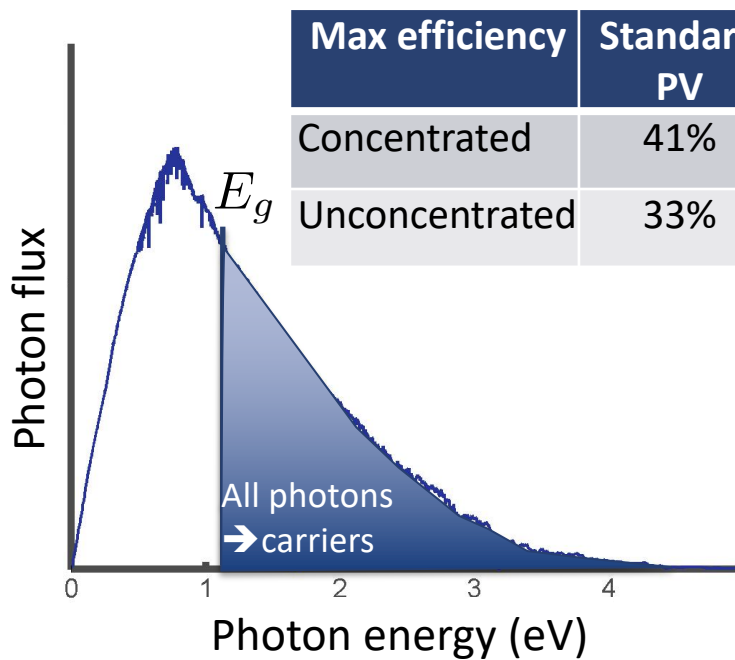
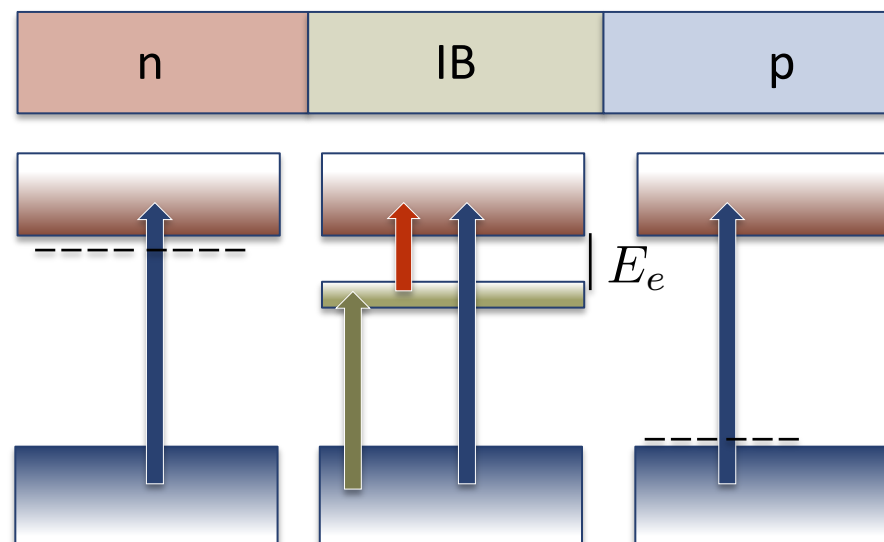
Outline

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

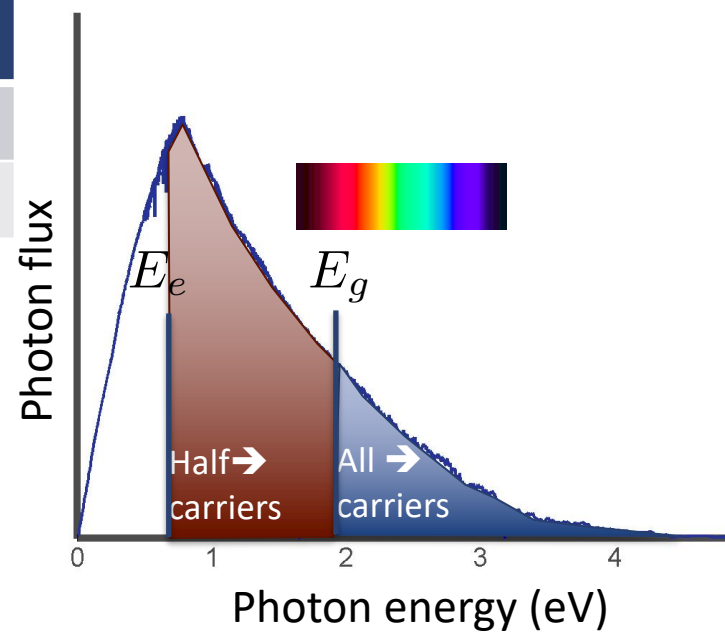
Standard PV



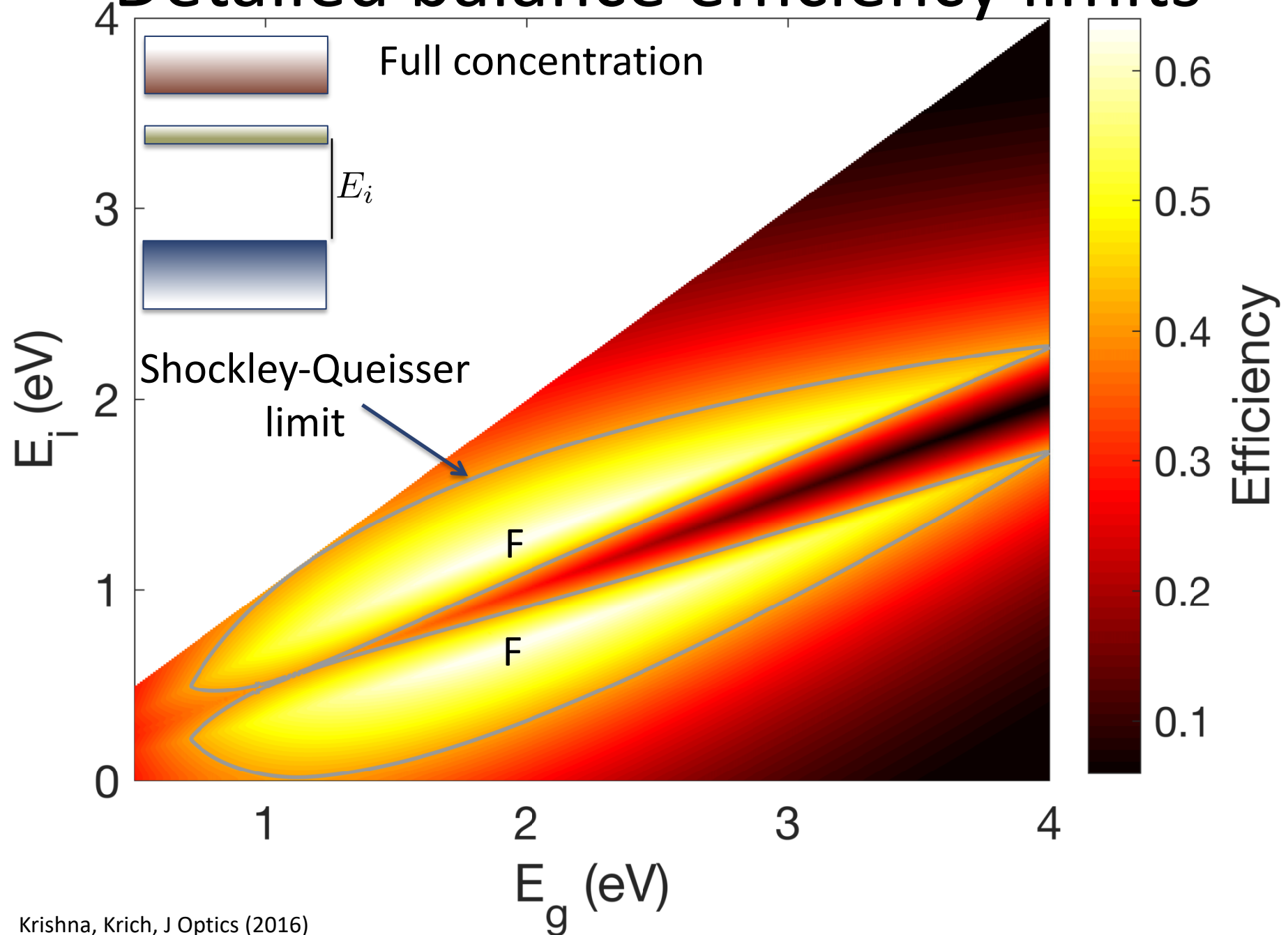
Intermediate band PV



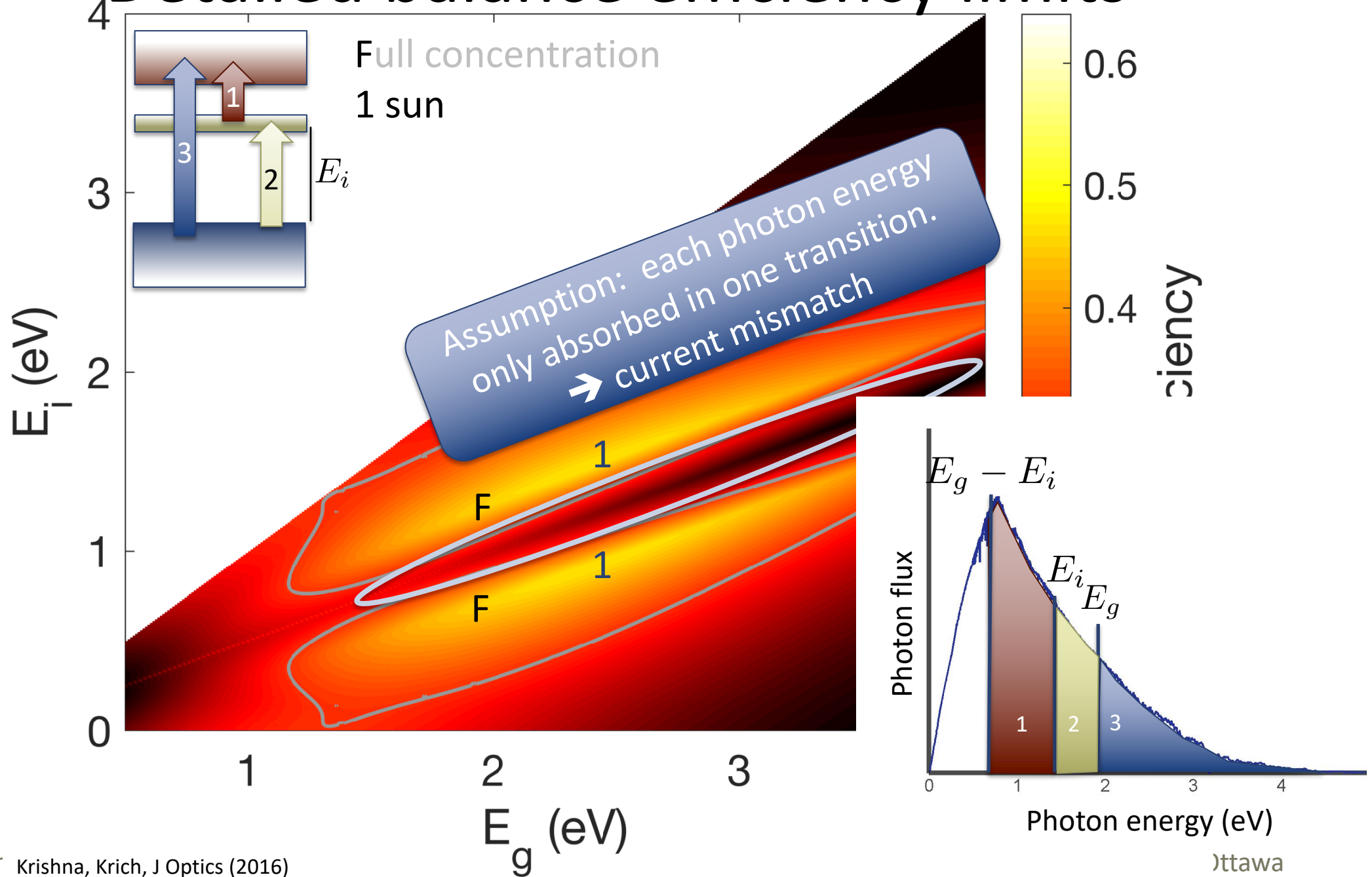
	Max efficiency	Standard PV	IBPV
Concentrated		41%	63%
Unconcentrated		33%	47%



