Multiscale Modeling and Simulation of Advanced Photovoltaic Devices

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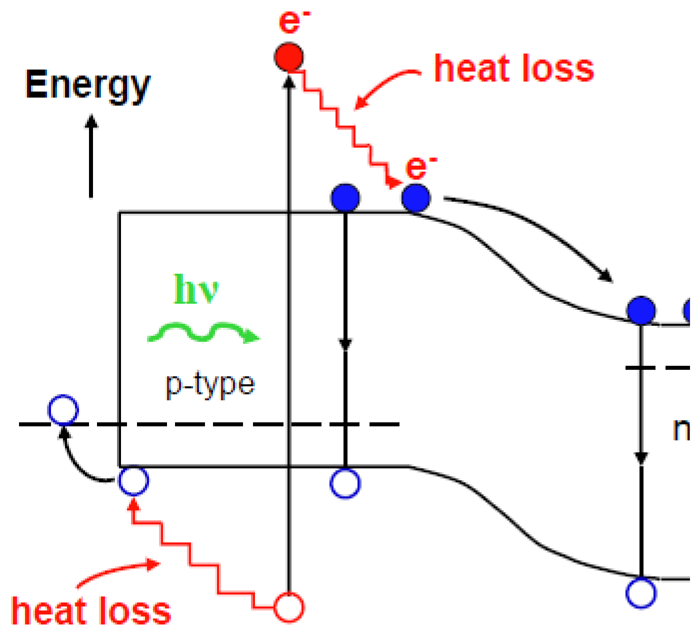
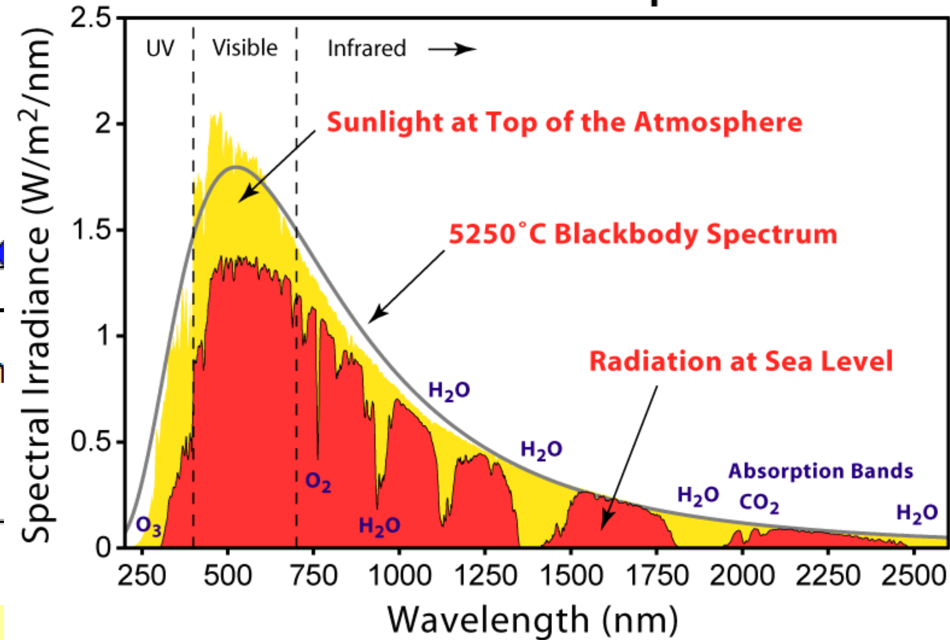
Outline

- **High efficiency photovoltaics and efficiency limits**
- **Multiscale modeling of c-Si/a-Si:H heterojunction solar cells**
- **Multiscale modeling of Si tandem solar cells**
- **Multiexciton generation in nanowires for advanced concept solar cells**

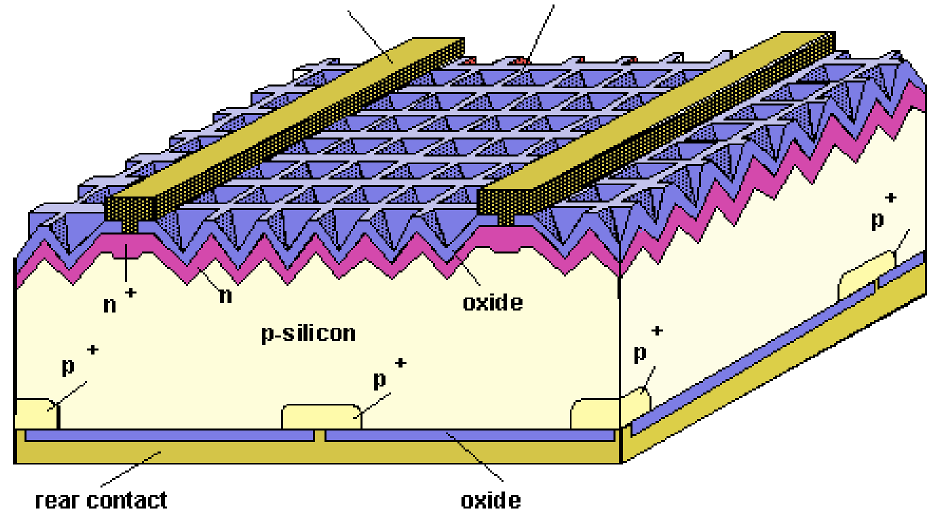
Photovoltaics (PV)



