A Deliberate Journey: Adapting Tools of Basic Science to Make Better Solar Cells, Hybrid Cars and Medical Devices

genuine utility

basic science

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Five pathways of basic science tools making direct impact in renewable energy and medicine

1. Strongly interacting electrons in perovskites	Boosting efficiency of energy conversion in solar cells
2. Metal-Insulator Transition	Improving charge extraction from solar cells
3. Quantum glassy dynamics	Mitigating performance degradation of world record holder Si solar cells
4. Renormalization group and scaling	Developing better magnets for the electromotor of the Toyota Prius
5. Test of Relativity and Nobel-winning femtosecond lasers	Creating LASIK and laser cataract eye surgery

UC Davis/Theory: F. Gygi, M. Voros, GTZ
UC Davis/Expt: S. Kauzlarich, E. Muthuswamy
UC Santa Cruz: S. Carter, C. Church,I. Carbone

Chicago:
G. Galli

Budapest:
A. Gali

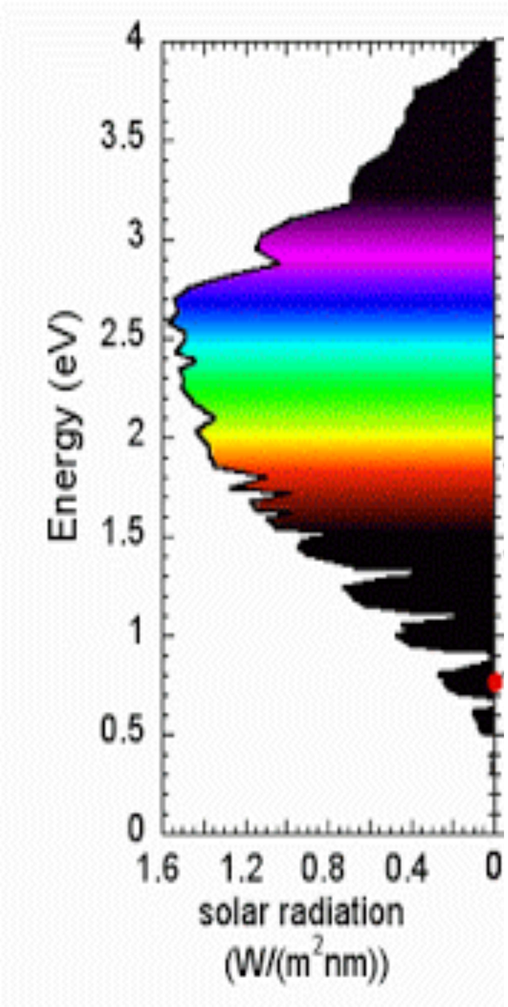
Harvard:
T. Kaxiras

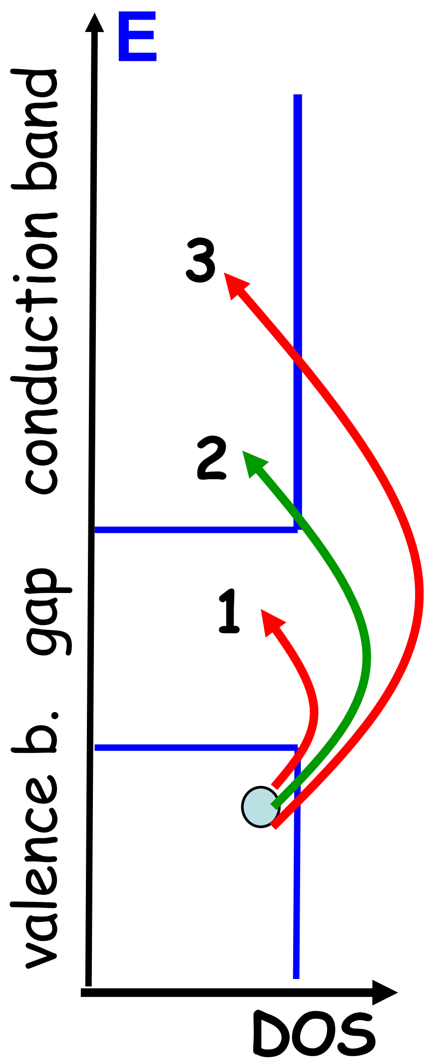
Max Planck:
S. Wippermann

Vienna
T. Schrefl

UC Irvine:
T. Juhasz

1. Boosting Solar Absorption Efficiency by Strongly Interacting Electrons in Perovskites





1. No absorption below gap:
   photon wasted

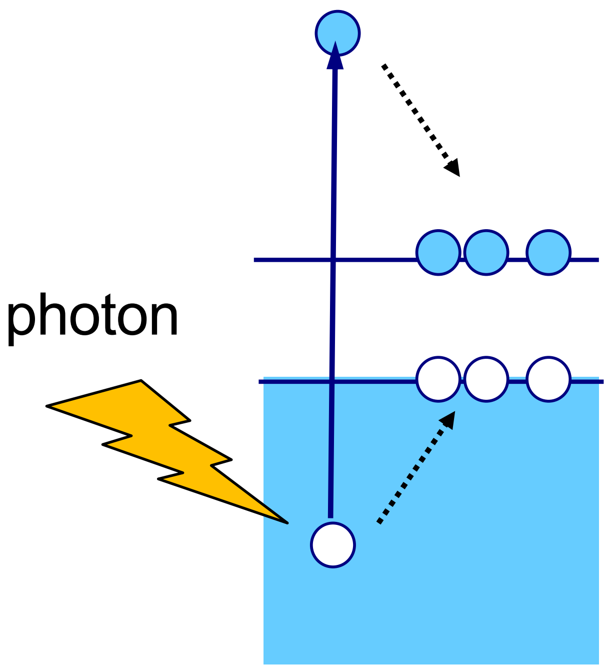
2. Absorption to bottom of
   conduction band: optimal

3. Absorption high into band:
   excess energy to phonons heats cell

Optimization of gap:
   max efficiency: **31%**

To boost efficiency substantially:
New physics needed: **3rd generation PV**

Break the Ruling PV Paradigm: Get two Electrons for One Photon



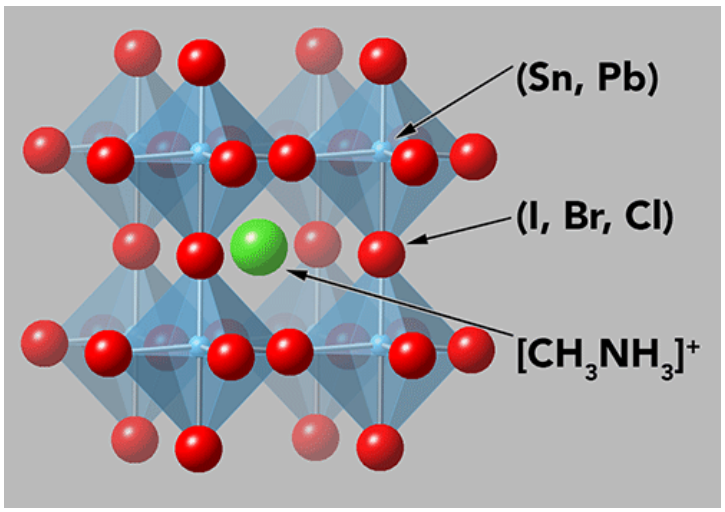
Carrier Multiplication (CM):
high-above gap photon excites electron that relaxes by exciting 2nd/3rd electron

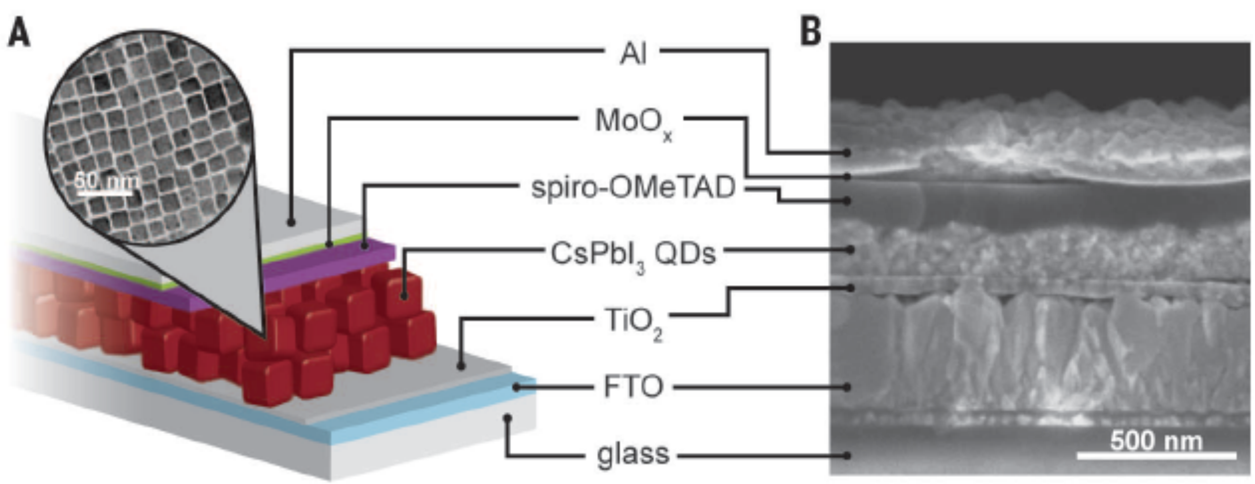
CM boosts absorption efficiency at high energies.
Theoretical max: 44%,
instead of 31%