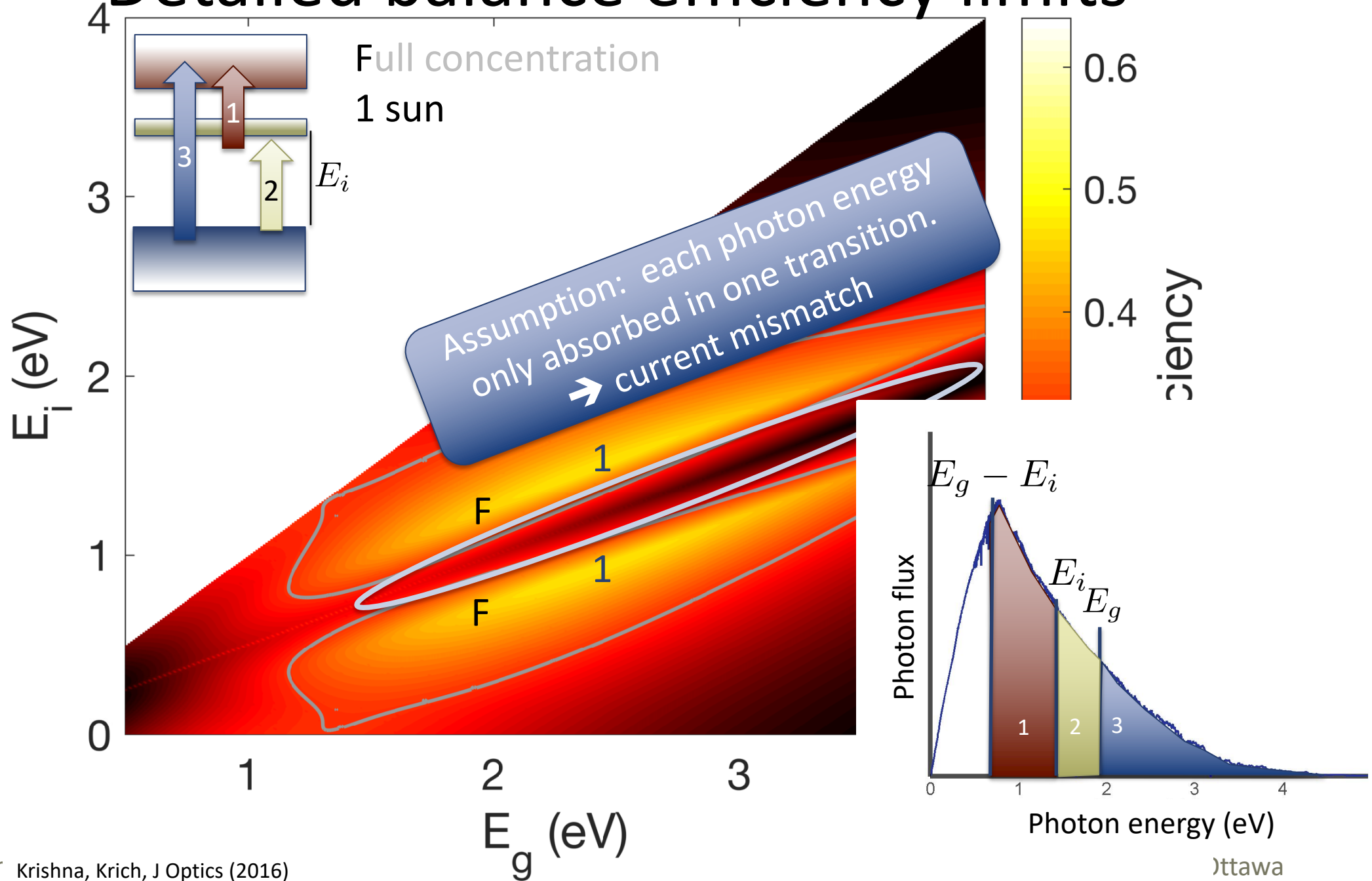
Detailed balance efficiency limits



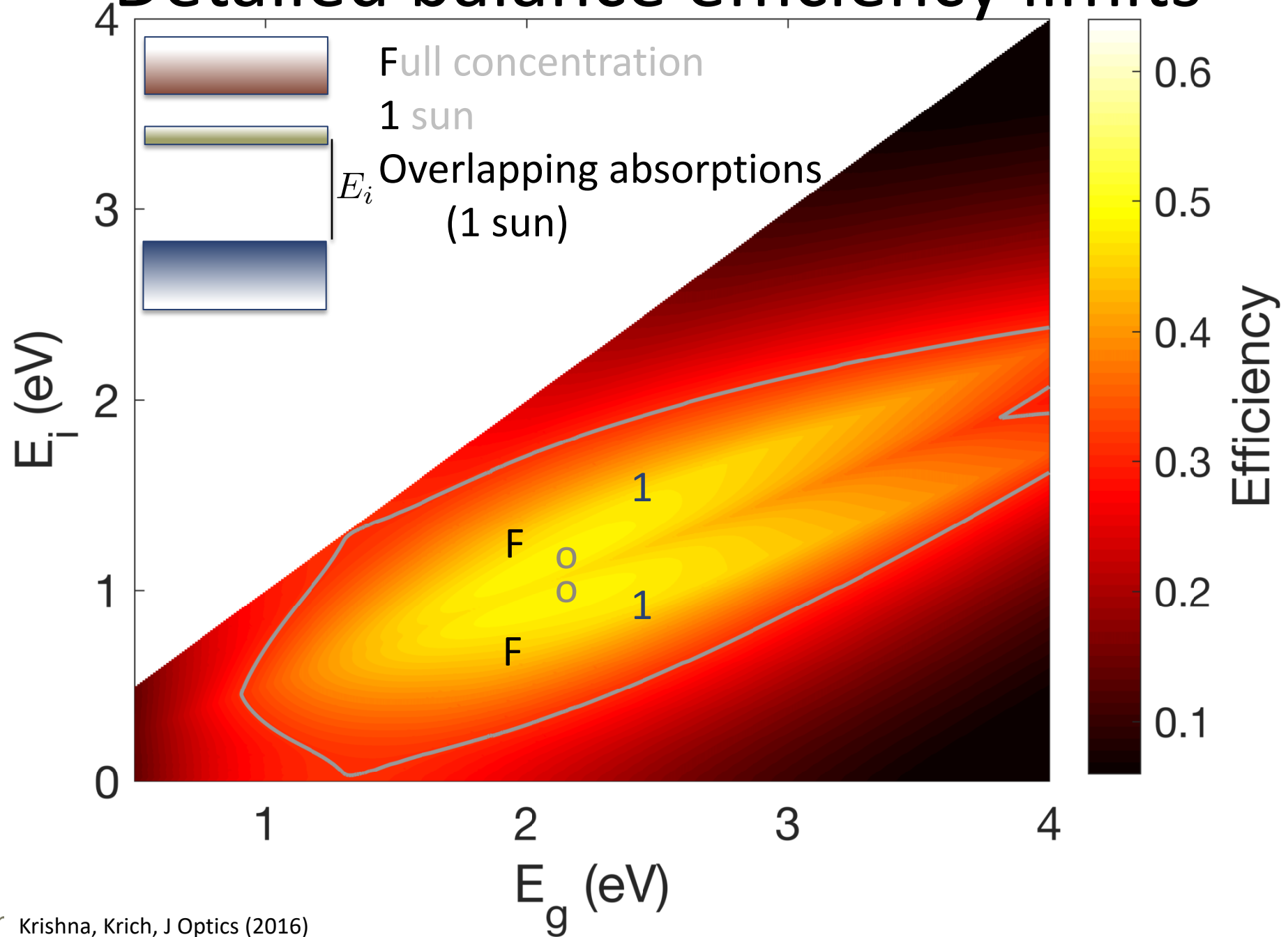
Detailed balance efficiency limits



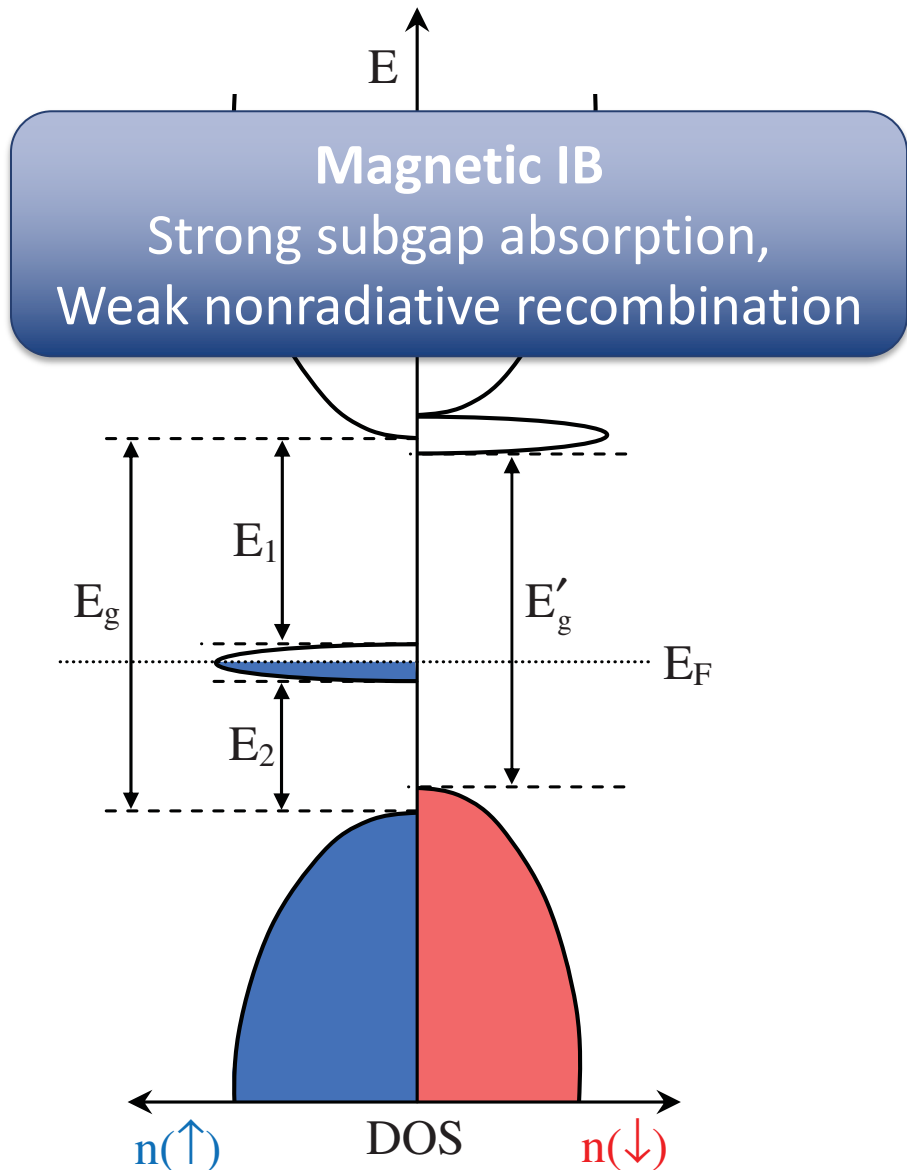
Detailed balance efficiency limits



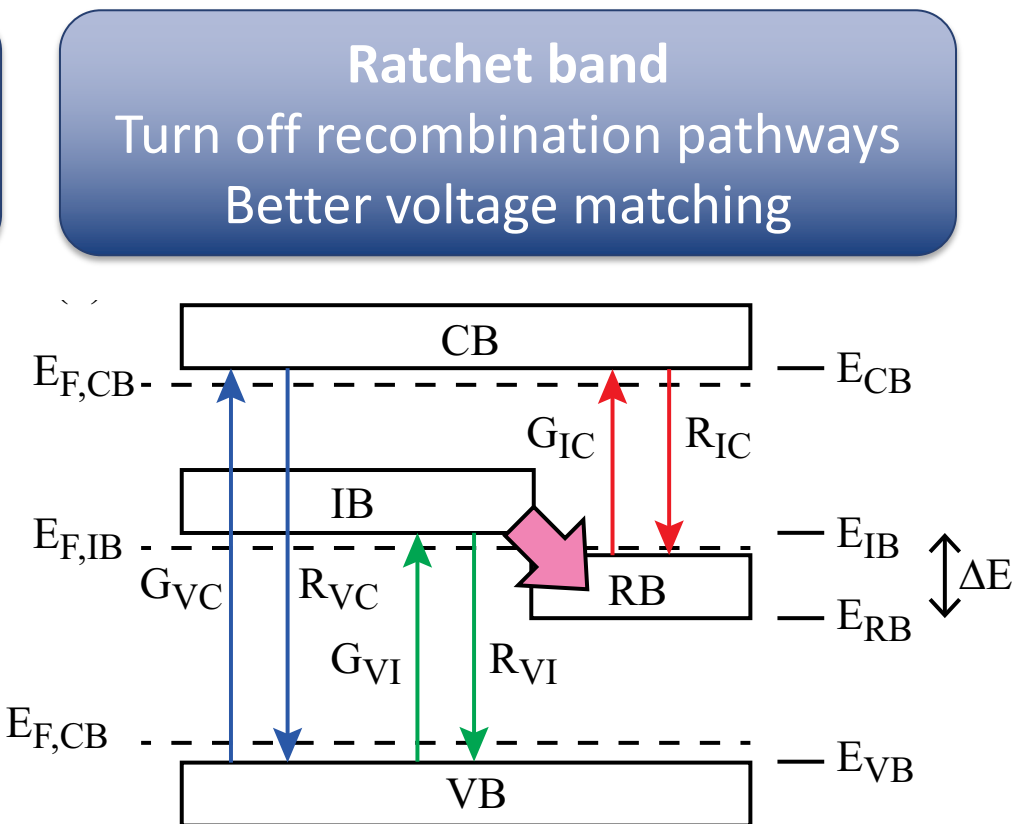
Detailed balance efficiency limits



IBPV variants



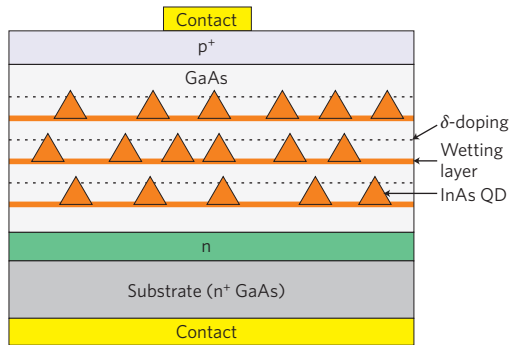
Olsson, Domain, Guillemoles, PRL 2009



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

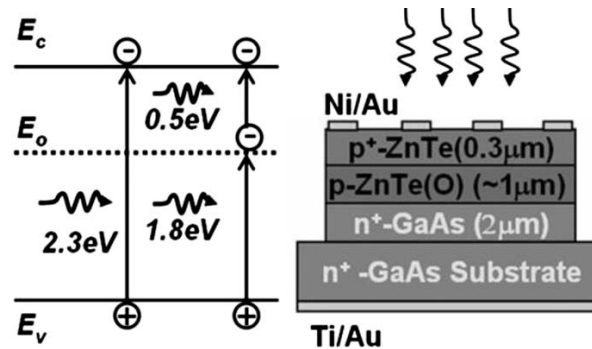
3 Candidate Materials Classes

1 Quantum dots



Luque et al., Nat Photon 2012

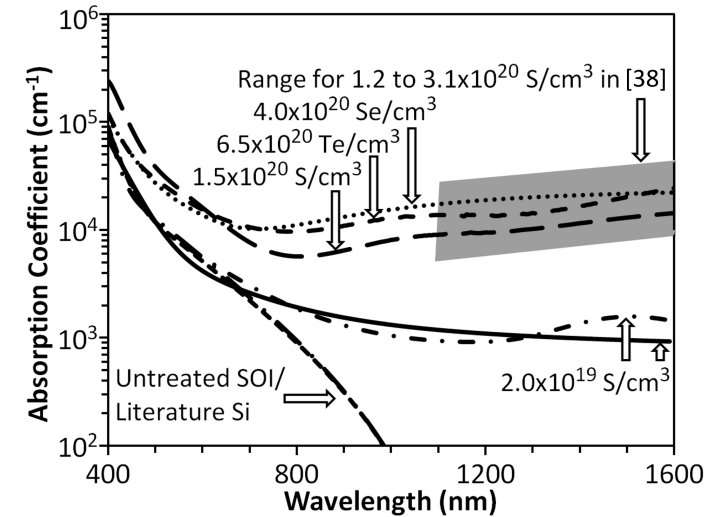
2 Highly-mismatched alloys



ZnTeO

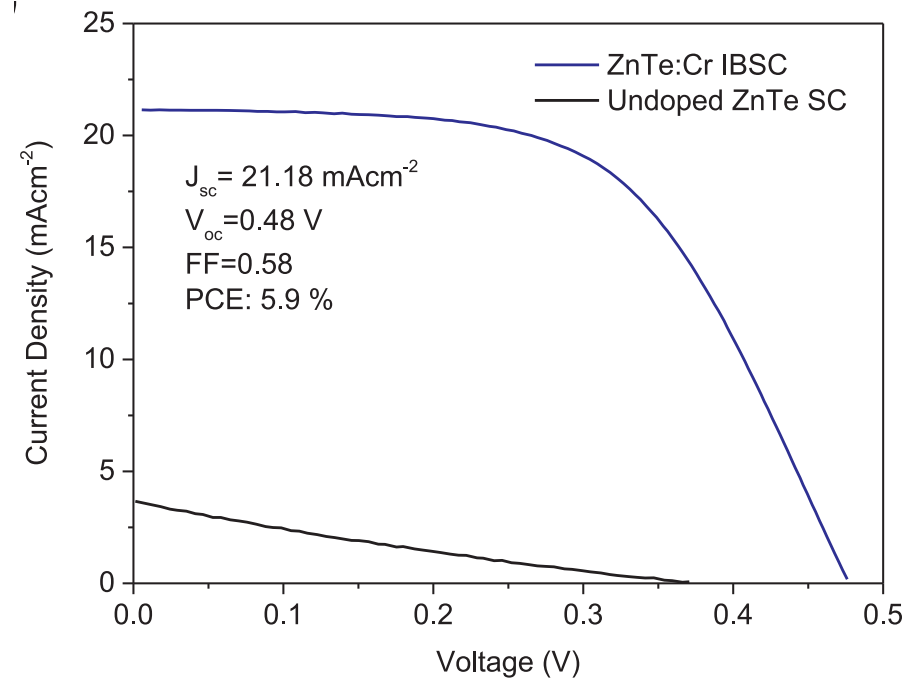
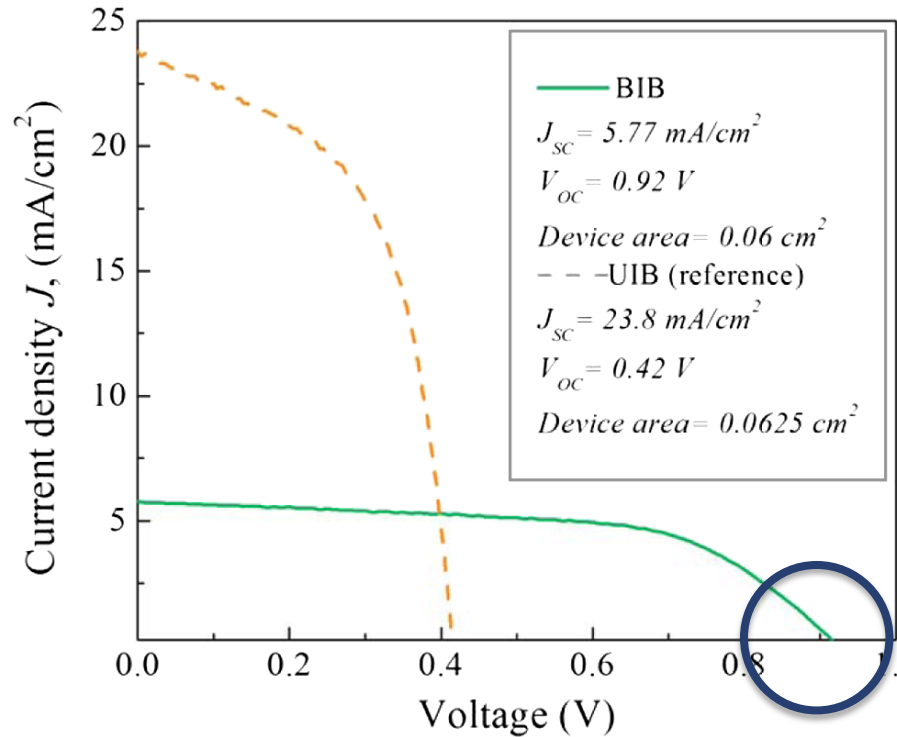
Wang et al., APL 2009