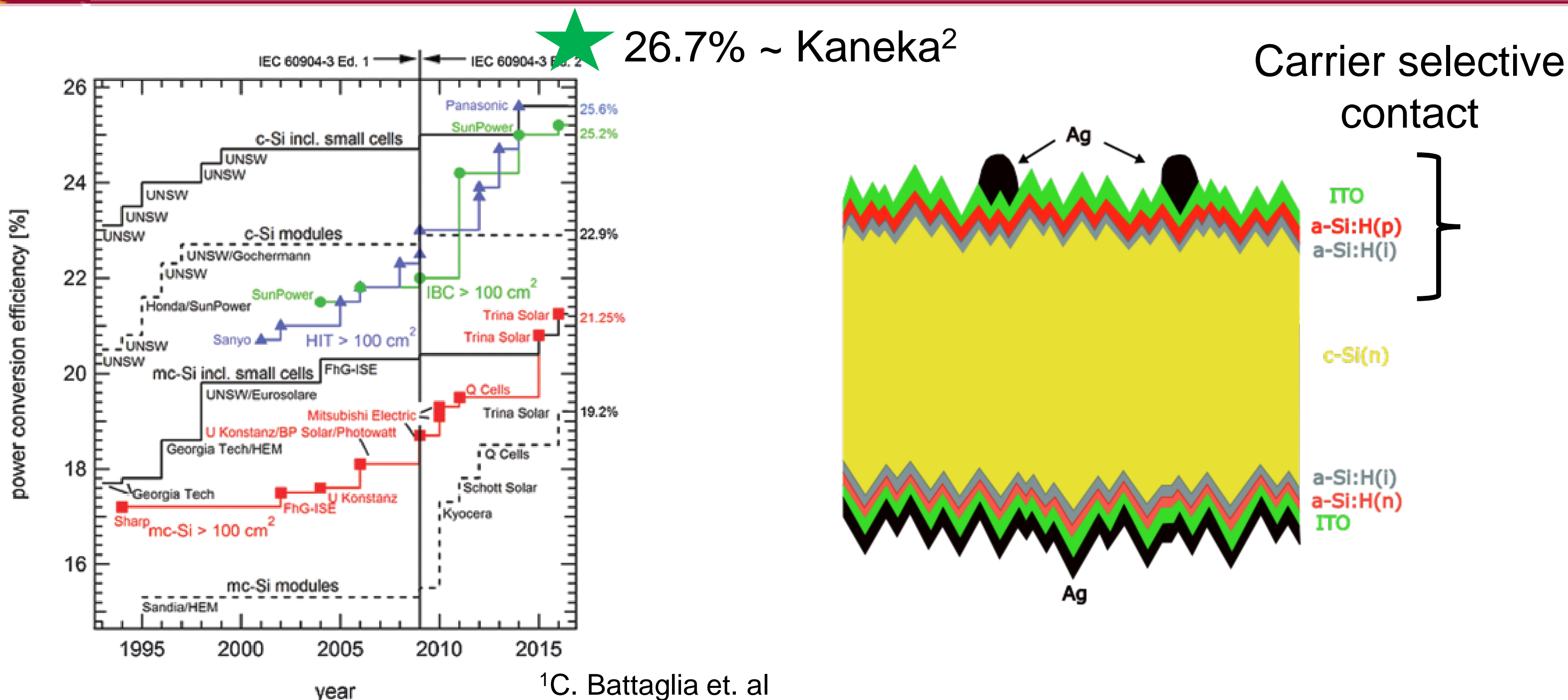


1 e- - h+ pair/photon

First Generation single crystal Si PV technology



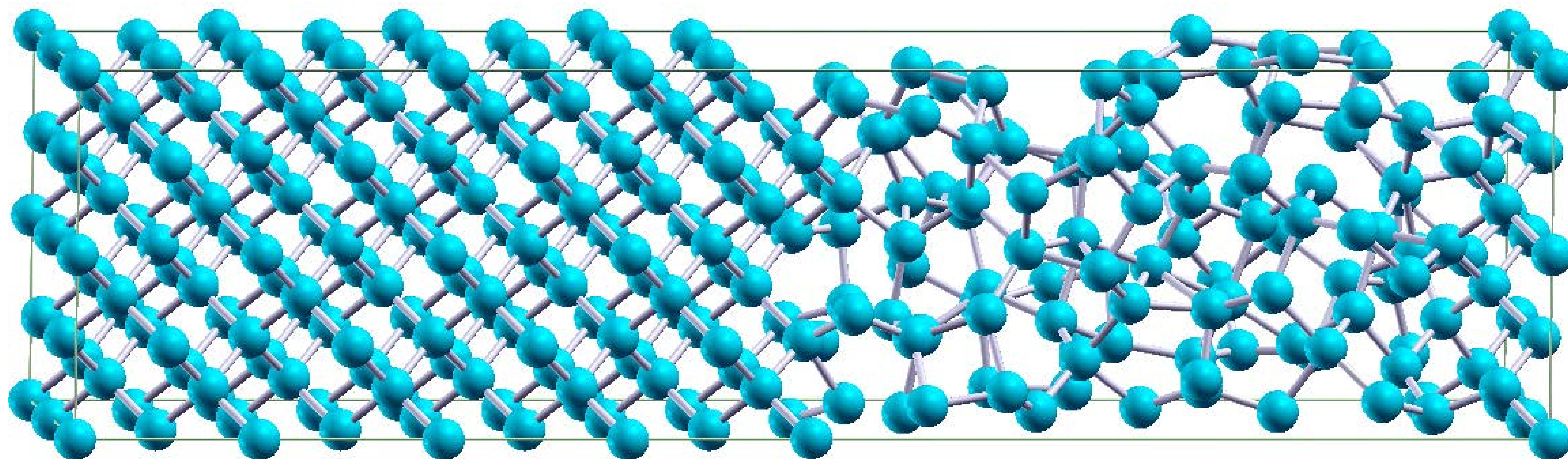
Silicon Heterojunction Solar Cells



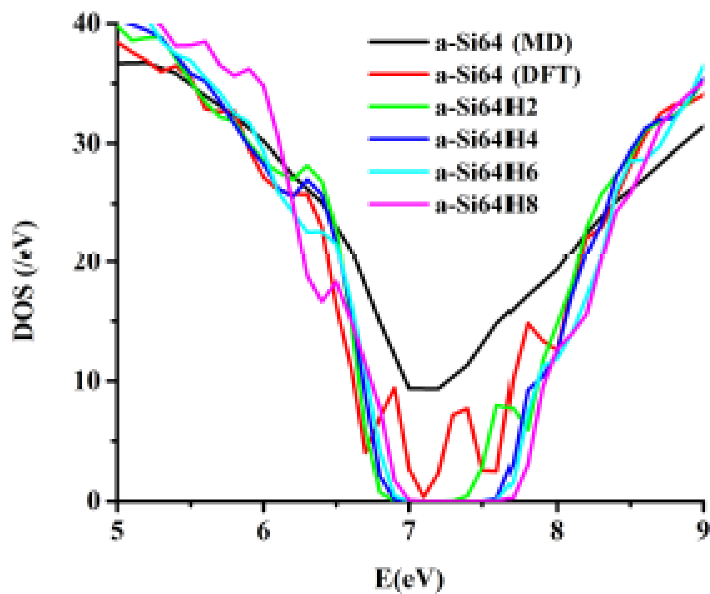
- Carrier selective contact structures are used to obtain high efficiencies
- The intrinsic hydrogenated amorphous silicon (a-Si:H(i)) is crucial as it provides passivation and carrier selectivity
- If the a-Si:H(i) layer is too thick, **photocurrent suppression** occurs
- Understanding defect transport through a-Si:H(i) is necessary to optimize the layer thickness and quality

[1]C. Battaglia *et al. Energy Environ. Sci.*, vol. 9,2016
[2]K. Yoshikawa *et al.*, *Nat. Energy*, vol. 2, no. 5, 2017

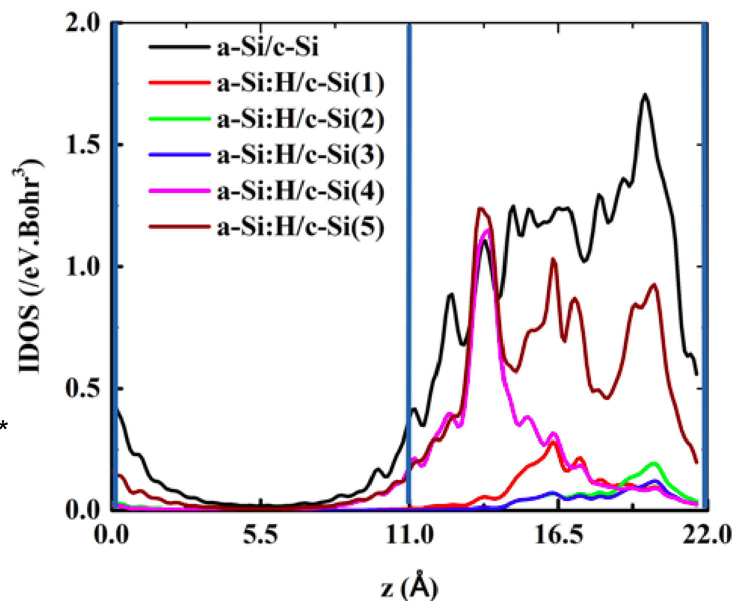
First Principles Study of c-Si/a-Si:H Interface



Simulated c-Si/a-Si:H interface using LAMMPS/DFT

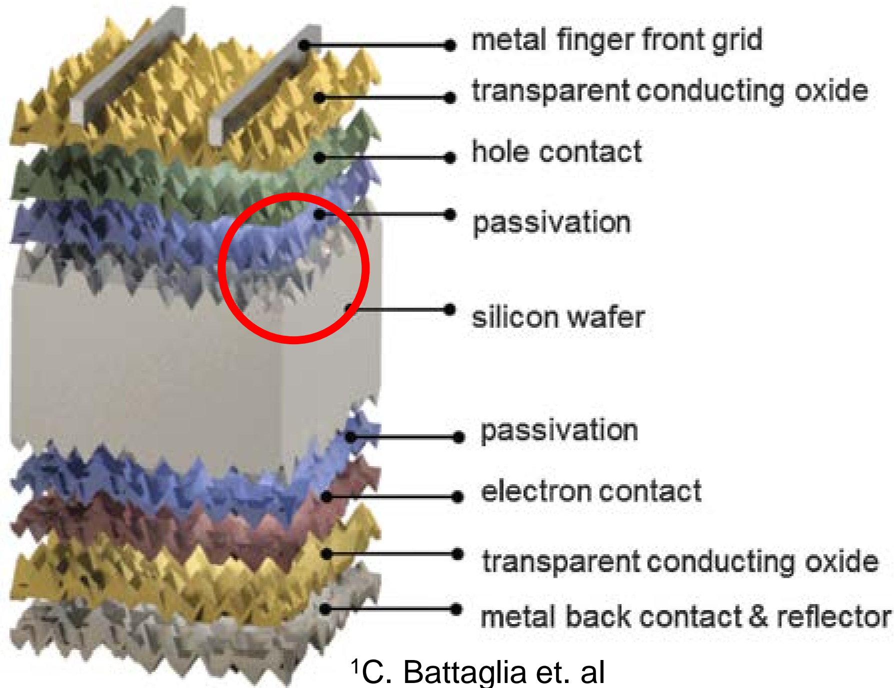


Density of states versus energy (left) and integrated bandgap DOS with different hydrogen concentrations*

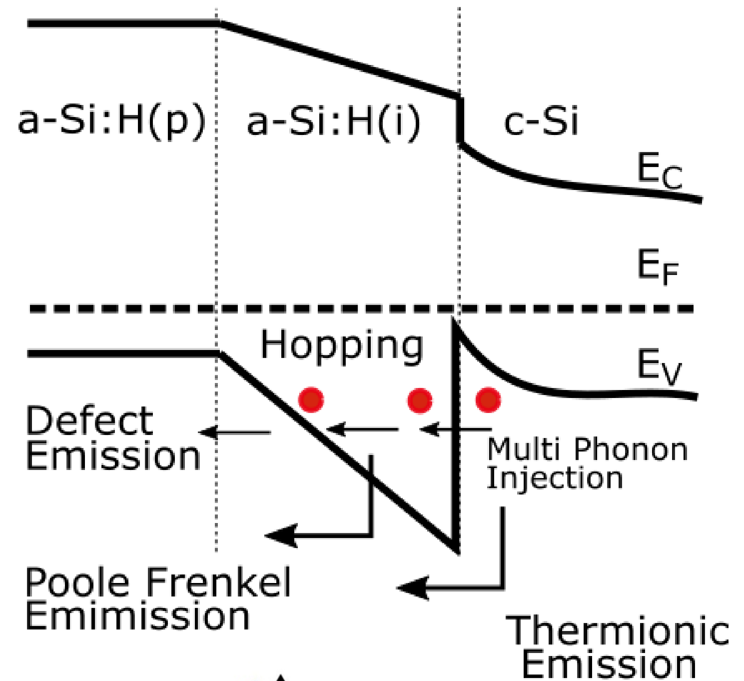


*R. Vatan, D. Vasileska, S. M. Goodnick, J. Phys. Chemistry (in review)

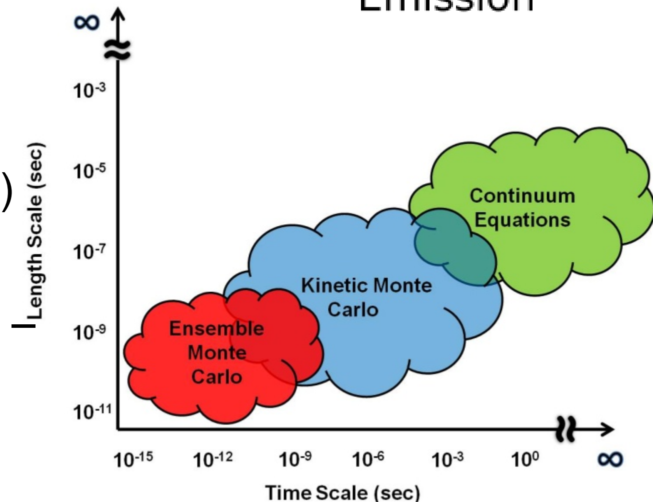
Transport Through a-Si:H(i)