Carrier Multiplication is driven by Strong Interactions

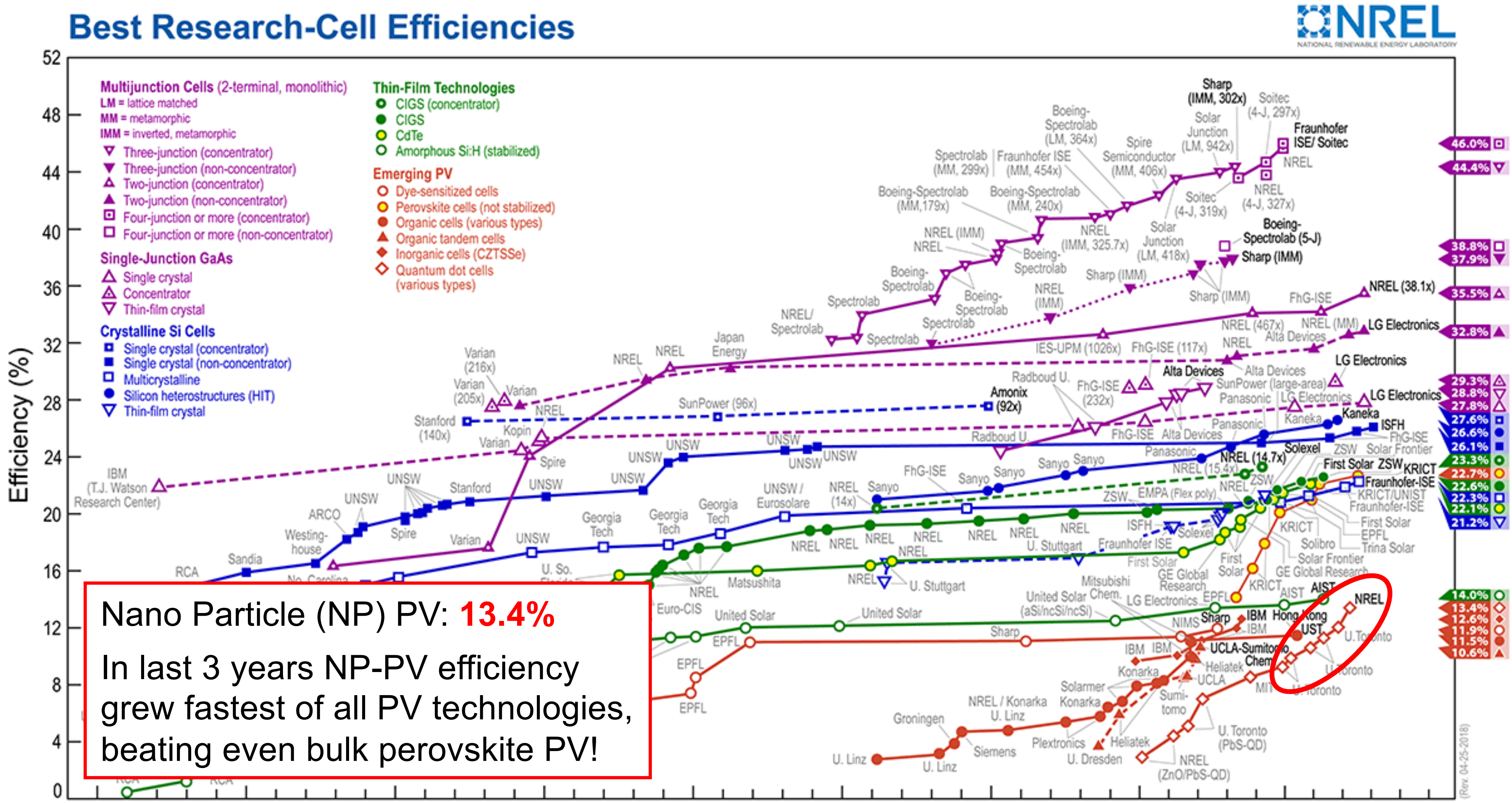
Carrier Multiplication requires enhanced Coulomb interaction: Quantum Confinement in Nanoparticles

Nanoparticles from inherently high PV efficiency bulk: Perovskites: 22.7%





Colloidal Nanoparticle Solar Cells Broke 10% Psychological Barrier in 2015, now 13.4%