3 Hyperdoped silicon



Pan et al, APL (2011)

Best bulk IBPV devices so far

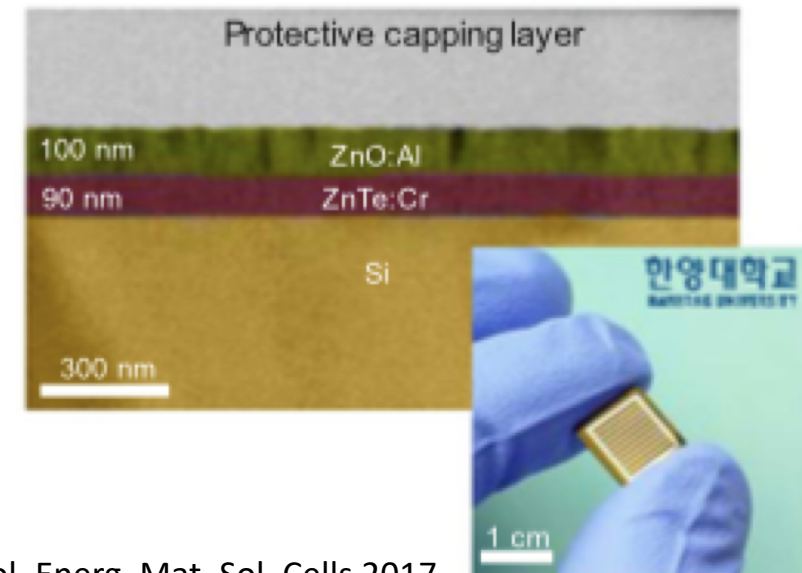
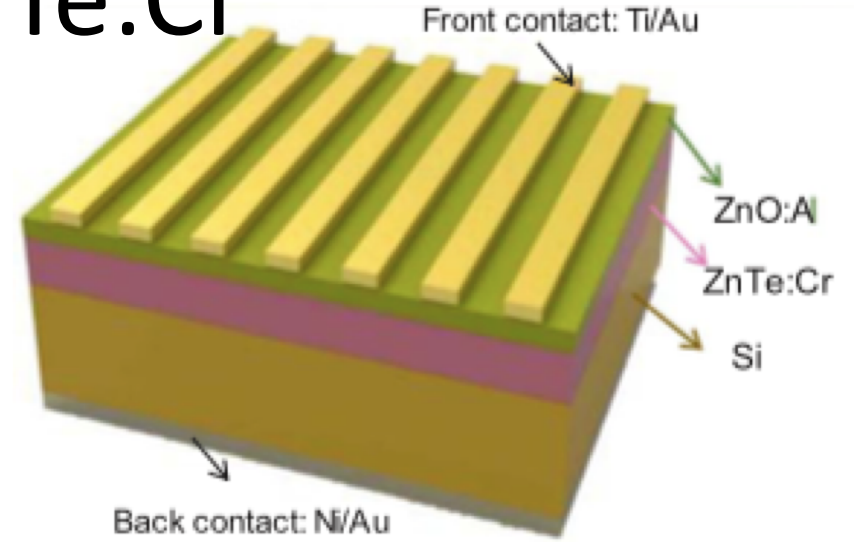
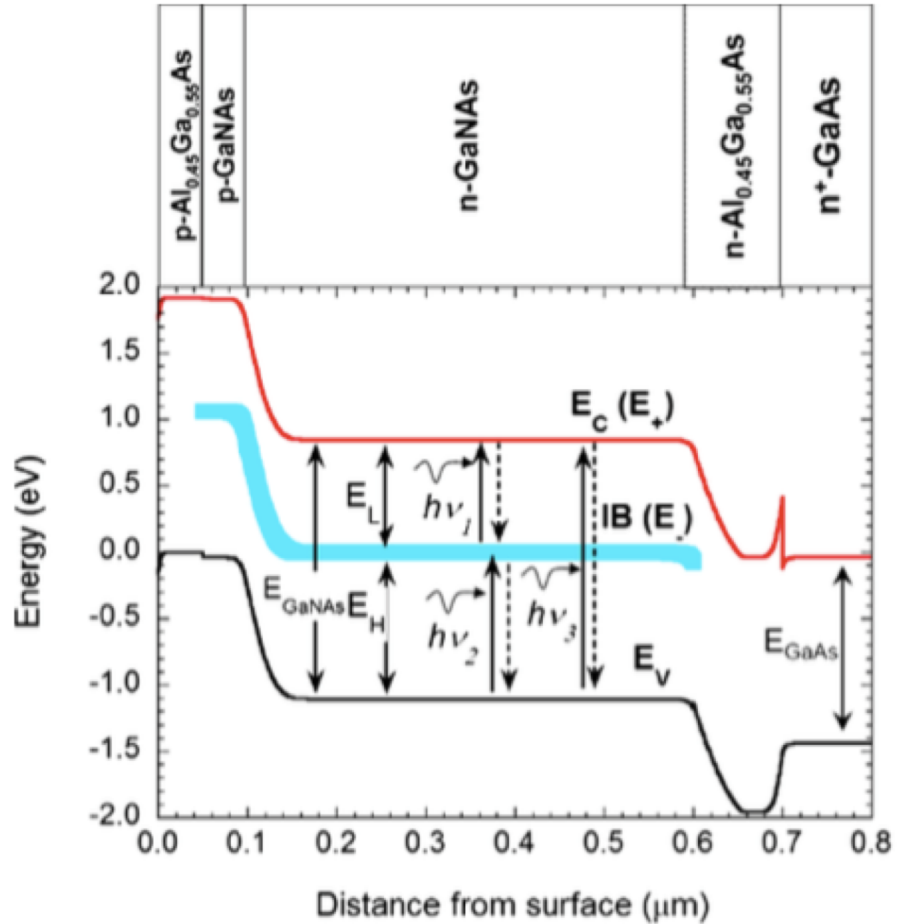


GaAs/GaNAs
<1% efficient
López et al., PRL 2011

Devices not
optimized, but
clear lifetime
problem.

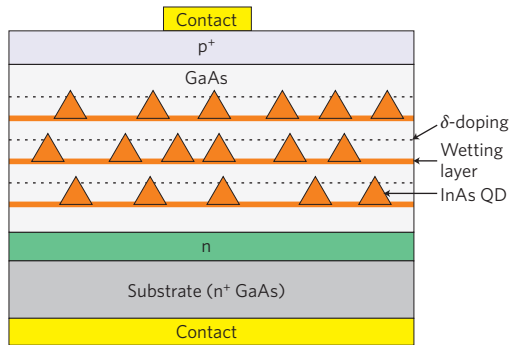
ZnTe:Cr
5.9% efficient
Lee et al., Sol. Energ. Mat. Sol. Cells 2017

GaNAs and ZnTe:Cr



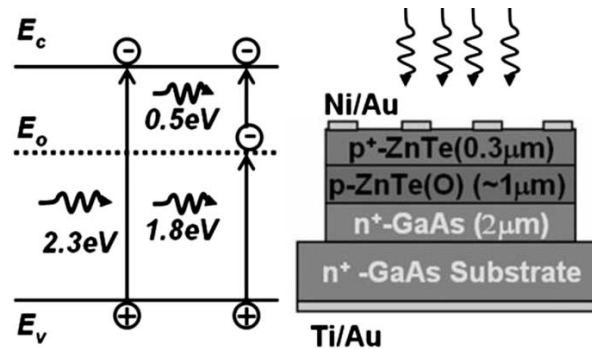
3 Candidate Materials Classes

1 Quantum dots



Luque et al., Nat Photon 2012

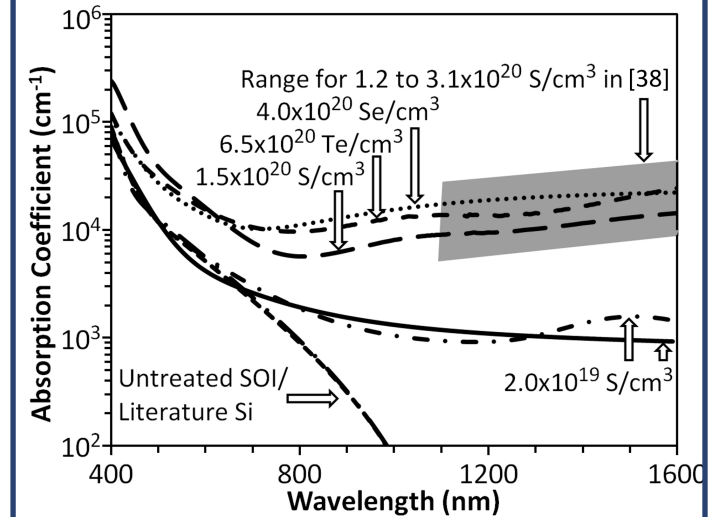
2 Highly-mismatched alloys



ZnTeO

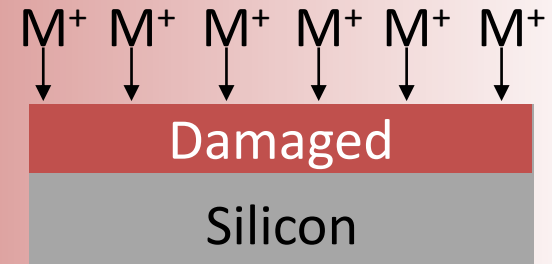
Wang et al., APL 2009

3 Hyperdoped silicon



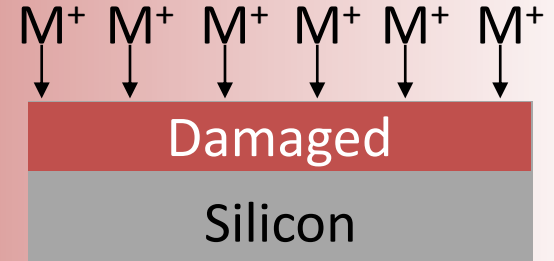
Pan et al, APL (2011)

Ion implantation



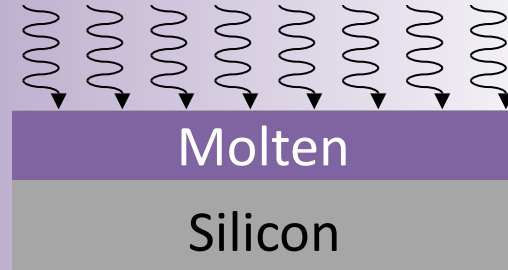
ANU

Ion implantation

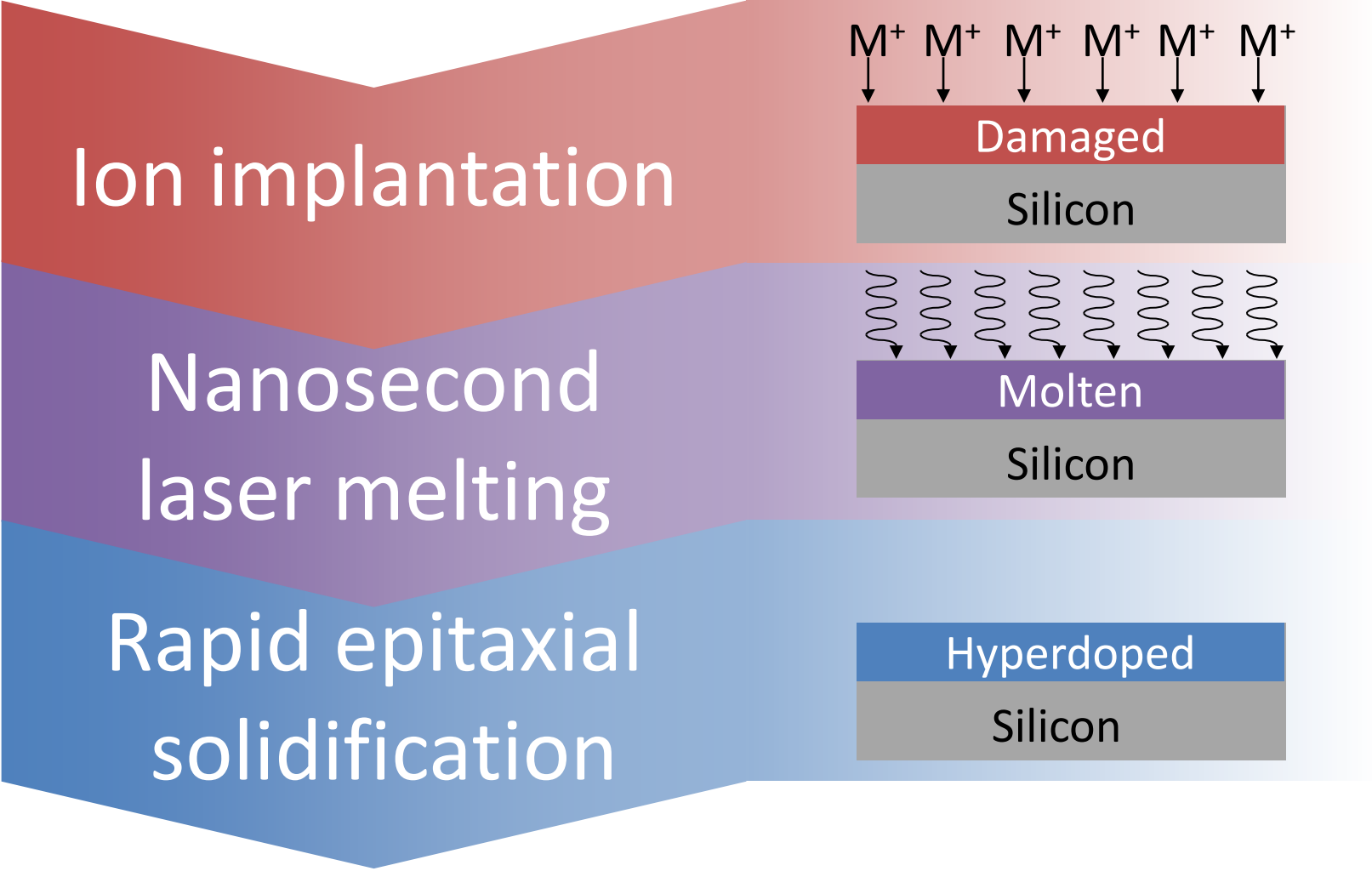


ANU

Nanosecond
laser melting



Benét Labs
New York



ANU

Benét Labs
New York

Hyperdoping in Silicon

Which materials are promising?
What doping to use?