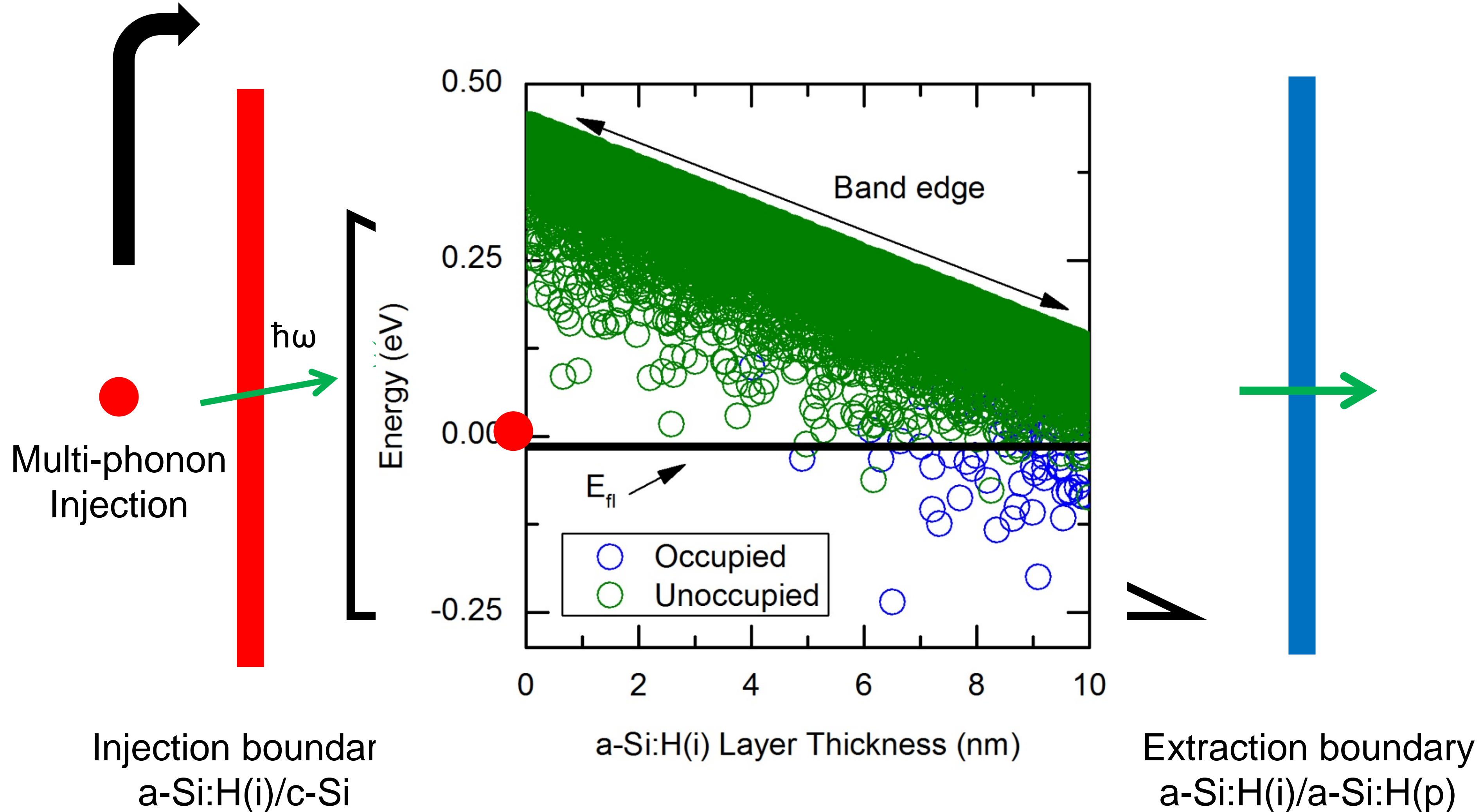
[1]C. Battaglia et. al



- Understanding the role of the a-Si:H(i)/c-Si heterointerface
  - High field transport – Scattering dependent(10^{-12} seconds)
- Understand the role of defects in the a-Si:H(i) layer
  - Defect assisted transport – Defect capture/emission (10^{-9} – 10^{-3} seconds)
- Traditional methods do not model non-local transport well



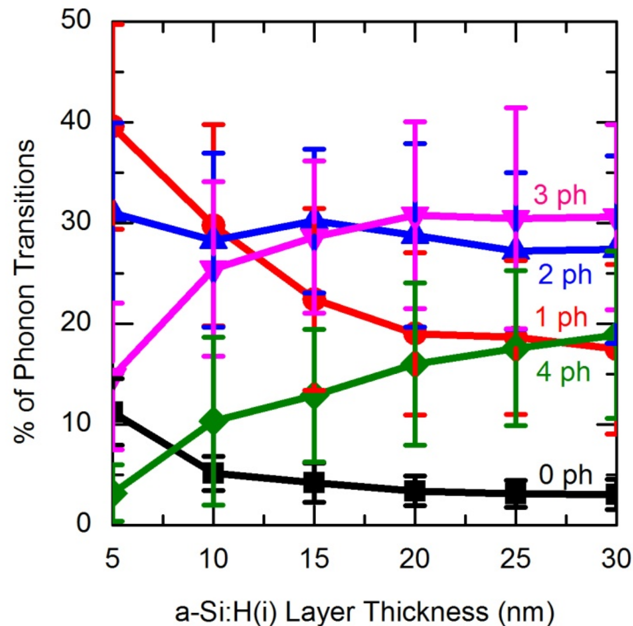
Transport Through KMC Domain



 P. Muralidharan, S. M. Goodnick, D. Vasileska *J. of Comp. Elect.* 18(4), 1152–1161 (2019)

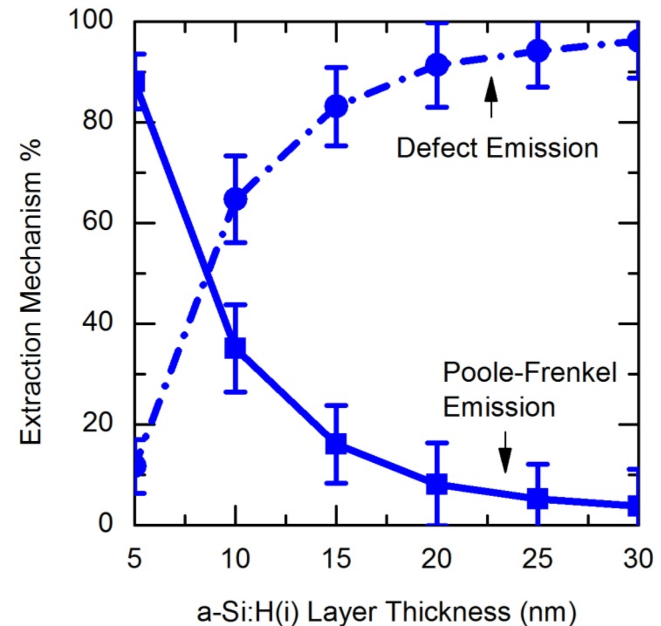
Injection and Extraction

How do carriers get into the a-Si:H(i) layer?
Multi-phonon injection



Injection depends on :
- ✓ Defect density
- ✓ Optical phonon energy
- ✓ Electric field in the a-Si:H(i)

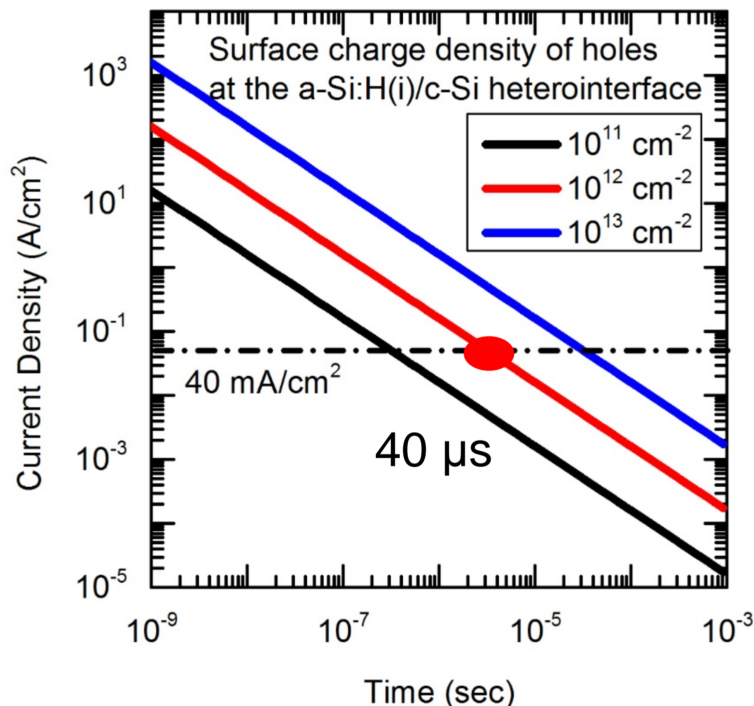
How do carriers get out of the a-Si:H(i) layer?
Poole-Frenkel and Defect Emission



Extraction depends on :
- ✓ a-Si:H(i) thickness
- ✓ Electric field in the a-Si:H(i)

Photocurrent Suppression

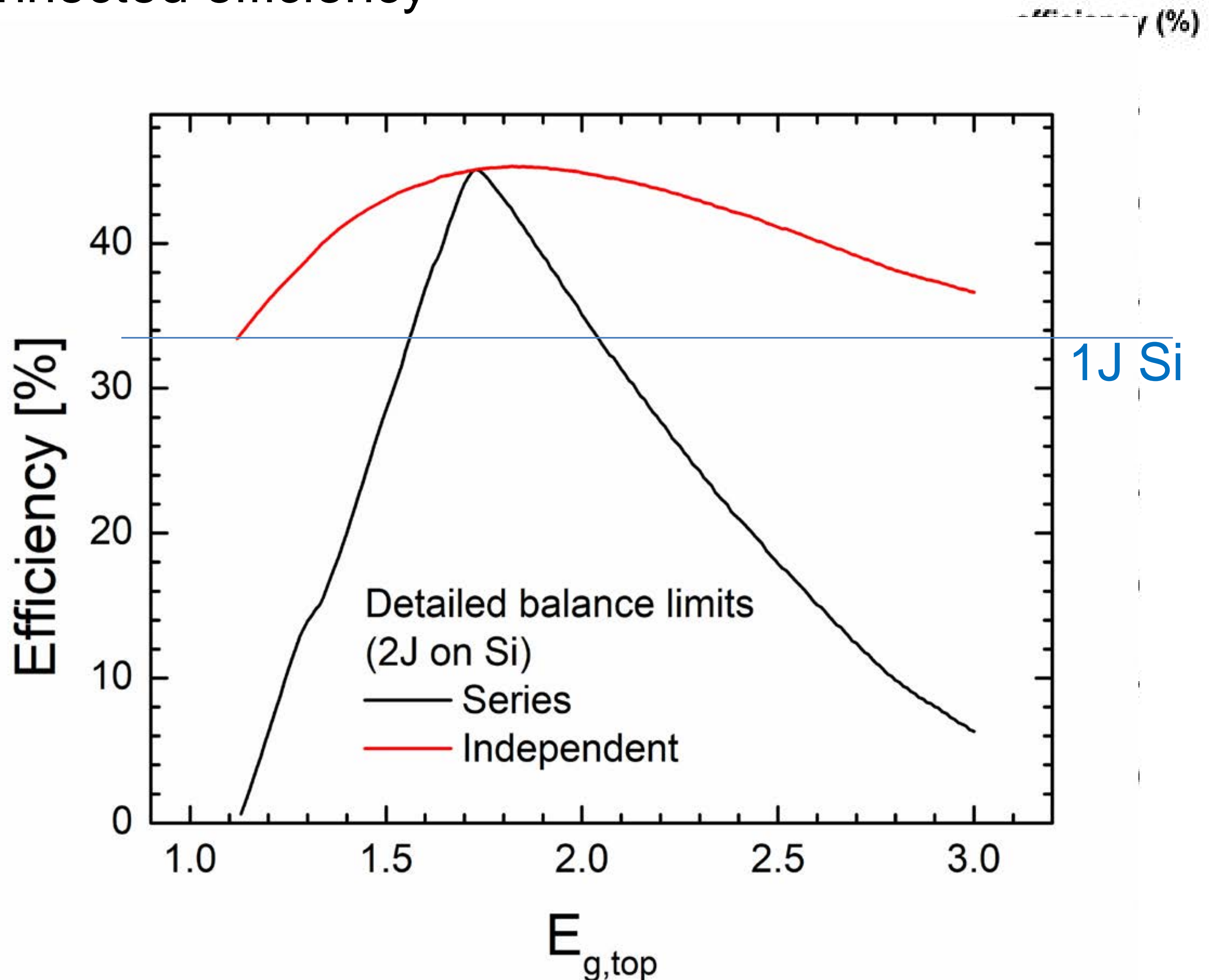
For Ohmic transport
Injection time = extraction time



- Current Density = Charge/Time
- For a surface density ~ 10^{12} cm^{-2} at the heterointerface, transit time required for ~ 40 mA/cm^2 is 40 μsec (Ohmic transport)
- The KMC predicts transit time $10^{-5} \rightarrow 10^{-1}$ sec
- Higher transit times → lower currents, higher surface charge density → higher currents
- KMC simulations indicates that the extraction supports lower currents, i.e. photocurrent suppression

Two Junction Si Tandems

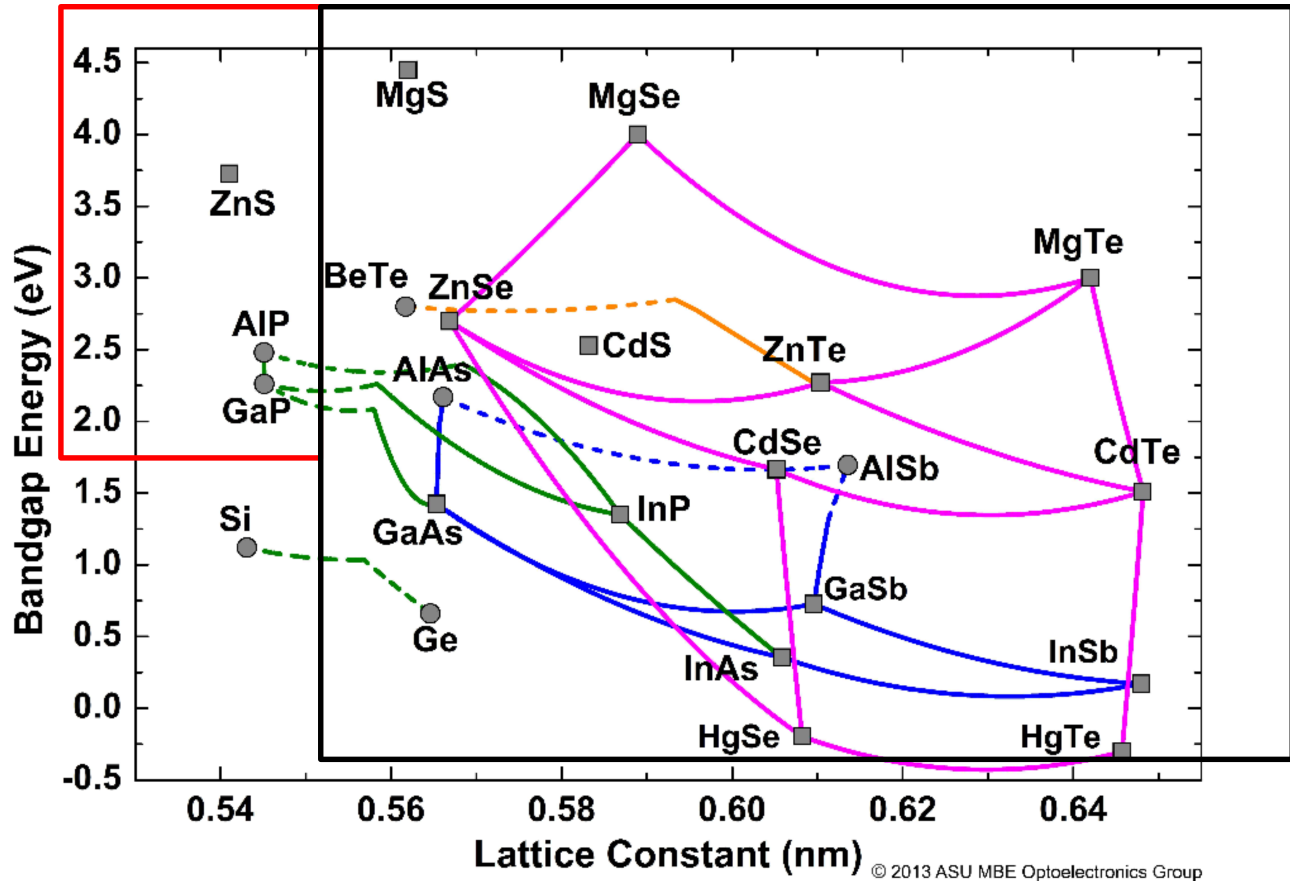
- Detailed balance calculation of the two-junction *series* connected efficiency



Epitaxial Combinations for Si

Bandgap too high

Large lattice mismatch

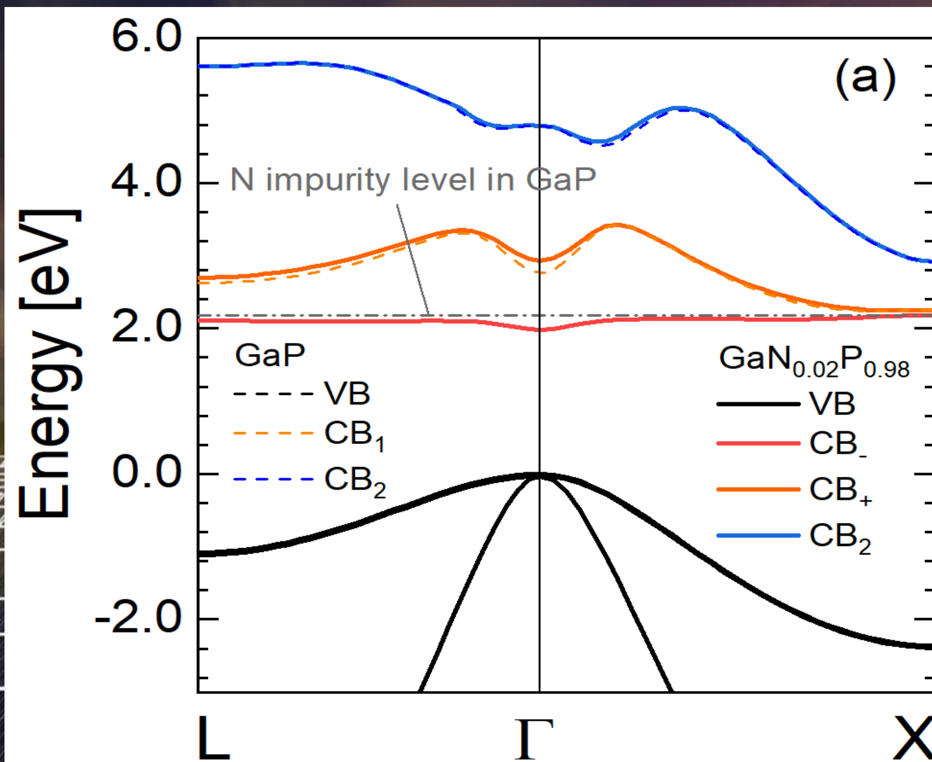


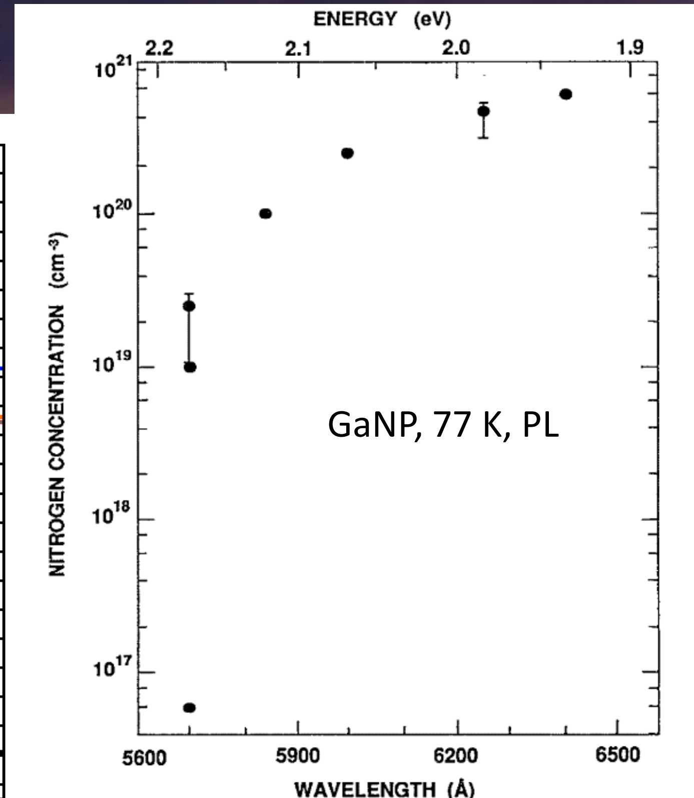
- **GaP is the only lower bandgap III-V which is nearly lattice-matched to Si**
- **Perovskite/Si tandems currently hold record (~27%)**