hydrogen 1 H 1.0079																	helium 2 He 4.0026						
lithium 3 Li 6.941	beryllium 4 Be 9.0122																	boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305																	aluminum 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078	scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80						
rubidium 37 Rb 85.468	strontium 38 Sr 87.62	yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29						
caesium 55 Cs 132.91	barium 56 Ba 137.33	lanthanum 57-70 * [223]	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	wolfram 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]					
francium 87 Fr [223]	radium 88 Ra [226]	actinide series 89-102 * *	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	unnilium 110 Uun [271]	ununium 111 Uuu [272]	ununium 112 Uub [277]	ununquadium 114 Uuq [289]										

* Lanthanide series

** Actinide series

lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

Figures of merit

Absorber materials

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

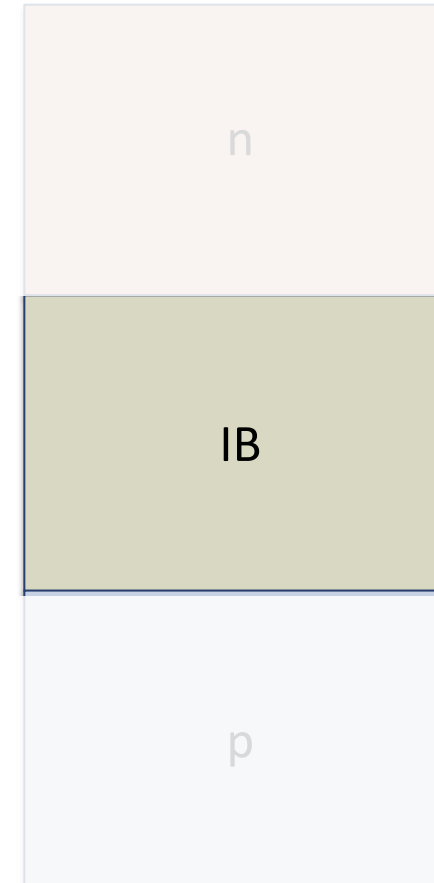
Devices

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

Want:

- Absorber only
- High predictive value

Indicate when to work on devices



Motivating a figure

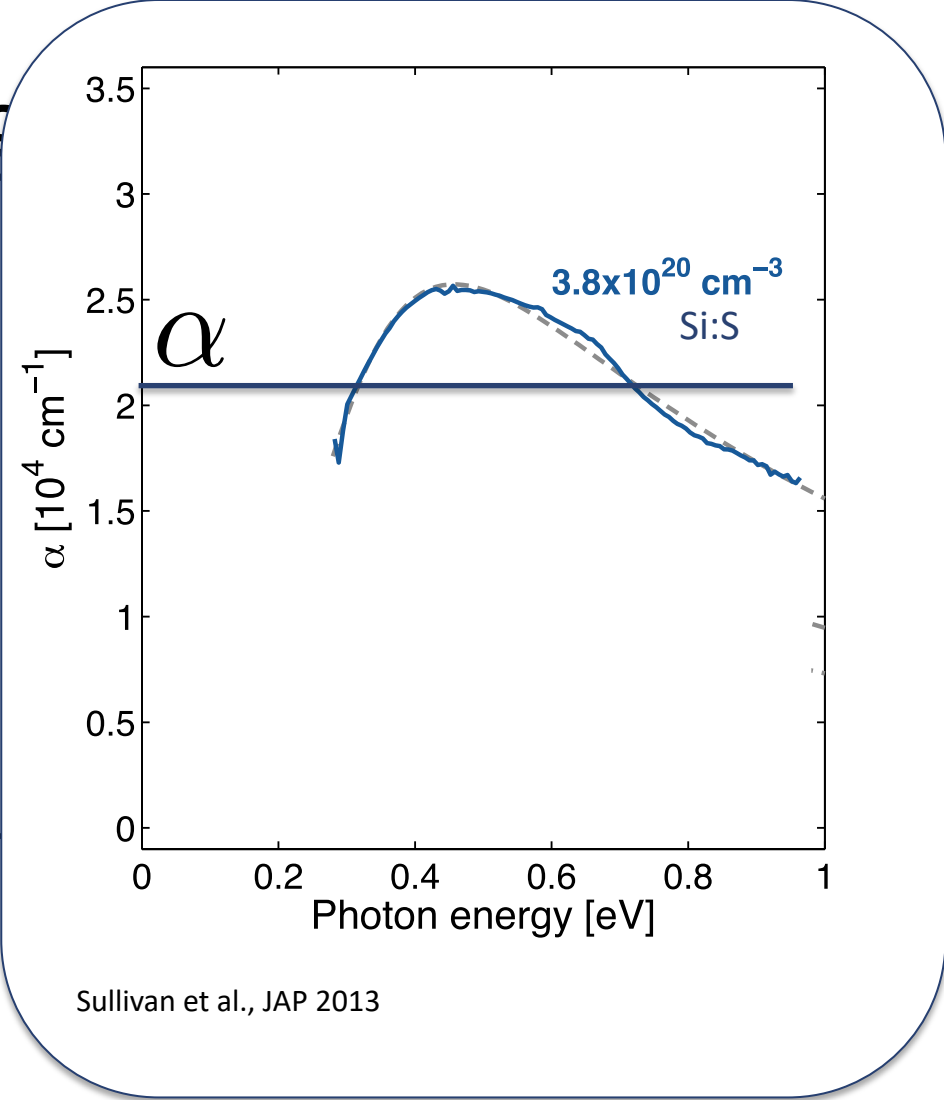
A good device has

carrier **lifetime** in IB region

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

transit time through IB region

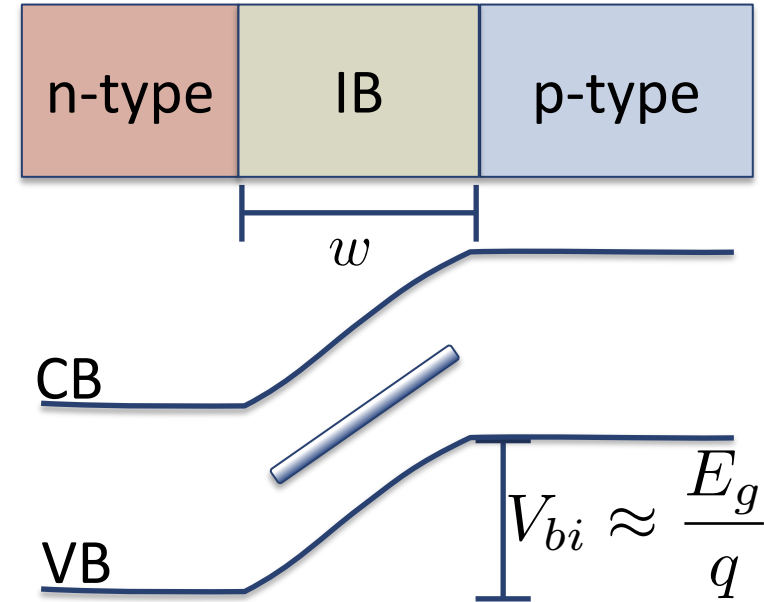
are



Drift Device

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

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

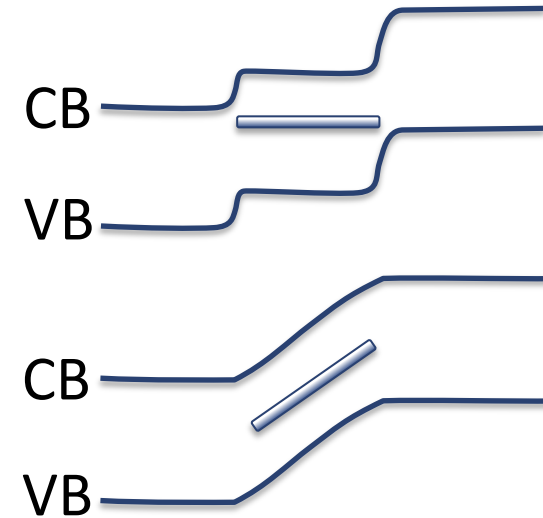


$$\frac{\tau}{t} \approx \nu_{\text{drift}} = \frac{E_g}{q} \mu \alpha^2 \tau$$

Comparison of figures of merit

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

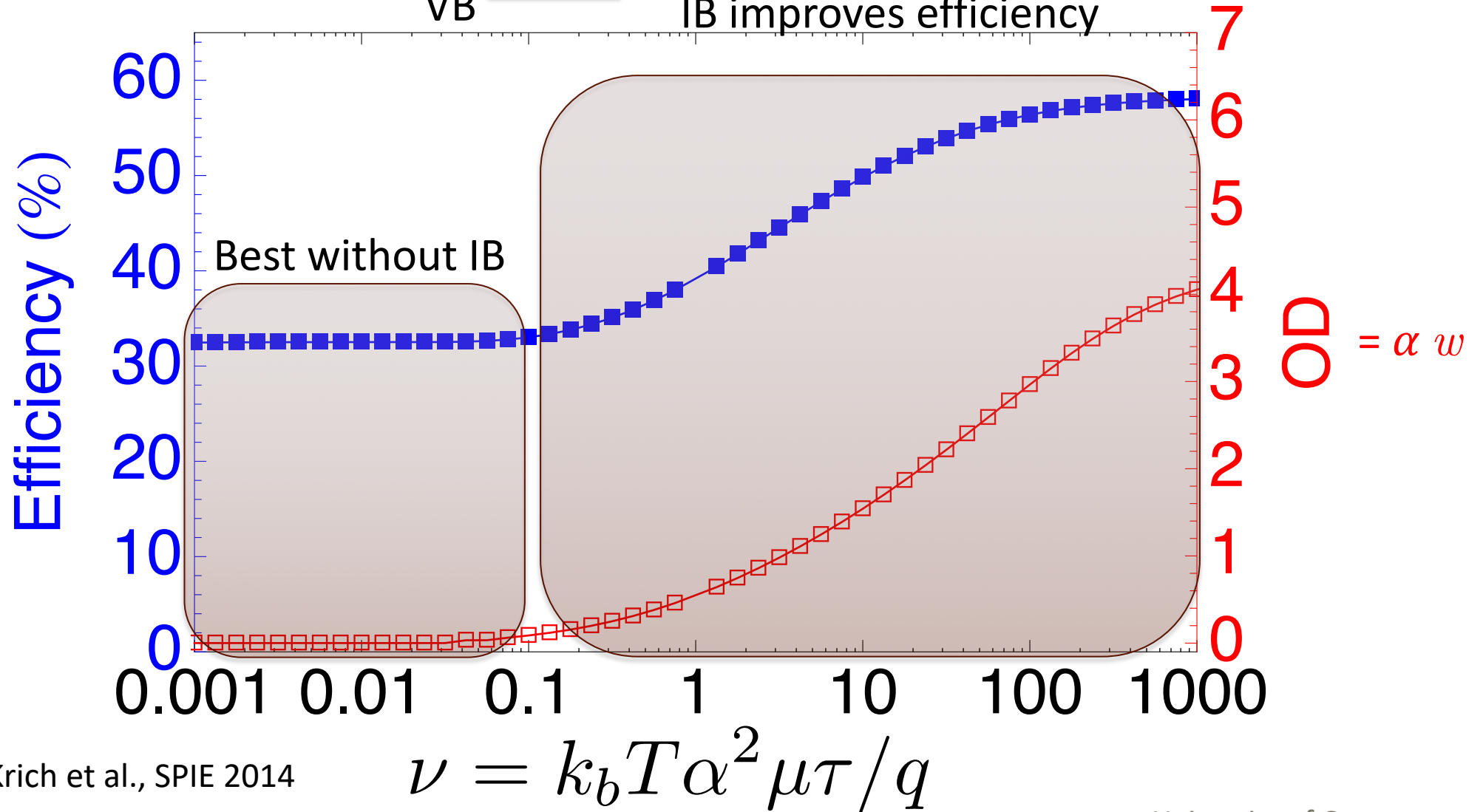
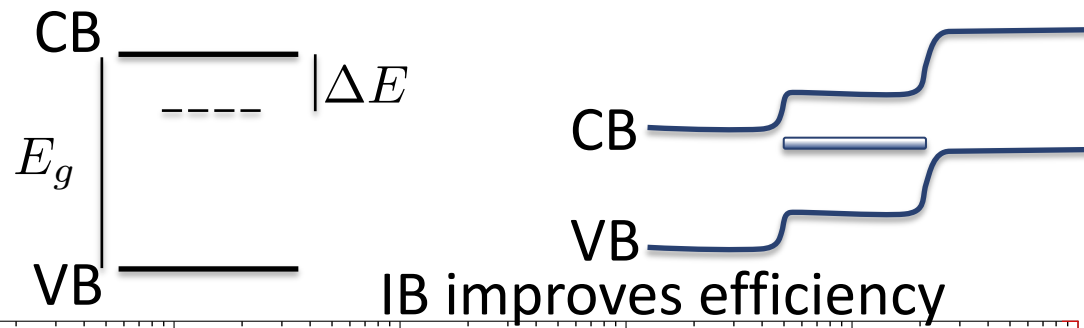
$$\nu_{drift} = \frac{E_g}{q} \mu \alpha^2 \tau$$



Measurable parameters of IB material alone.

Good devices: large ν for both electrons and holes.