Dilute GaNP Nitrides

Large bandgap reduction through incorporation of a small fraction of N in III-Vs

- Tight binding model: $sp^3d^5s^*s_N$





(J. N. Baillargeon, *et al.*, Appl. Phys. Lett., 60, 1992)

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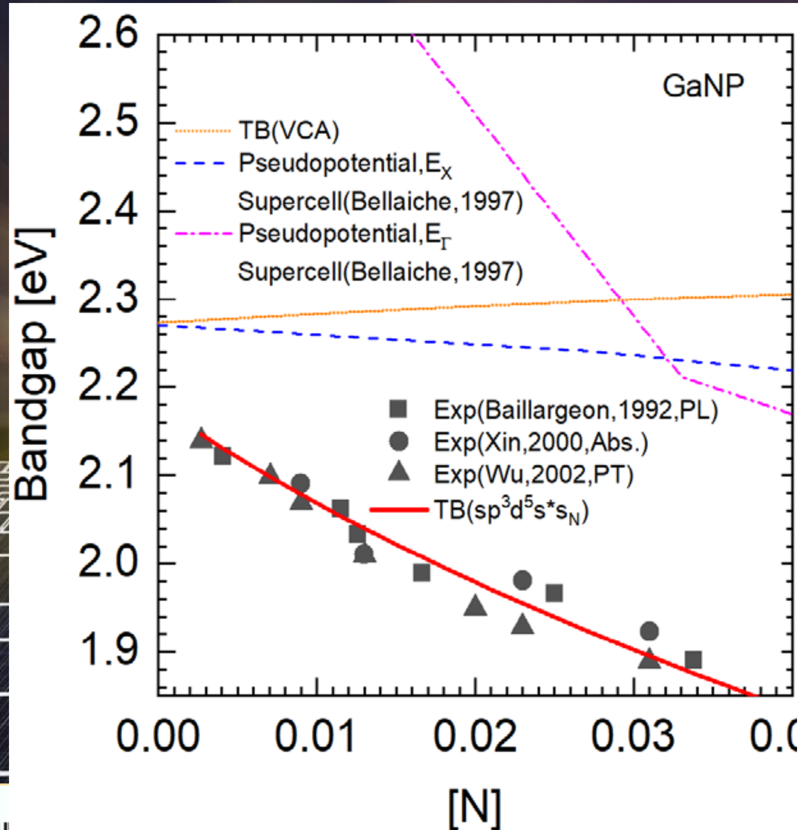
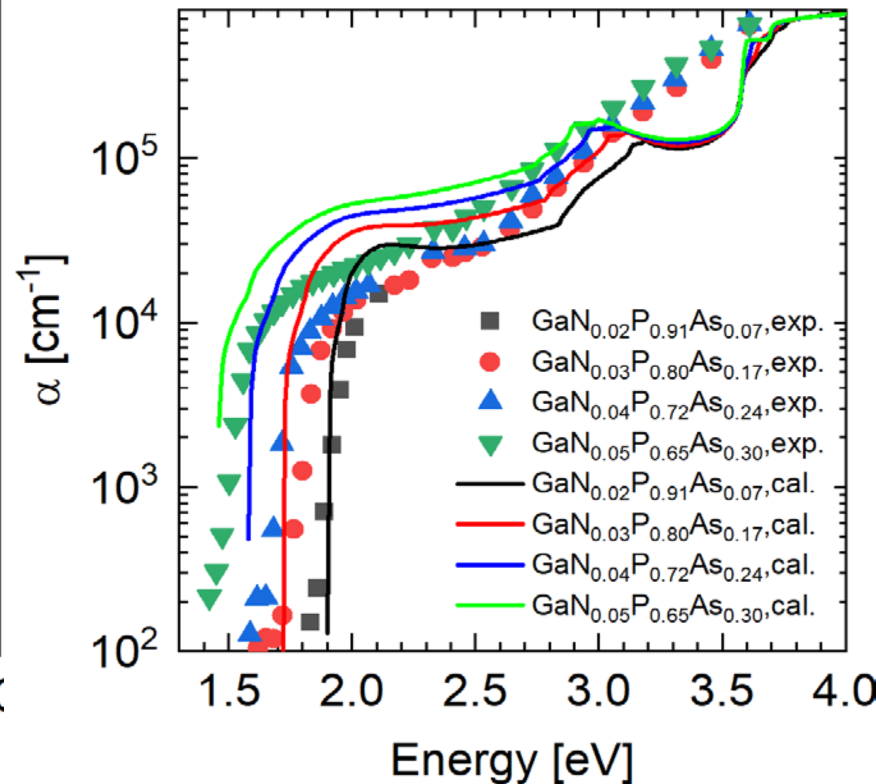
Tight Binding Modeling of Dilute Nitrides

- Excellent agreement with experimental bandgap versus N mole fraction data
- Optical absorption calculated from direct allowed transition in dipole approximation

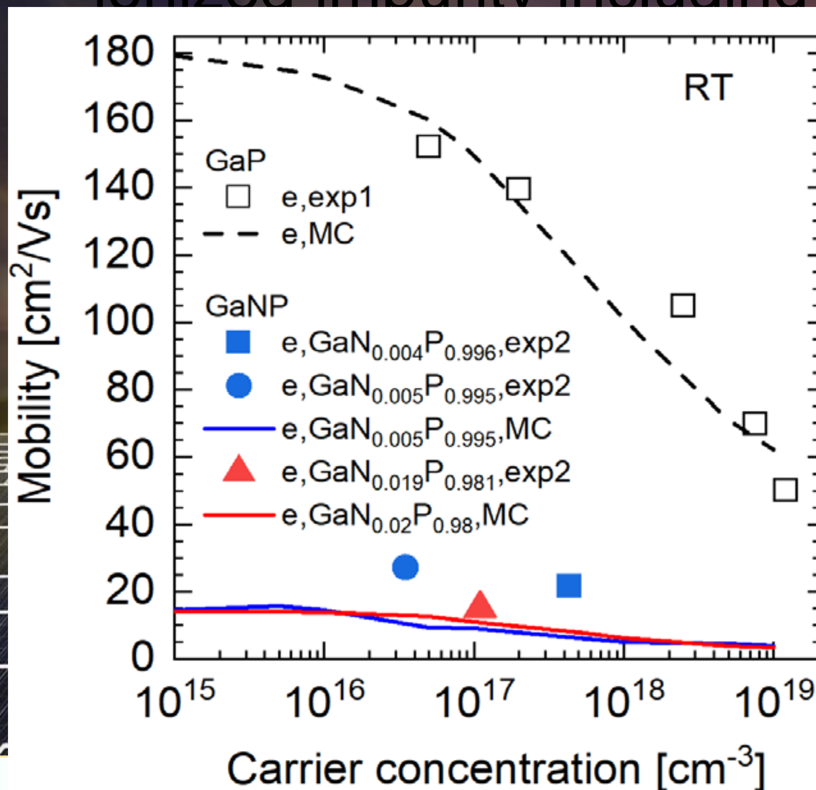


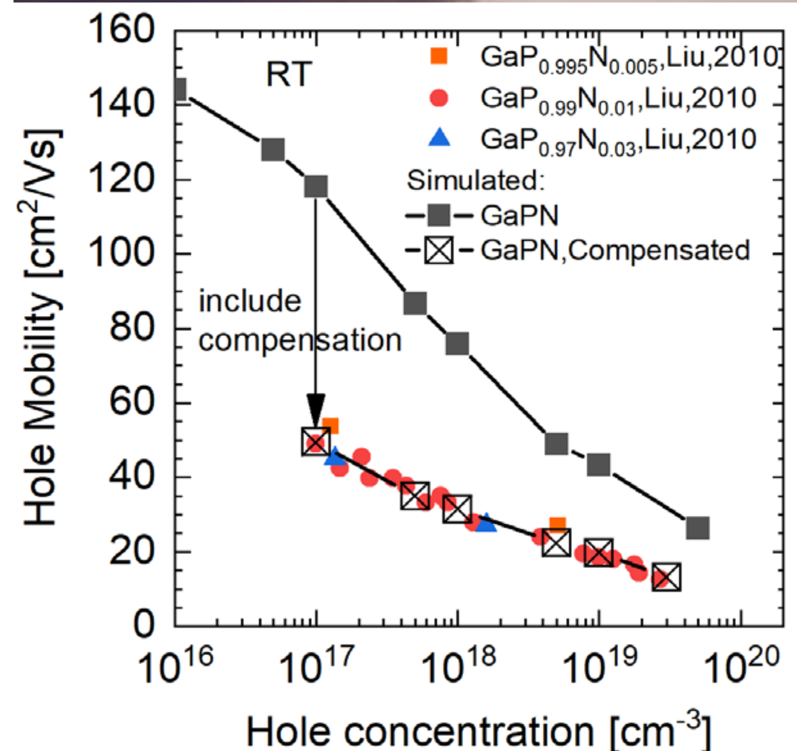


Y. Zou, S. M. Goodnick, J. Appl. Phys. 127, 075703 (2020)

Transport Simulation

- The TB basis was used in full band cellular Monte Carlo simulation of the mobility of electrons and holes in binary GaP and alloys of GaNP
- Polar optical, acoustic, deformation potential optical, ionized impurity including compensation





Y. Zou and S. M. Goodnick, *AIP Advances* 11, 035207 (2021)

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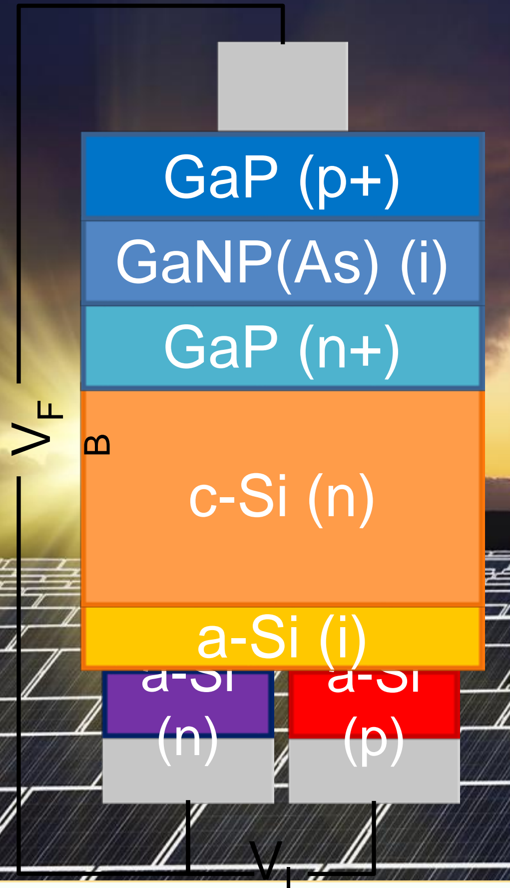
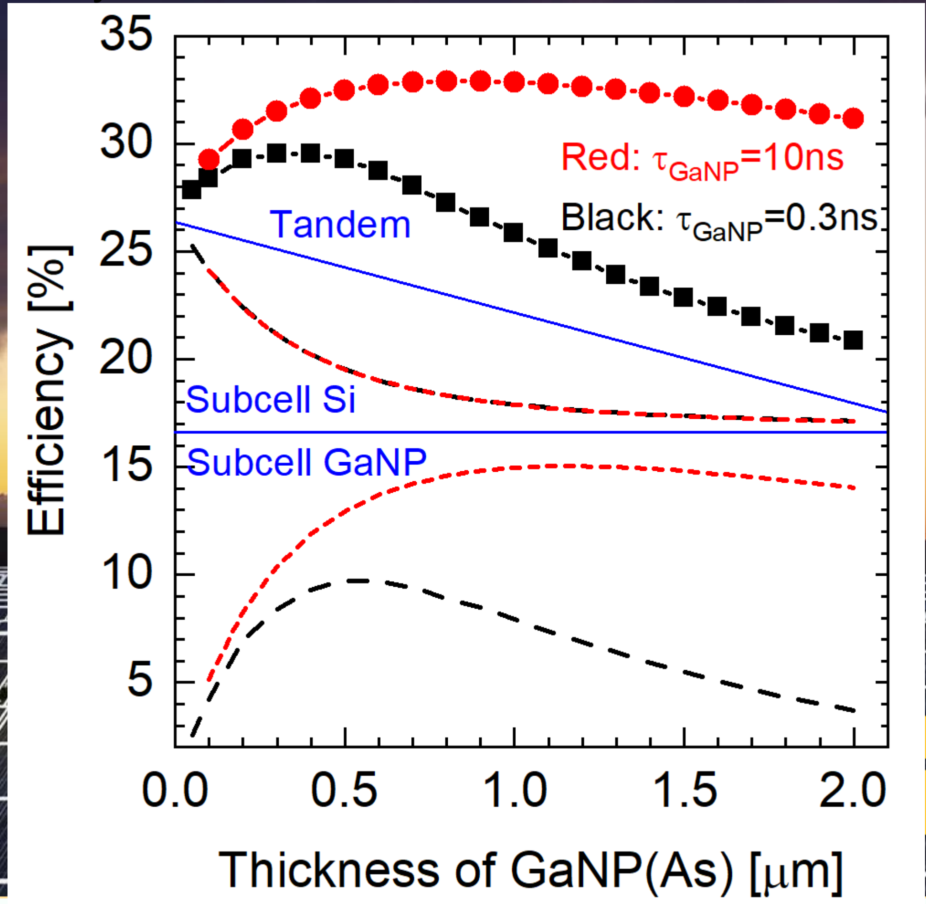
TCAD Device Simulation

- Silvaco ATLAS simulation of 3-terminal device using simulated optical absorption and transport data
- Lifetime of the GaNP layer critical parameter in determining the maximum conversion efficiency

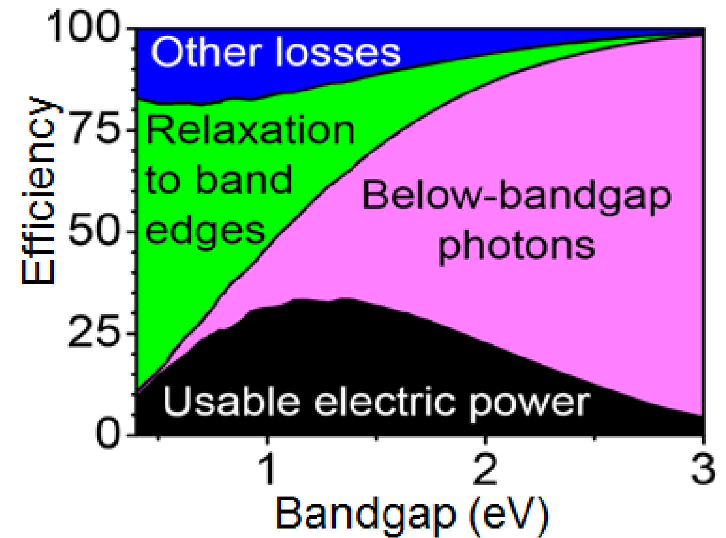


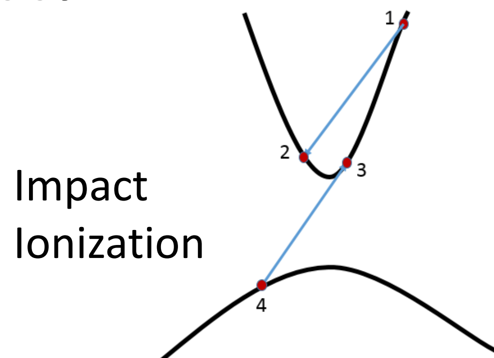


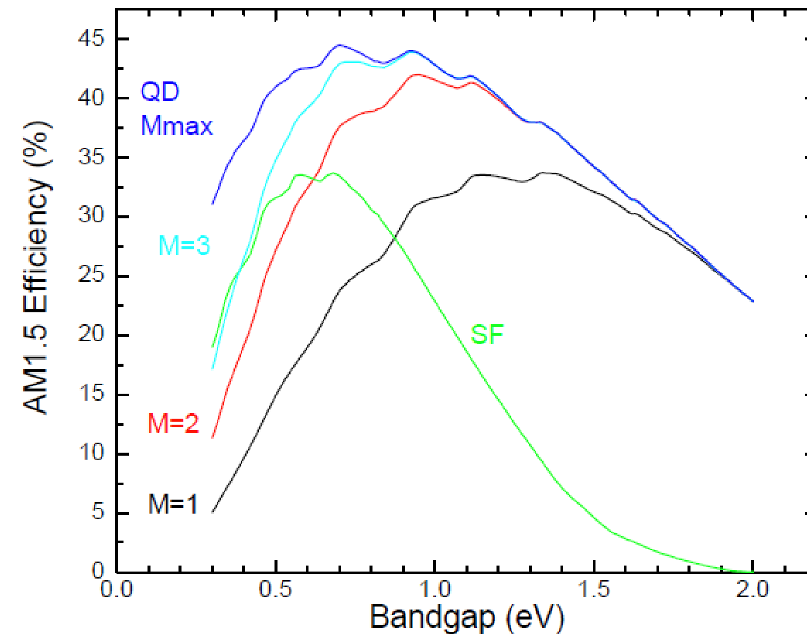
Y. Zou, C. Zhang, C. Honsberg, D. Vasileska, R. King, and S. M. Goodnick, Proceedings of the 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion (WCPEC)

Multi-Exciton Generation Solar Cells

- Ultrafast energy relaxation processes a major loss mechanism in photovoltaic devices
- **Impact ionization** or **multi-exciton generation** uses the excess photon energy to increase the quantum yield above 100%