$E_g = 1.9 \text{ eV}$
 $\Delta E = 0.7 \text{ eV}$
 full concentration



Krich et al., SPIE 2014

$$\nu = k_b T \alpha^2 \mu \tau / q$$

Light trapping

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

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

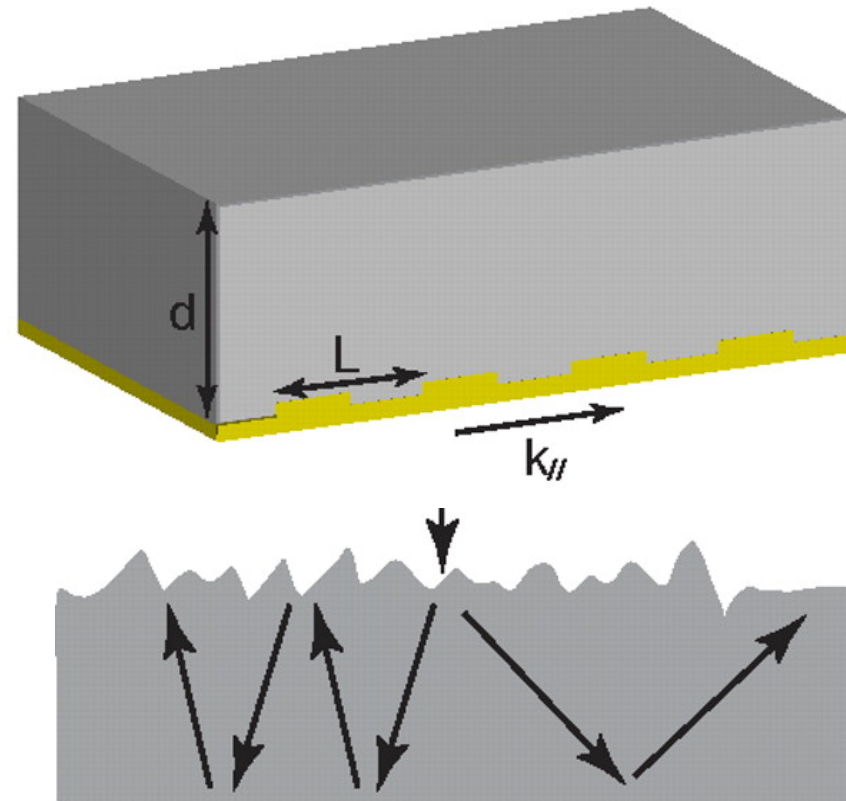


Figure from Yu et al, PNAS 2010

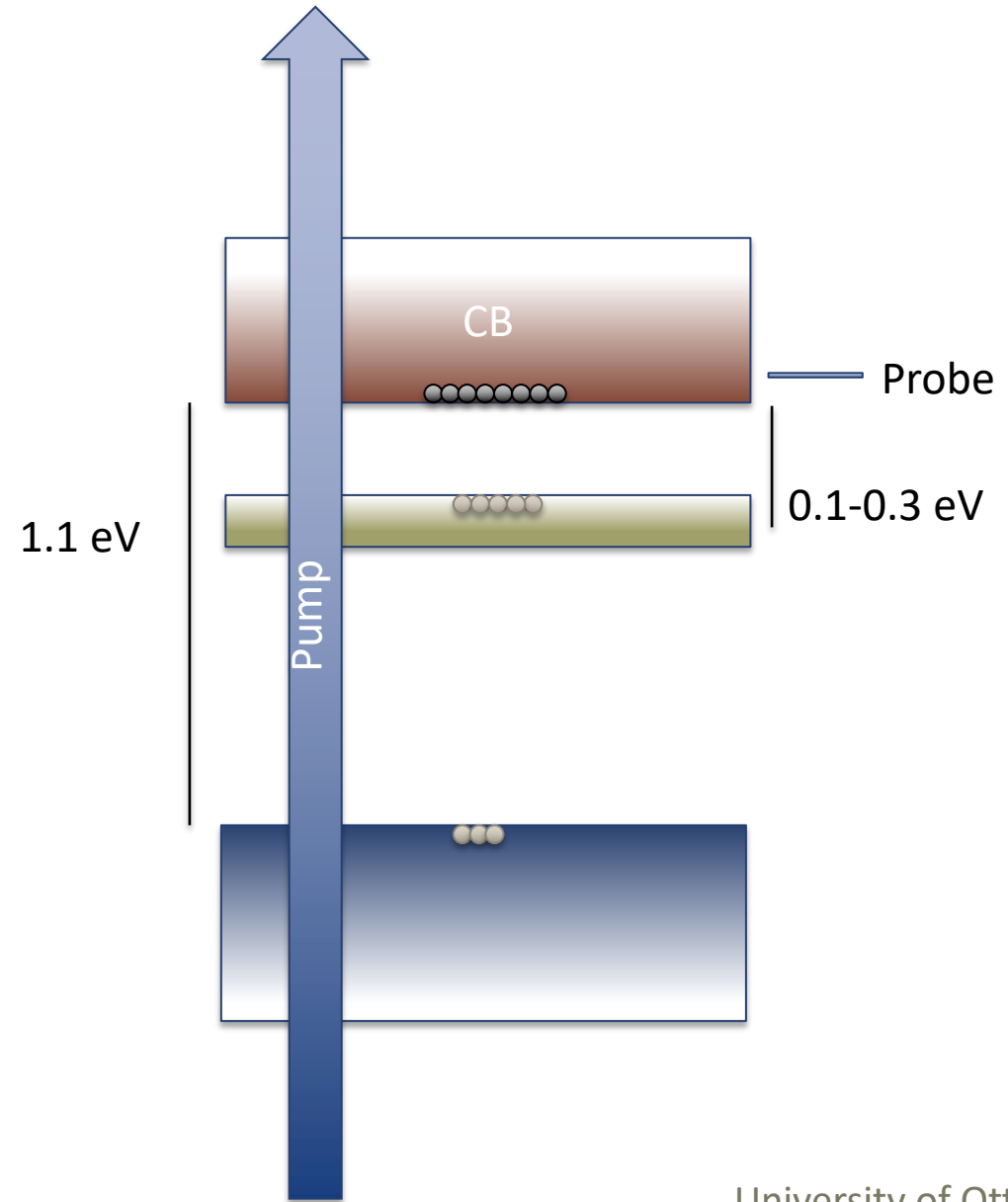
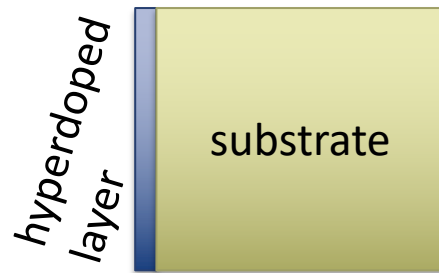
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 - 3 material classes
- Figure of merit
 - **Measurements**
 - Predictions
- New developments
 - InGaN quantum dots in nanowires
 - Device model