MEG in Nanowires

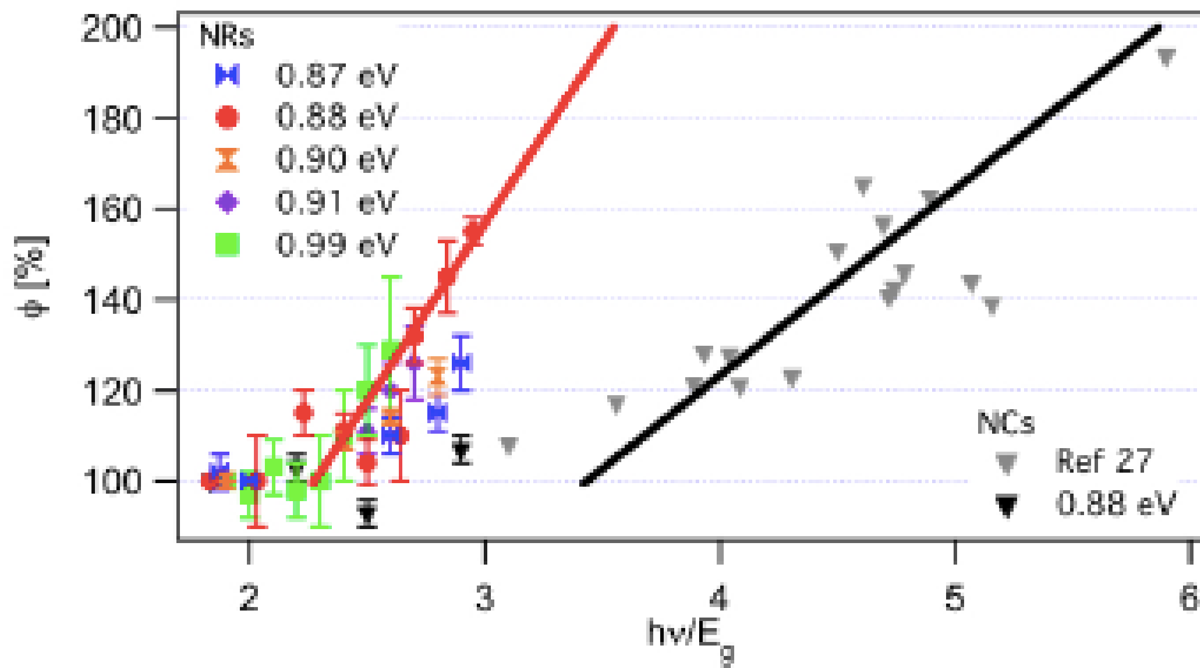
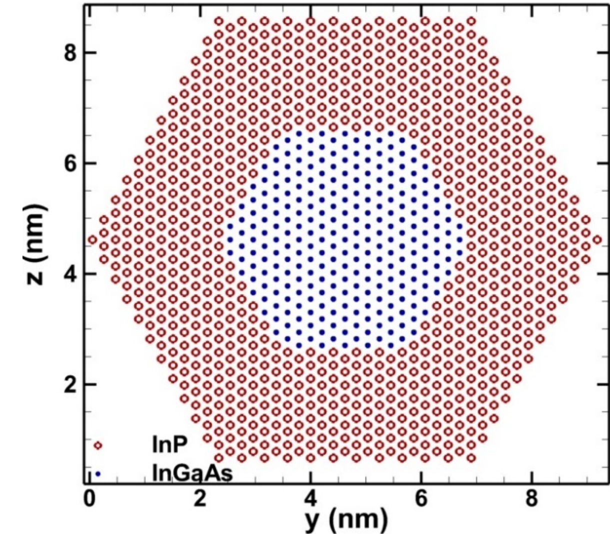


Figure 4. The exciton quantum yield as a function of relative photon energy ($h\nu/E_g$) for PbSe nanorods and nanocrystals. The energies of the first excitonic absorption are listed for each batch of nanostructures. Lines are best fits to equation 2. The MEG efficiency is 0.78 for nanorods and 0.41 for nanocrystals. Literature values taken from Beard, et al. [27].

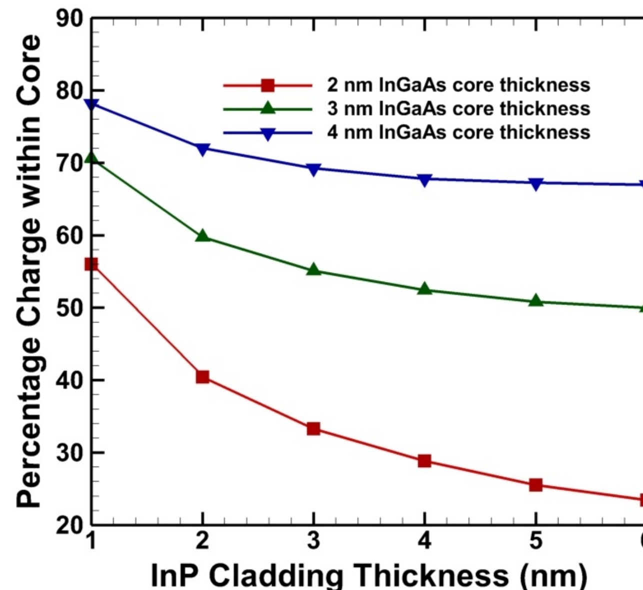
P. D. Cunningham et al., Proc. SPIE
Vol. 8256, 2012,

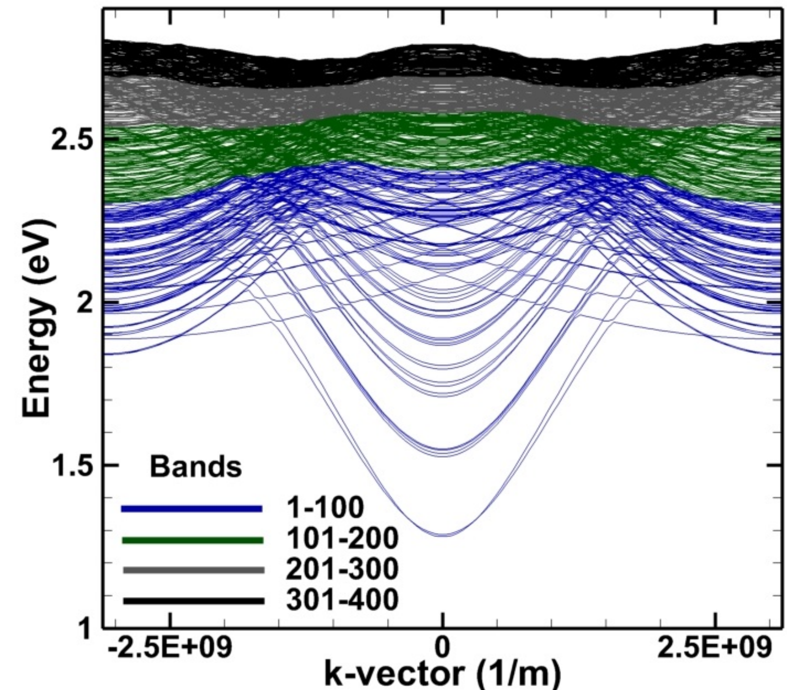
Band Structure of Hexagonal Cladded Nanowires along 111

- Empirical TB $sp^3d^5s^*$ including spin-orbit interaction. Parameters taken from Purdue group.**
- The periodicity and the supercell of the nanowire is created using the primitive basis vectors of the material and the nanowire cross-section dimensions.



**TB Boykin, G Klimeck, F Oyafuso , Physical Review B 69 (11), 115201



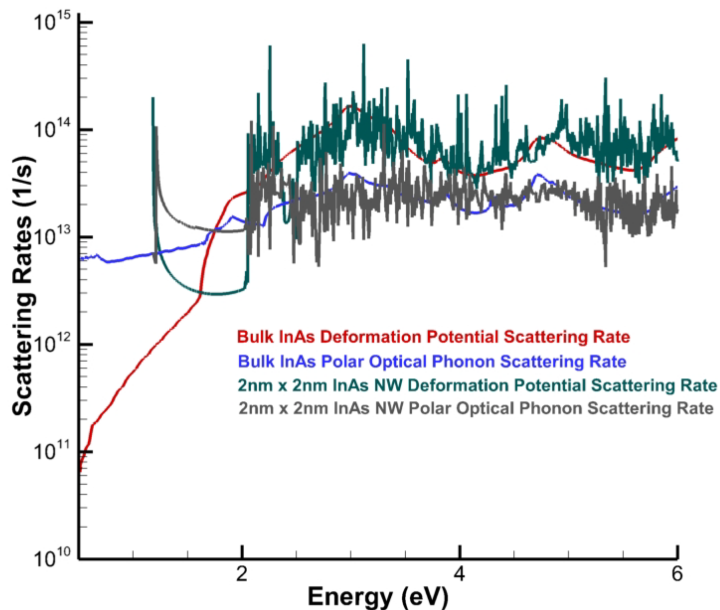


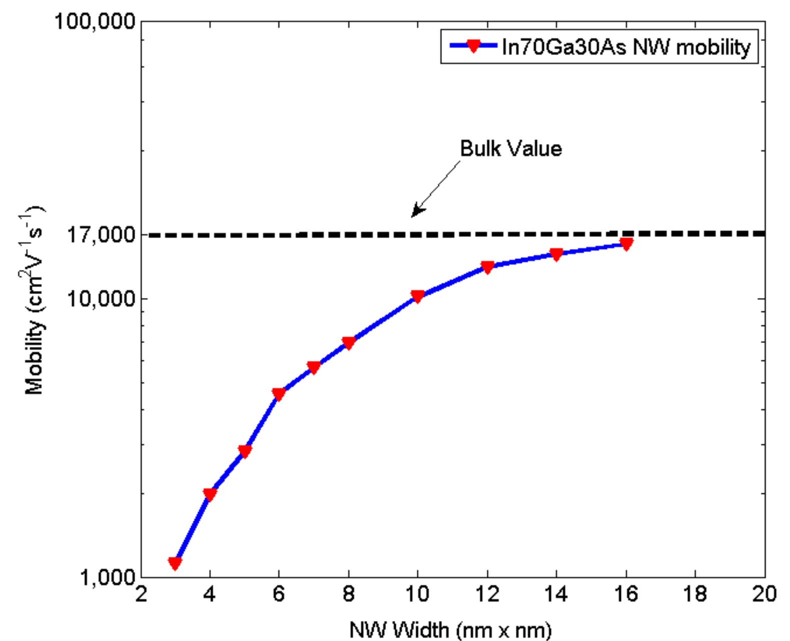
Scattering Rates

- Fermi's Golden Rule is used to calculate all scattering rates:

$$W(k_\mu, k_\nu', \mathbf{q}) = \frac{2\pi}{\hbar} \left| \left\langle \psi_{k_\nu', q} \middle| \delta H \middle| \psi_{k_\mu, q} \right\rangle \right|^2 \delta\left(E_{k_\nu'} - E_{k_\mu} \pm \hbar\omega_q \right)$$

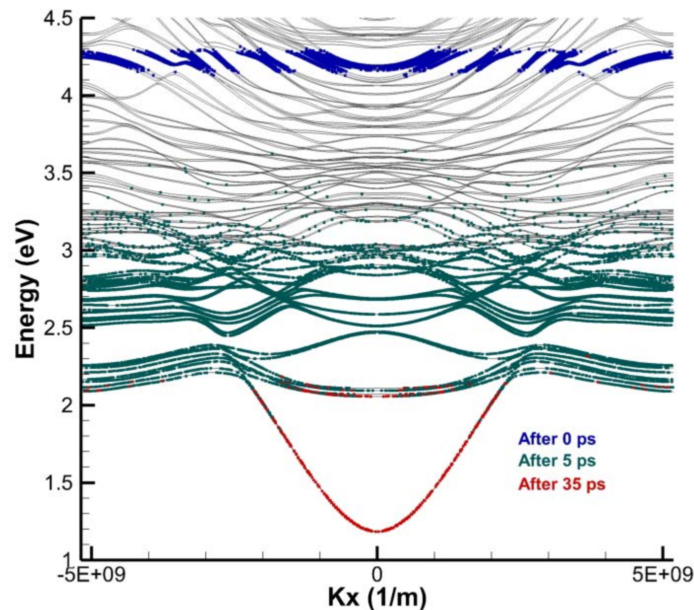
- Bulk-like phonons are assumed in the cases of def. potential and polar optical phonon scattering.