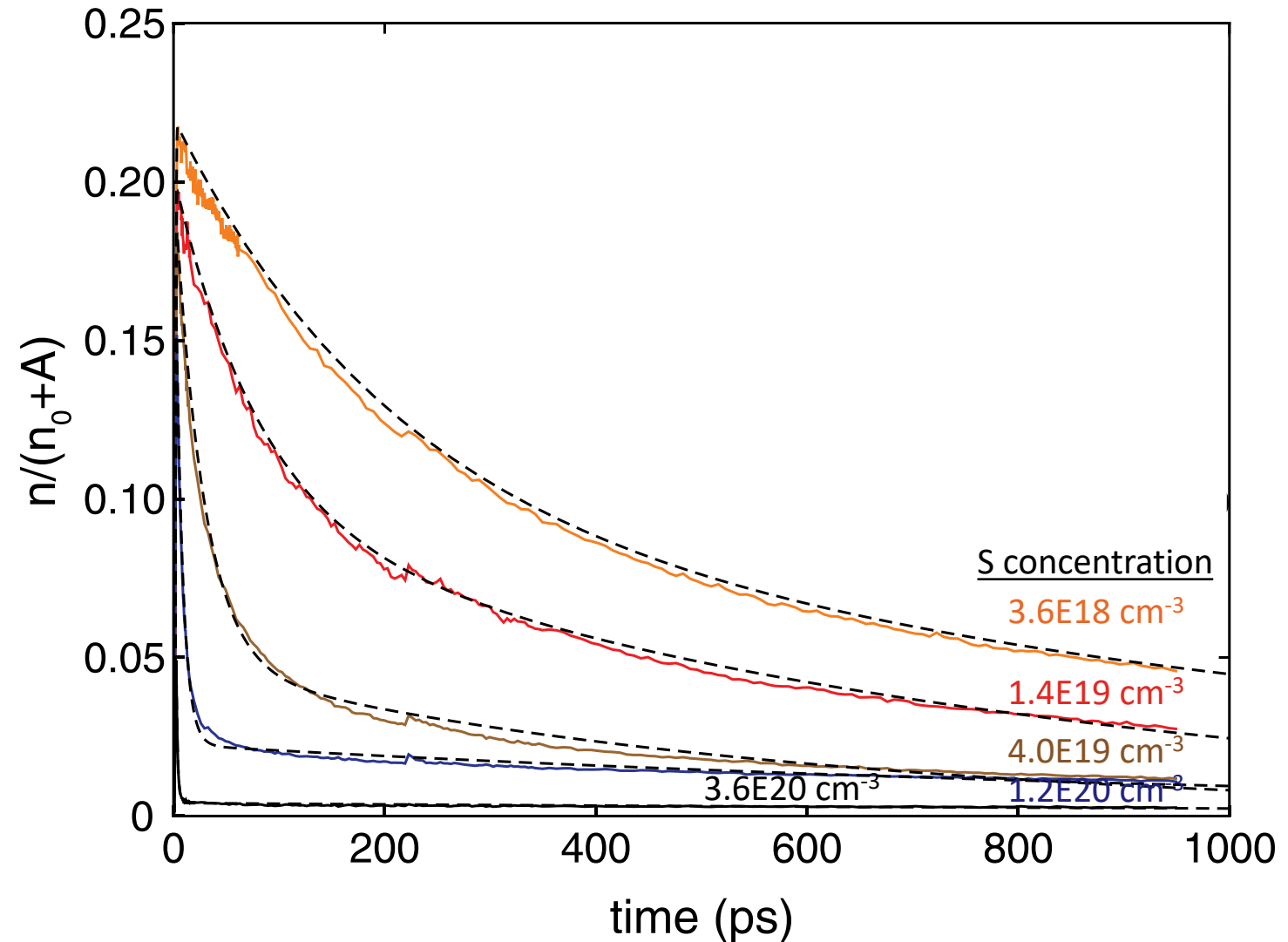
THz measurements of carrier lifetime

Pump

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

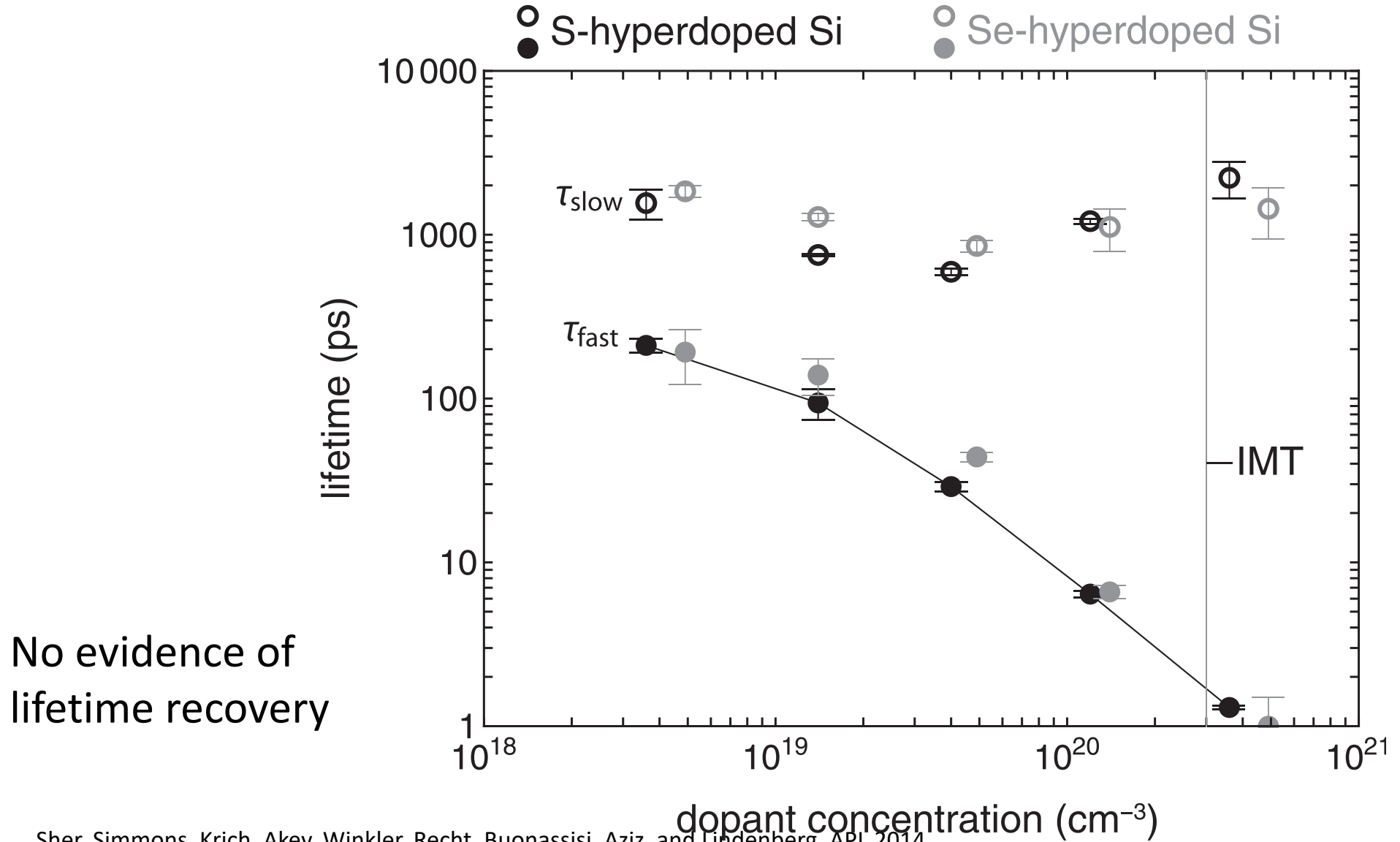


fs THz study of trapping times in Si:S and Si:Se



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

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



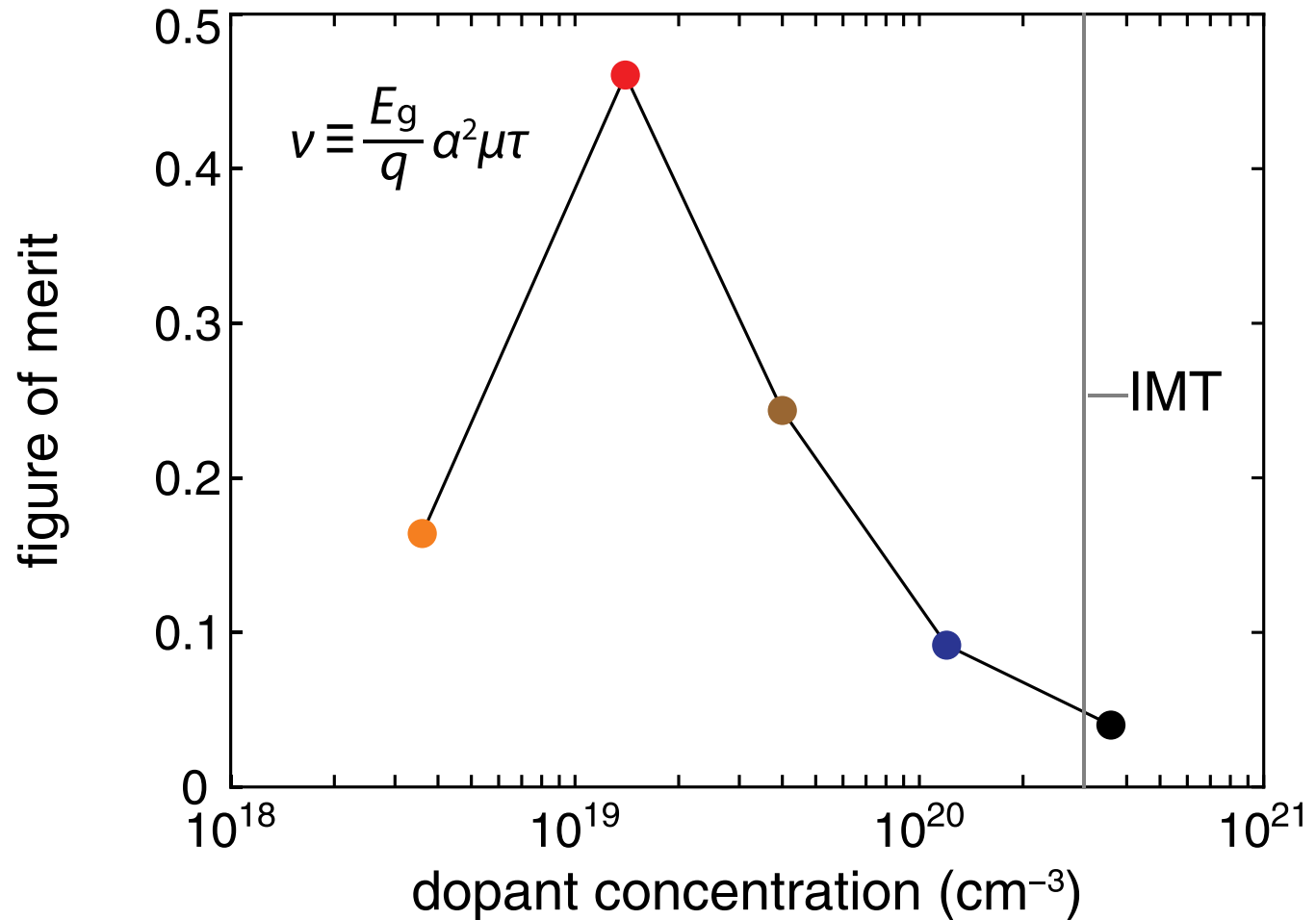
No evidence of
lifetime recovery

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

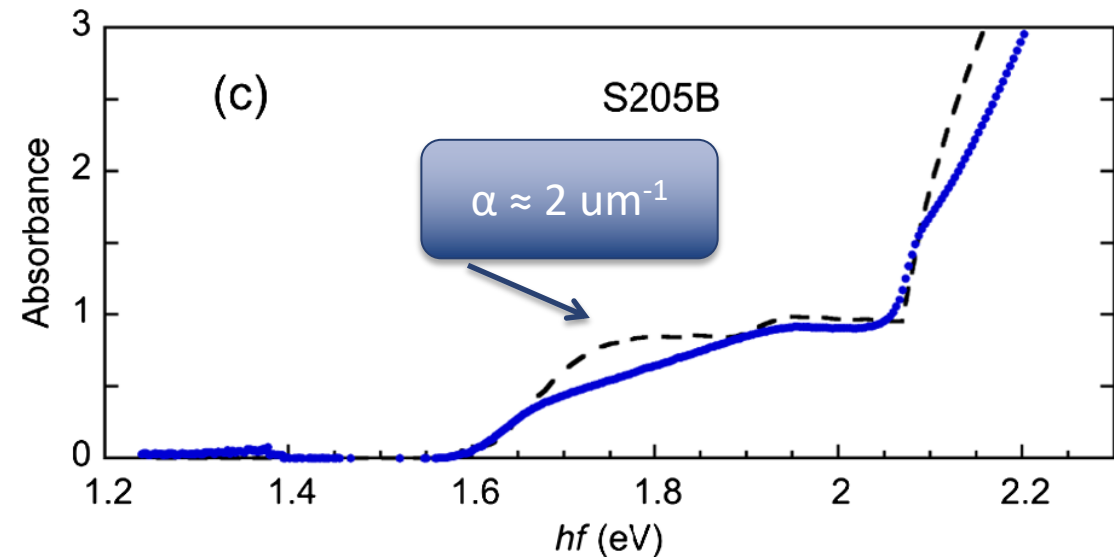
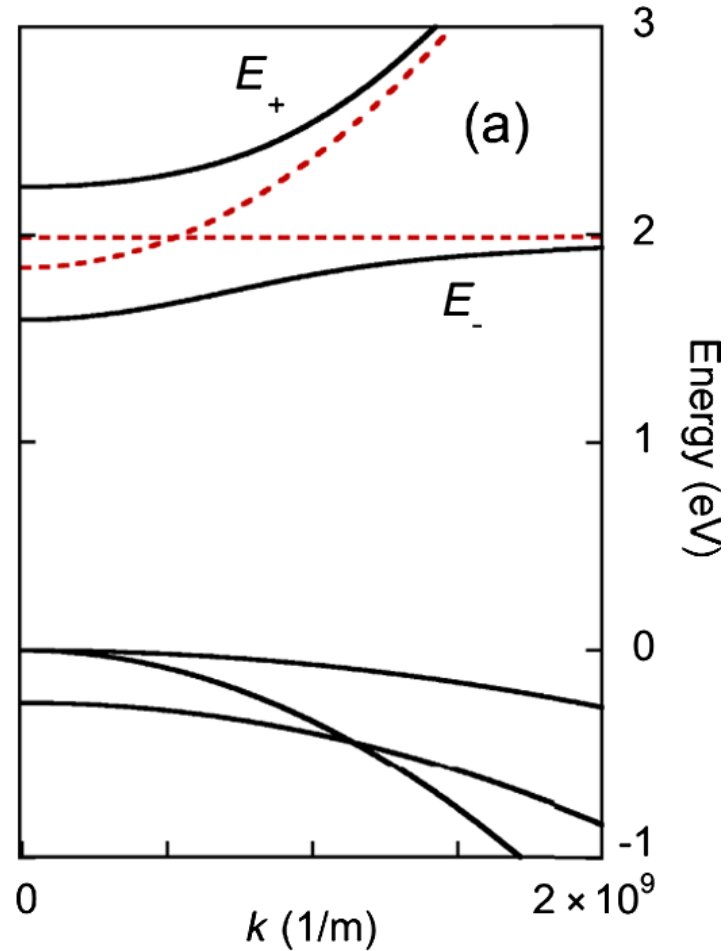
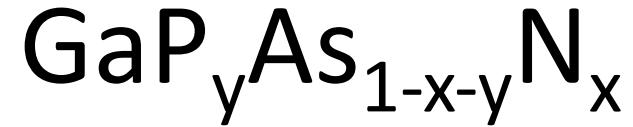
ν peaks at lower concentration.

Still hyperdoped.

Hole figure of merit not measured.



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



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

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

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

Heyman et al, PR Applied (2017)

OPEN

Multicolor emission from intermediate band semiconductor $\text{ZnO}_{1-x}\text{Se}_x$

Received: 06 December 2016

Accepted: 03 February 2017

Published: 13 March 2017

M. Welna¹, M. Baranowski^{1,2}, W. M. Linhart¹, R. Kudrawiec¹, K. M. Yu^{3,4}, M. Mayer³ & W. Walukiewicz³

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.

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Predicting ν

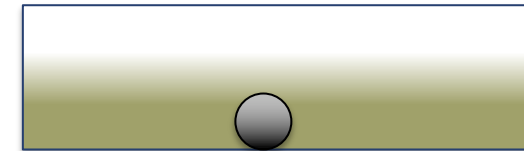
$$\nu_{drift} = \frac{E_g}{q} \mu \tau \alpha^2$$

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

μ_{latt} is constant
 $\mu_{ni} \propto \frac{1}{N_I}$

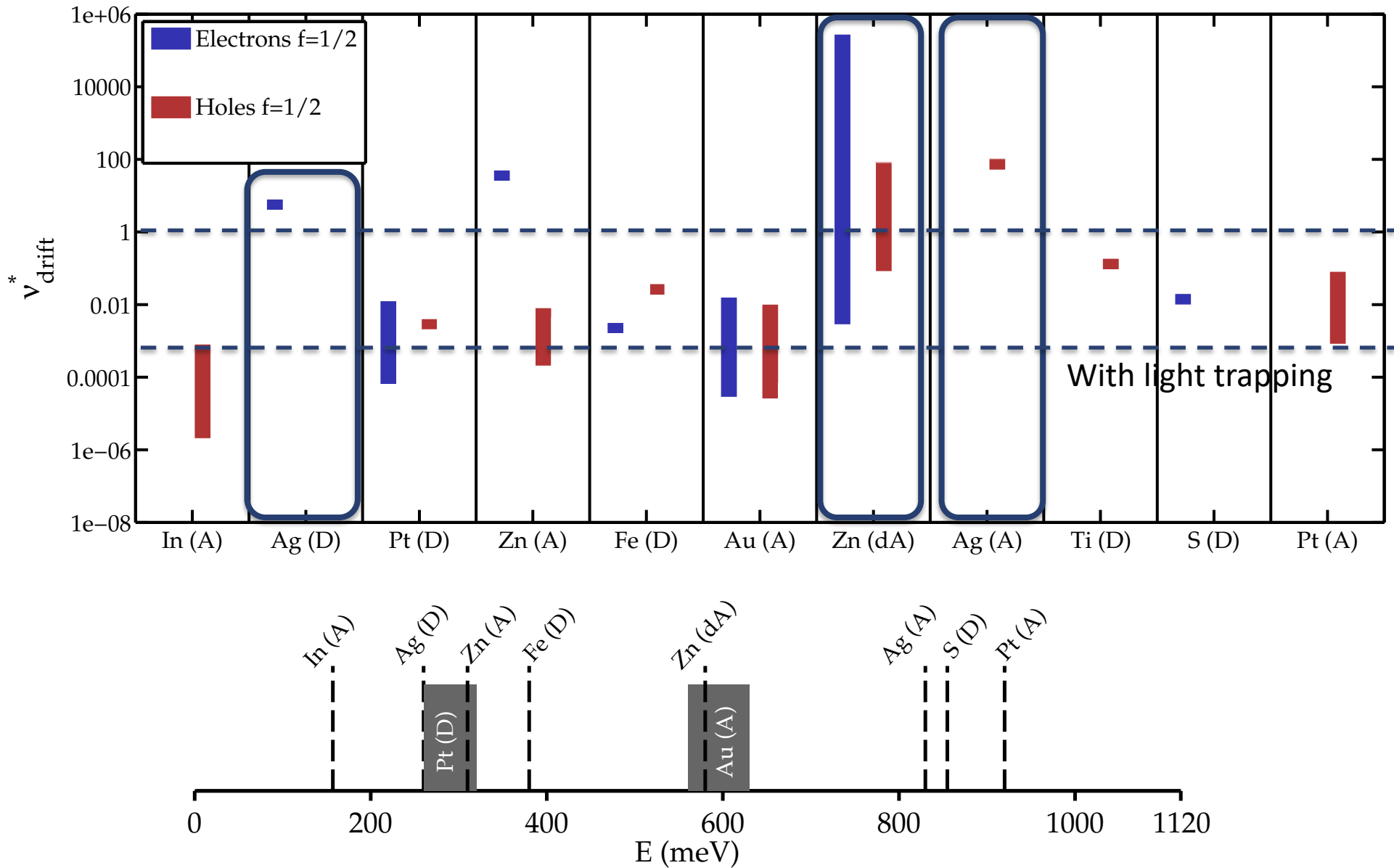
$$\tau \propto \frac{1}{N_I}$$

$$\alpha \propto N_I$$



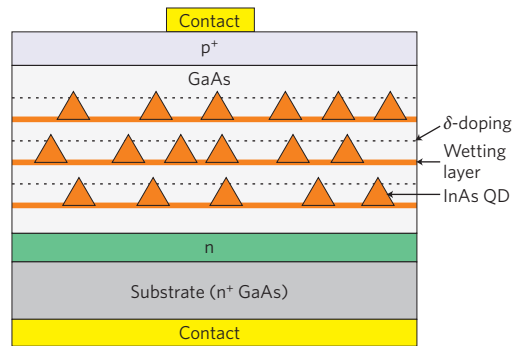
Small N_I : $\nu \propto N_I$

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



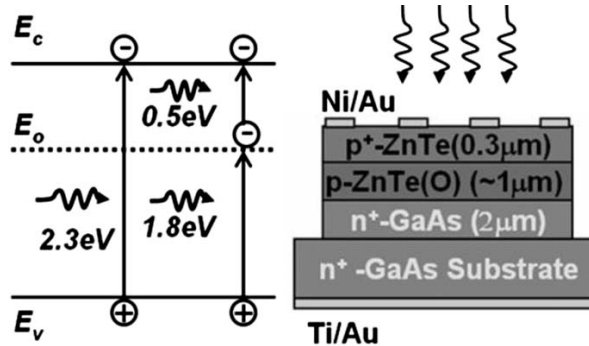
3 Candidate Materials Classes

1 Quantum dots



Luque et al., Nat Photon 2012

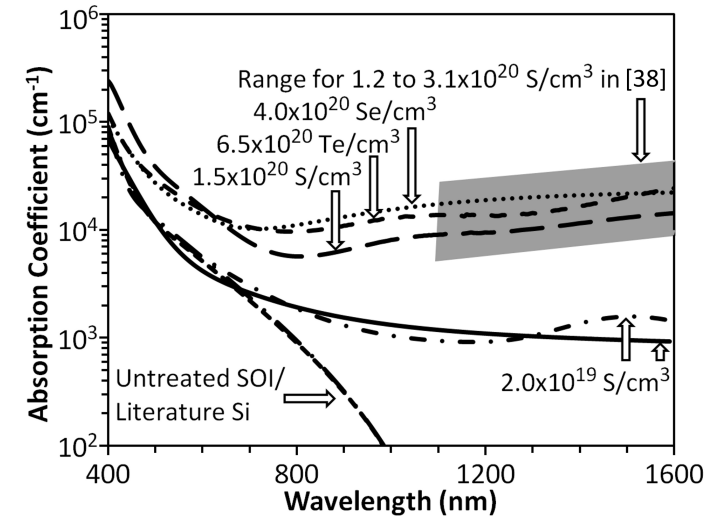
2 Highly-mismatched alloys



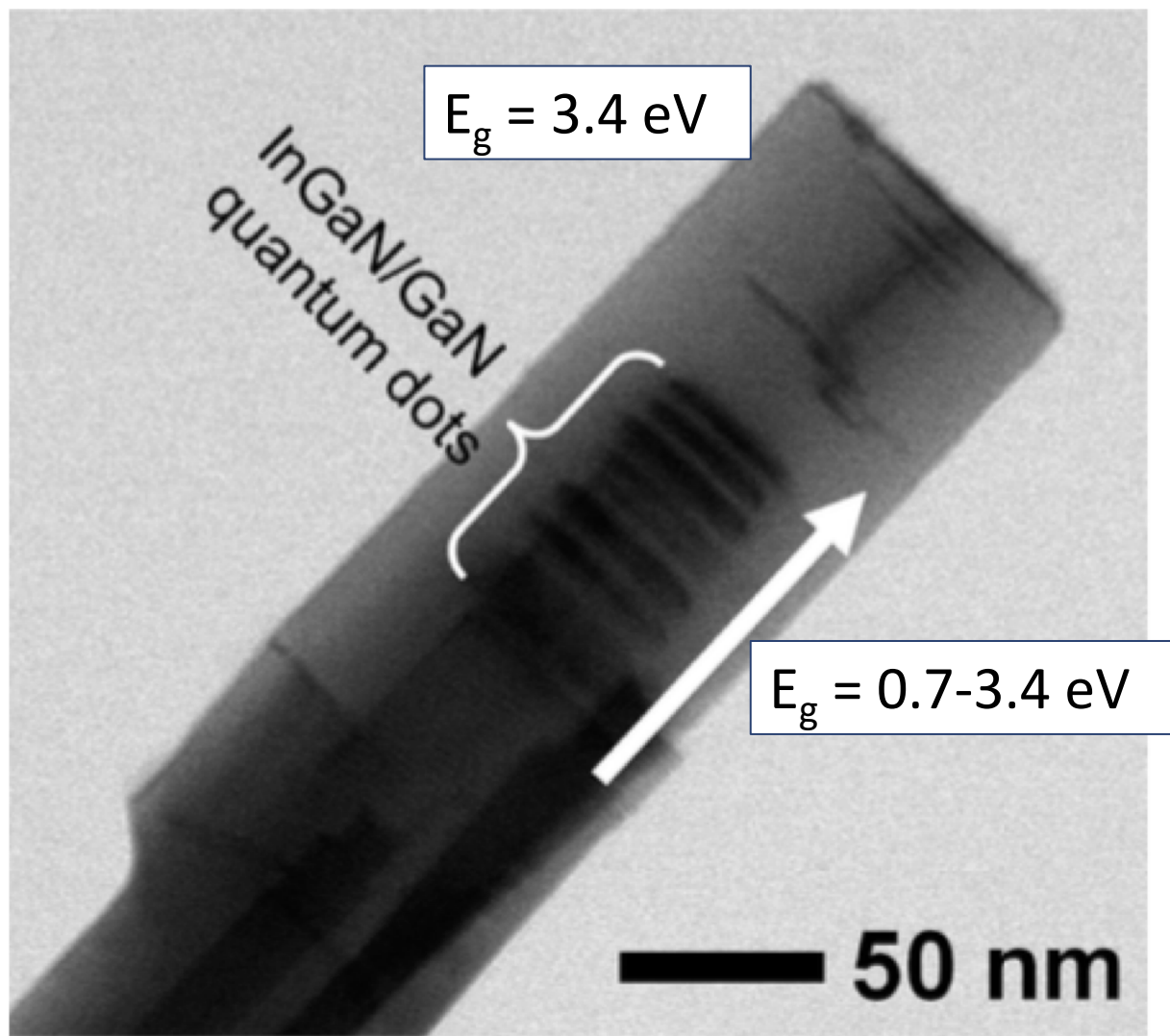
ZnTeO

Wang et al., APL 2009

3 Hyperdoped silicon

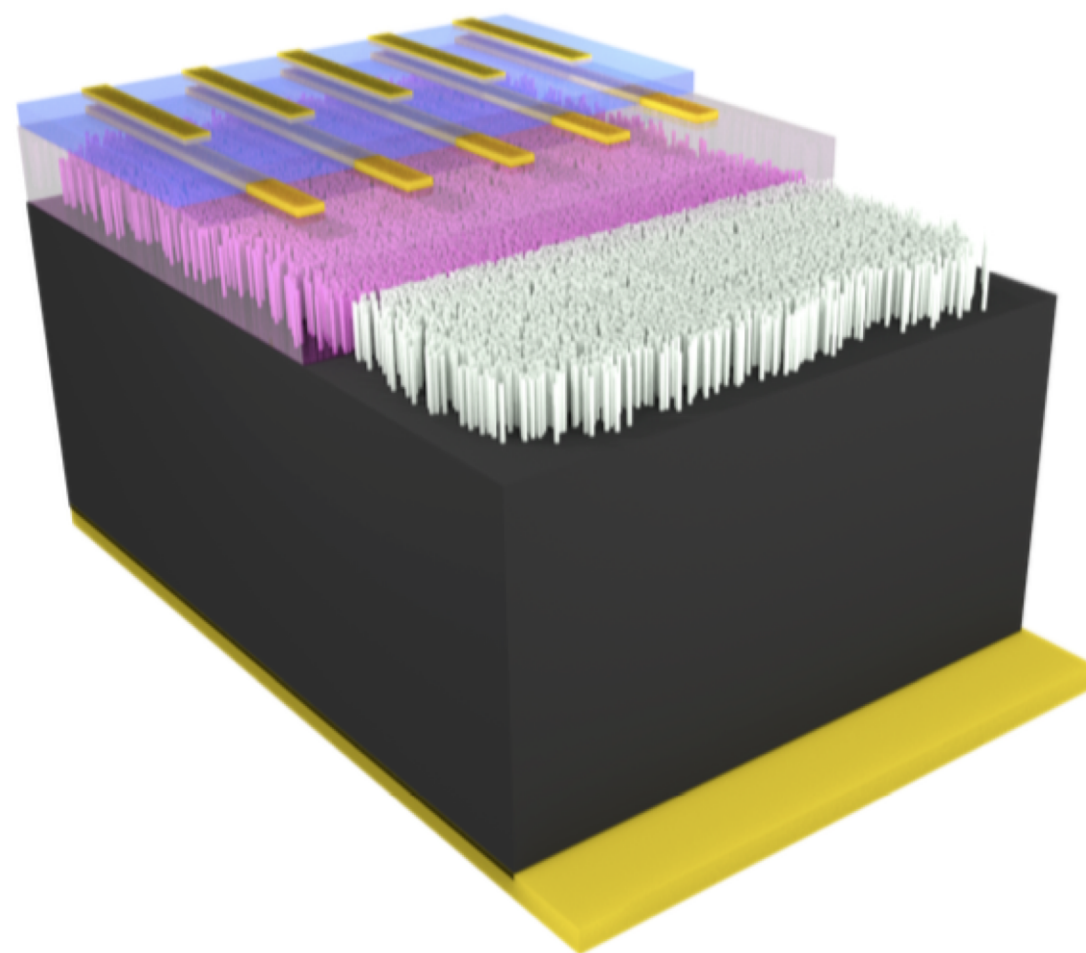


Pan et al, APL (2011)



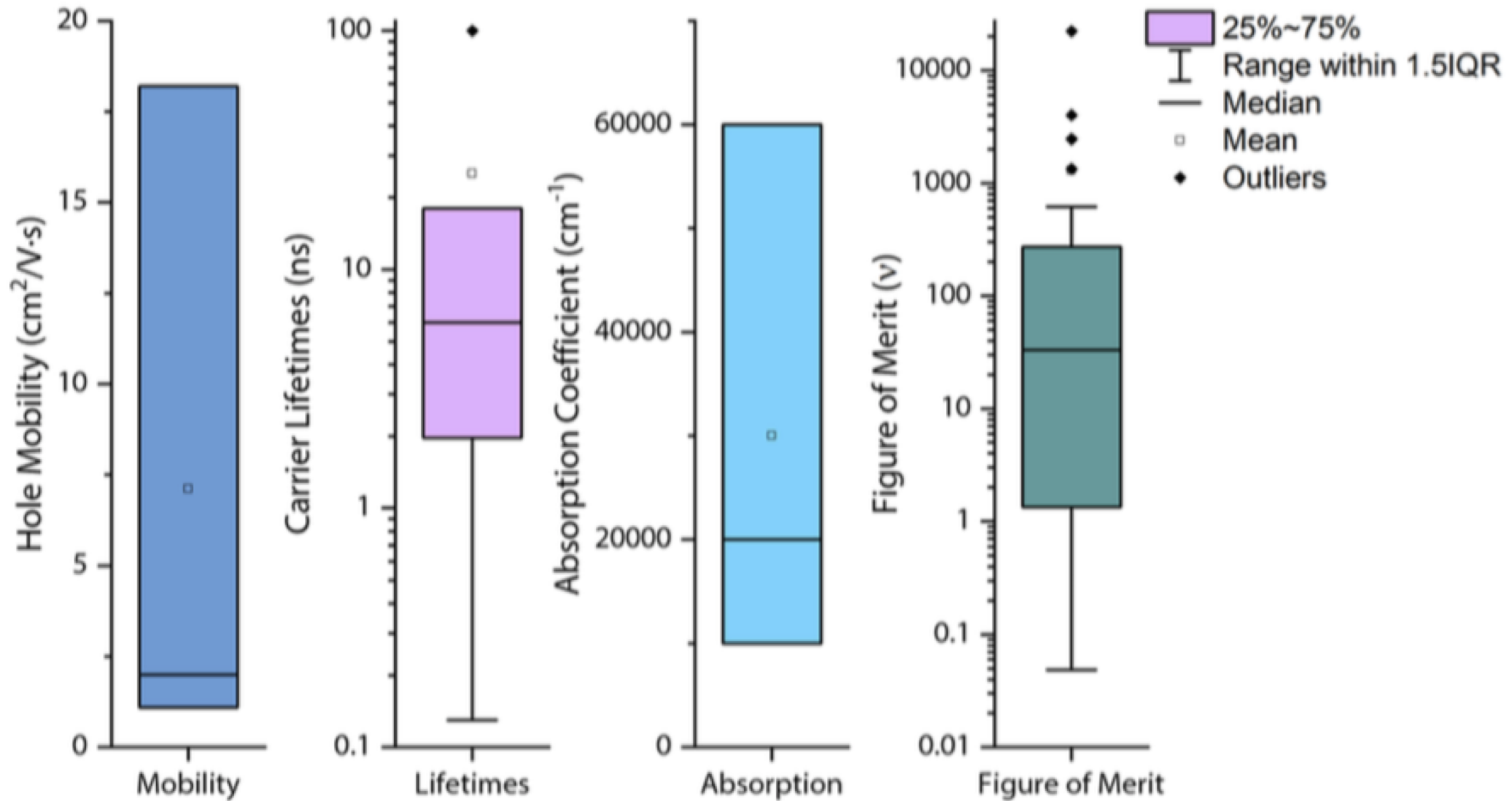
Nguyen et al., Nano Lett 2011

Jacob J. Krich



Ross Cheriton, PhD thesis, 2018

University of Ottawa



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.

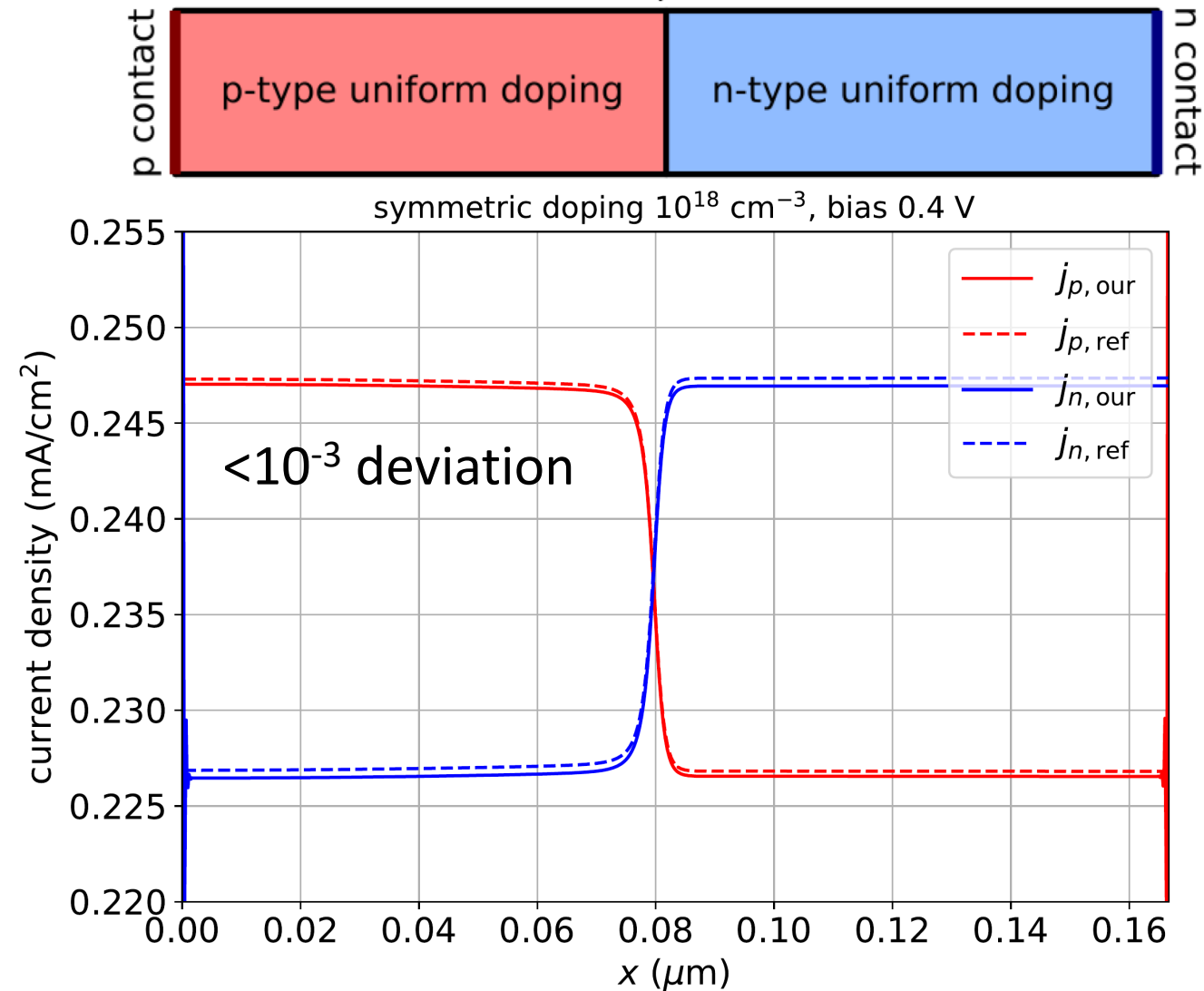
Martí, Cuadra, Luque IEEE TED 2002

- Diffusive only. Radiative recombination only.

Many detailed-balance based models

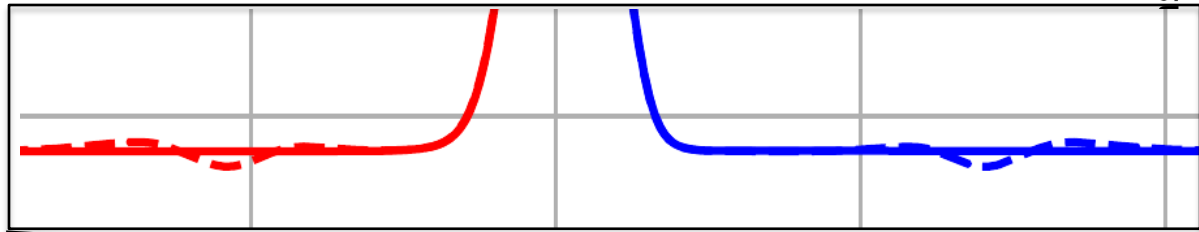
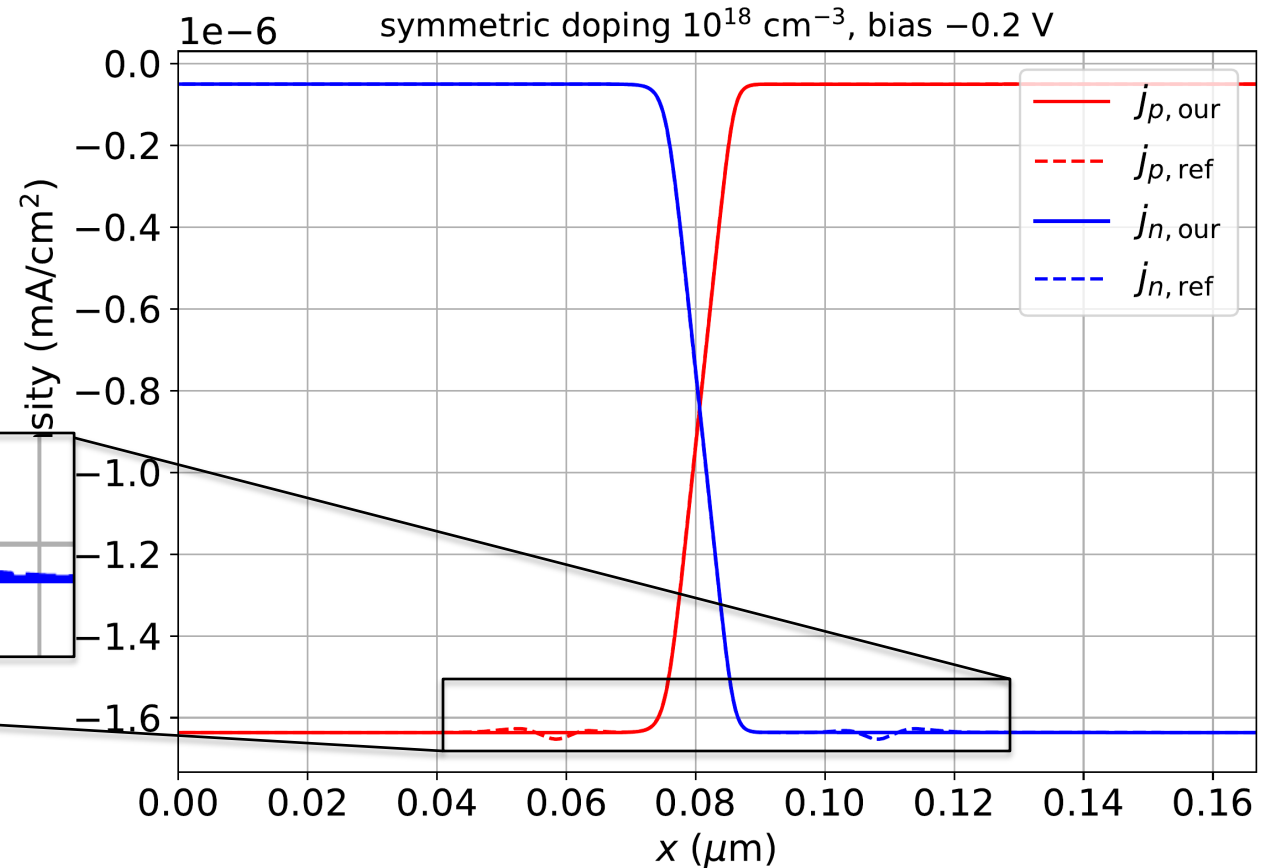
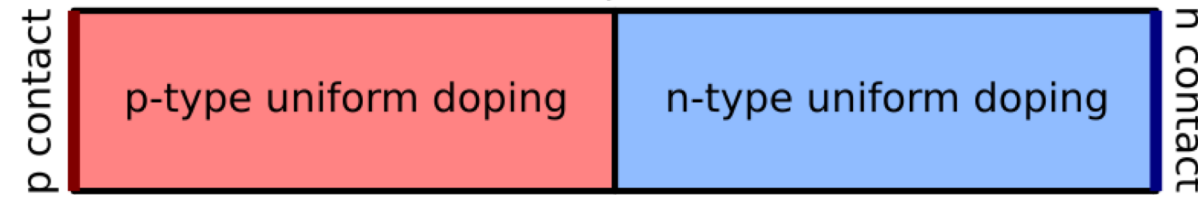
Our device model