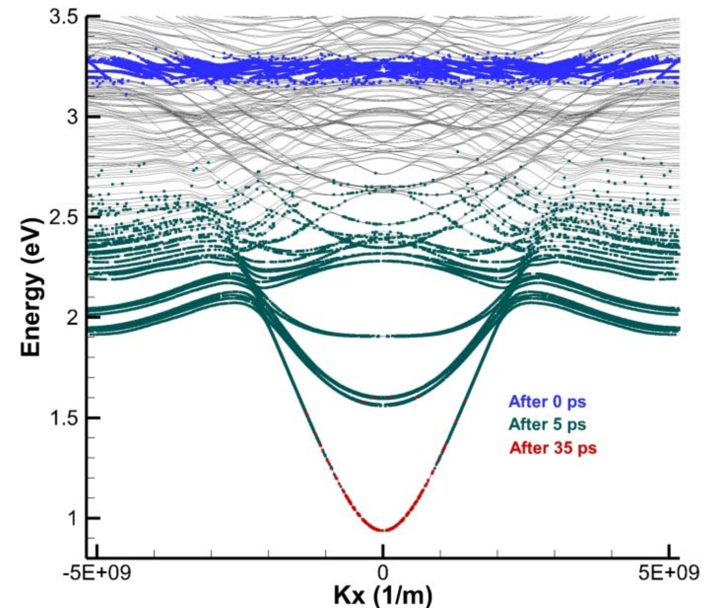


Cellular Monte Carlo Simulation of Energy Relaxation in Nanowires

- The plots below show the relaxation of electrons after the initial excitation at t = 0 ps.



2nm x 2nm InAs Carrier Relaxation



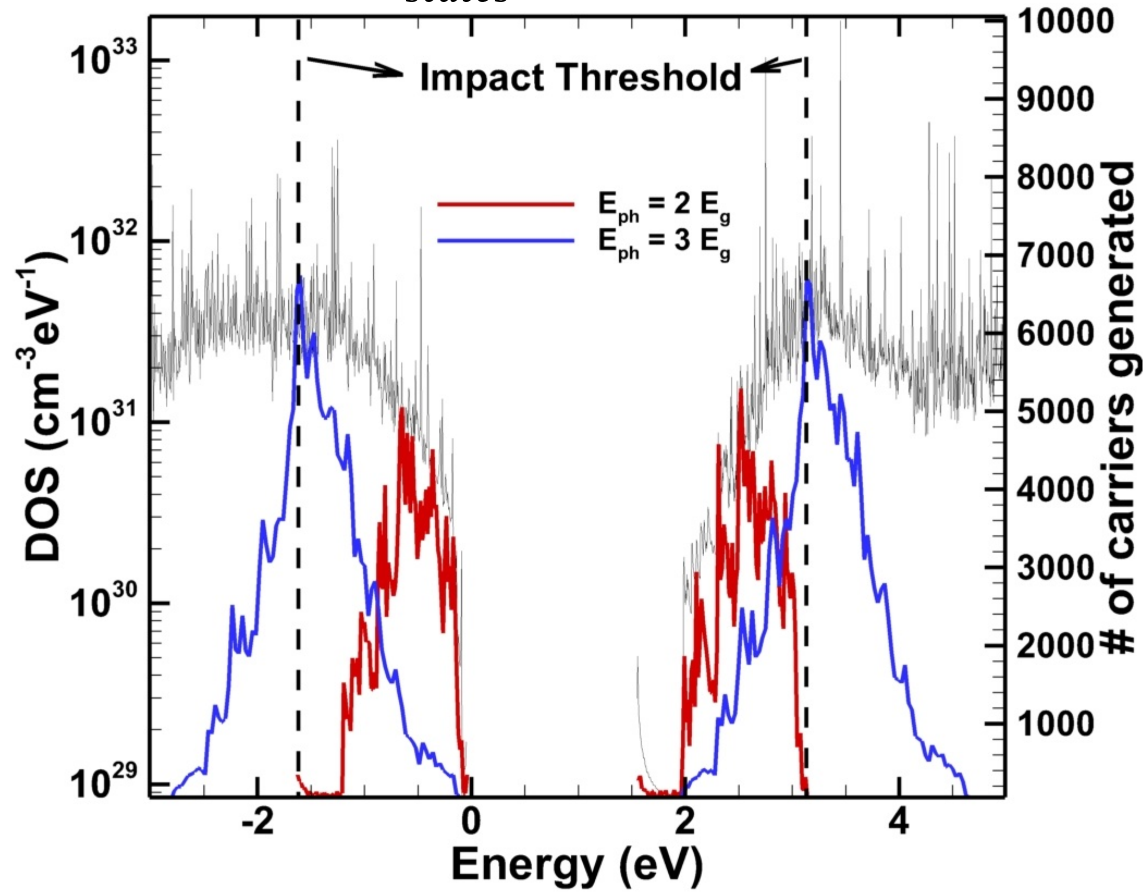
3nm x 3nm InAs Carrier Relaxation

- **Electrons' energy is initialized to a Gaussian distribution with a half-width of 100 meV at *t* = 0.**

Hathwar et al., J. Phys. D 52 (2019)

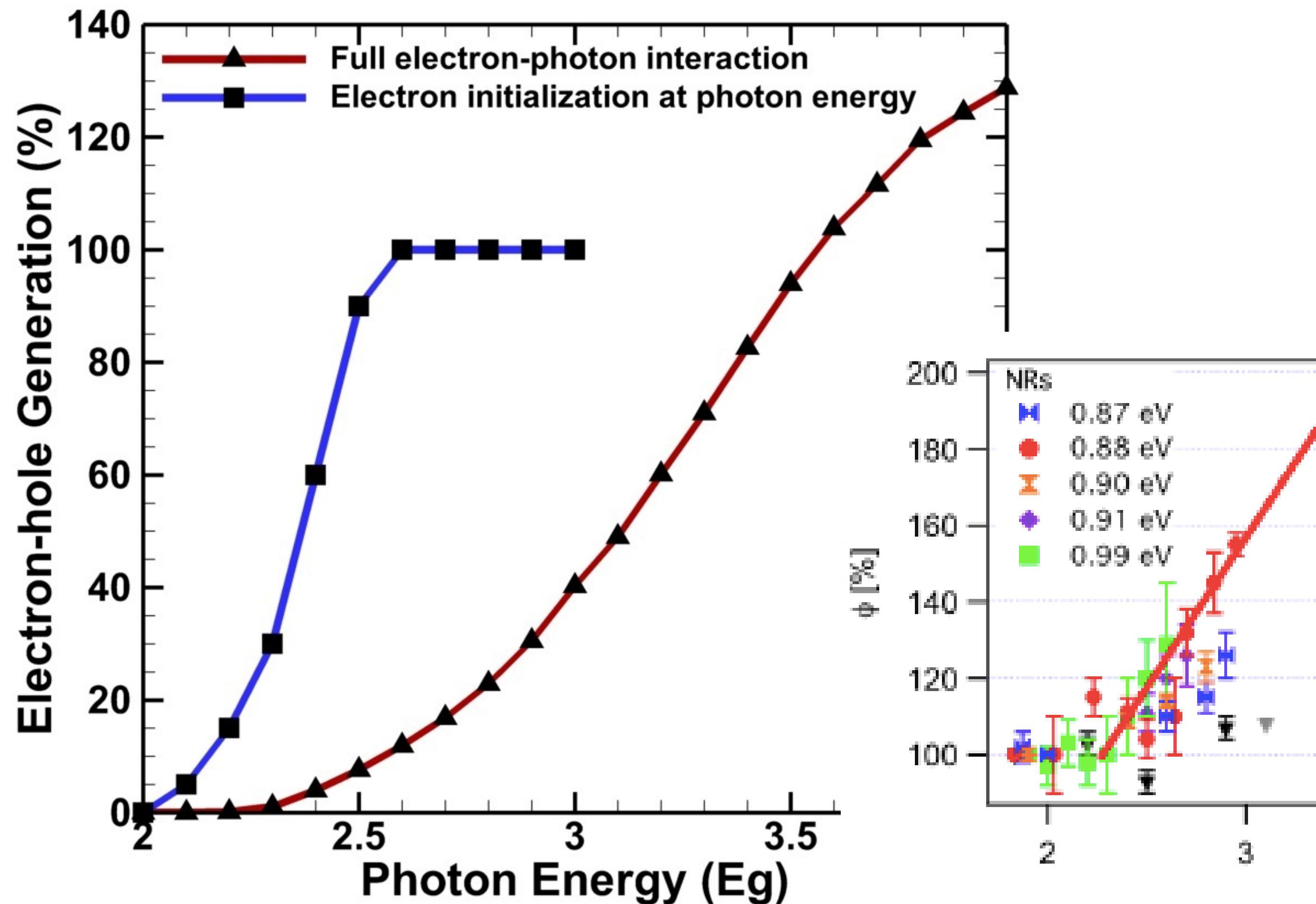
Carrier Generation due to Electron-Photon Interaction

$$W_{abs} = \frac{2\pi}{\hbar}\frac{e^2}{m_0^2}\left(\frac{\hbar n_{ph}}{2\omega\varepsilon}\right)\sum_{states}|(a.p)_{cv}|^2\delta(E_e - E_h - \hbar\omega)$$



- The excess energy of electrons in the CB is significantly reduced due to partitioning between VB and CB.

MEG for 2 nm InGaAs with 1 nm InP



- Linear behavior in MEG excitation curve due to partitioning of photon energy between VB and CB

Acknowledgements

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