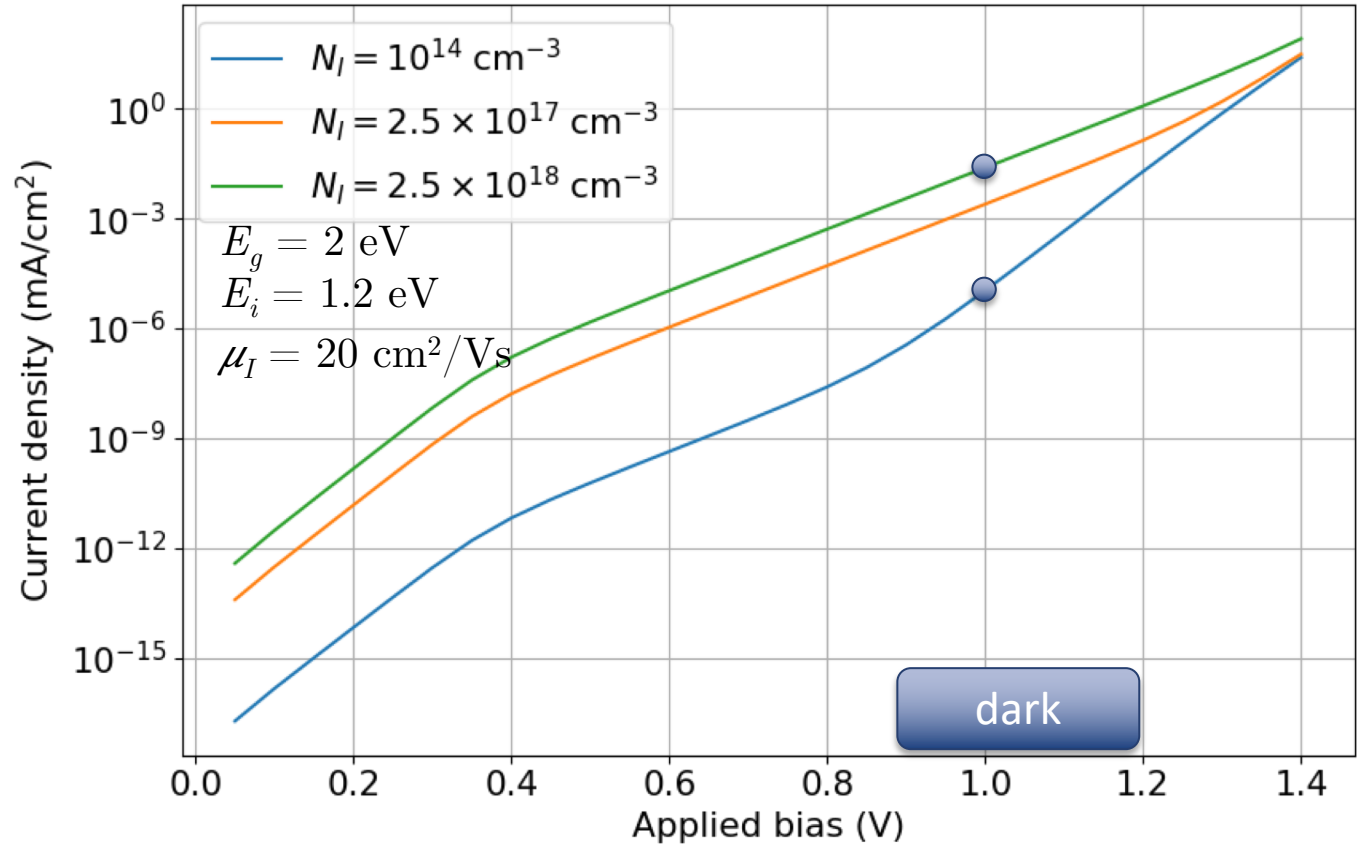
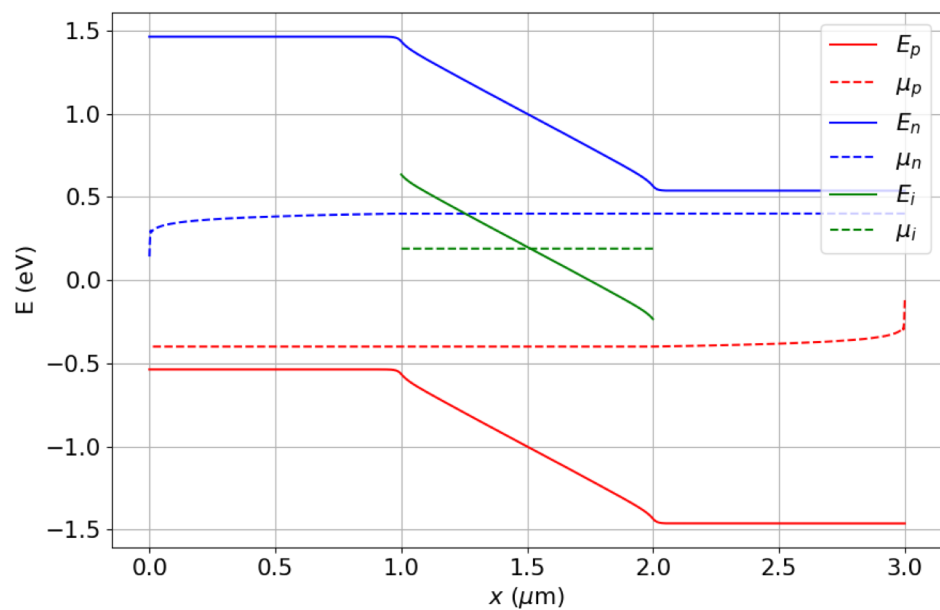
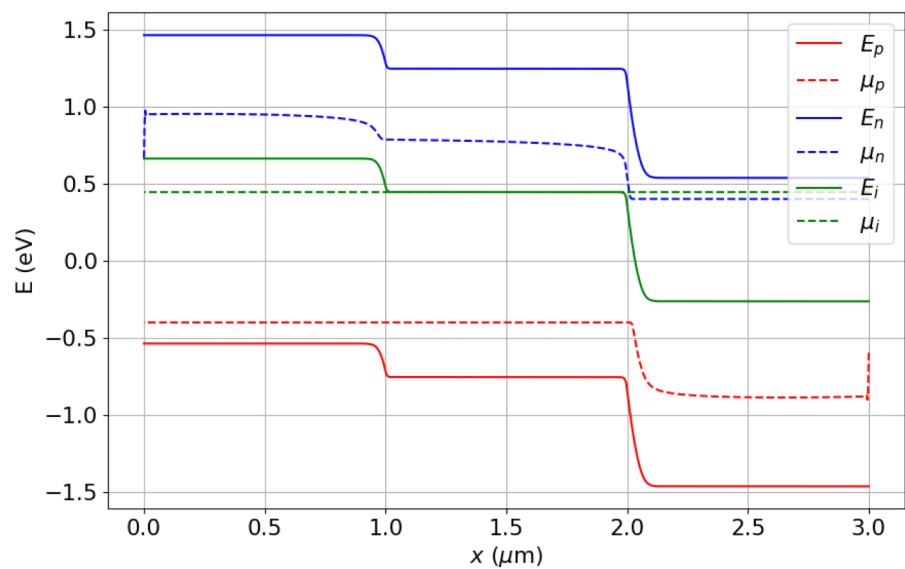
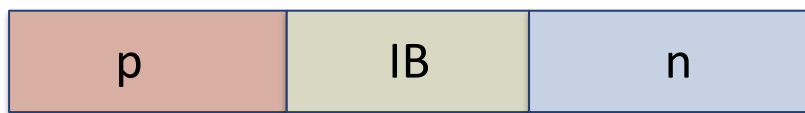
- 2D
- Finite element – built using FEniCS
- Benchmark against Synopsys Sentaurus

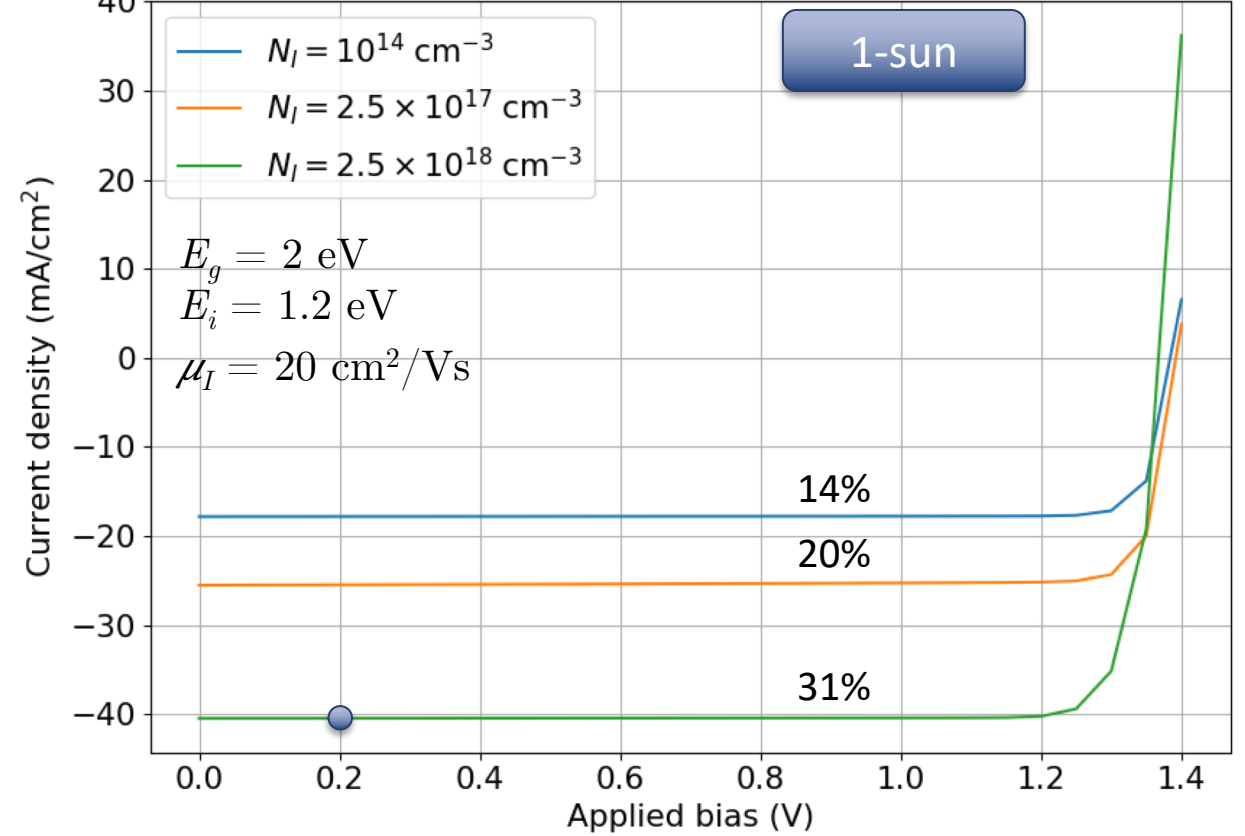
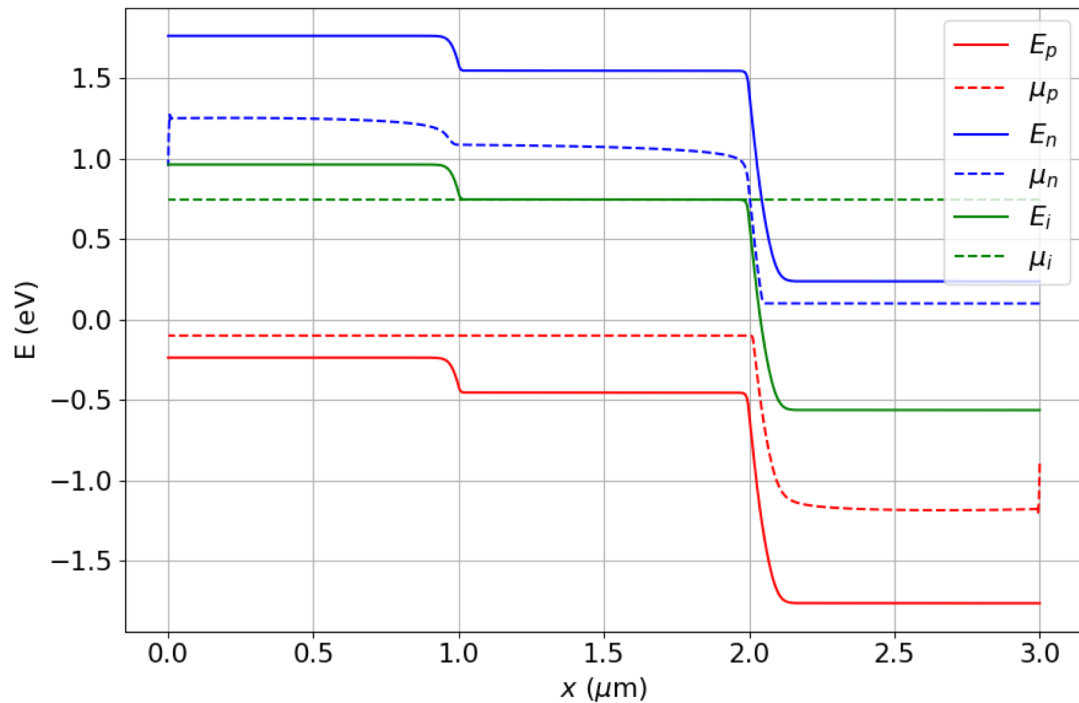
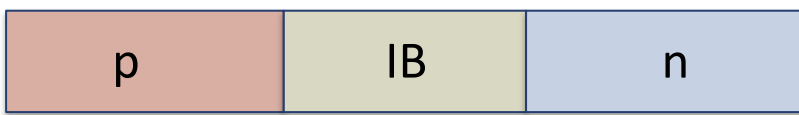


Our device model

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







- 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