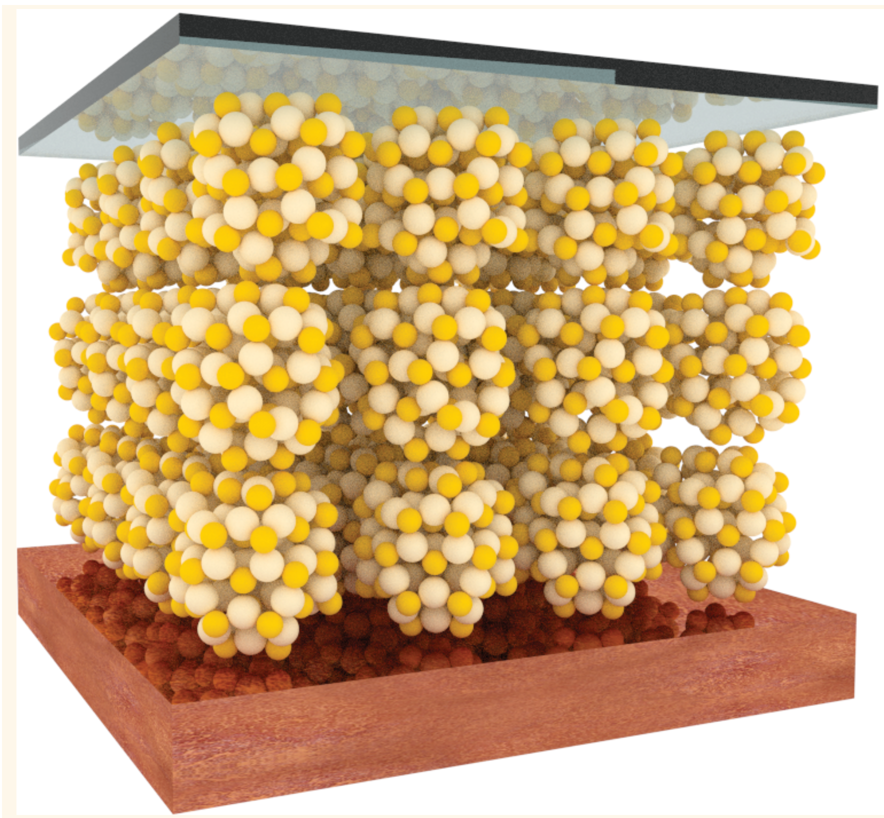


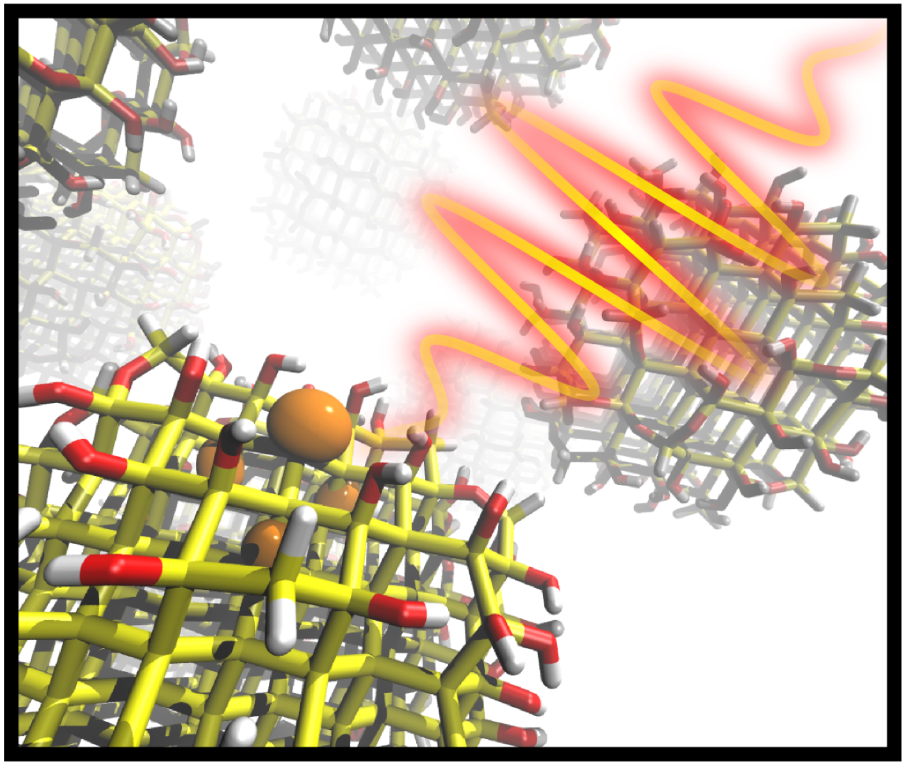
Nano Particle (NP) PV: **13.4%**

In last 3 years NP-PV efficiency grew fastest of all PV technologies, beating even bulk perovskite PV!

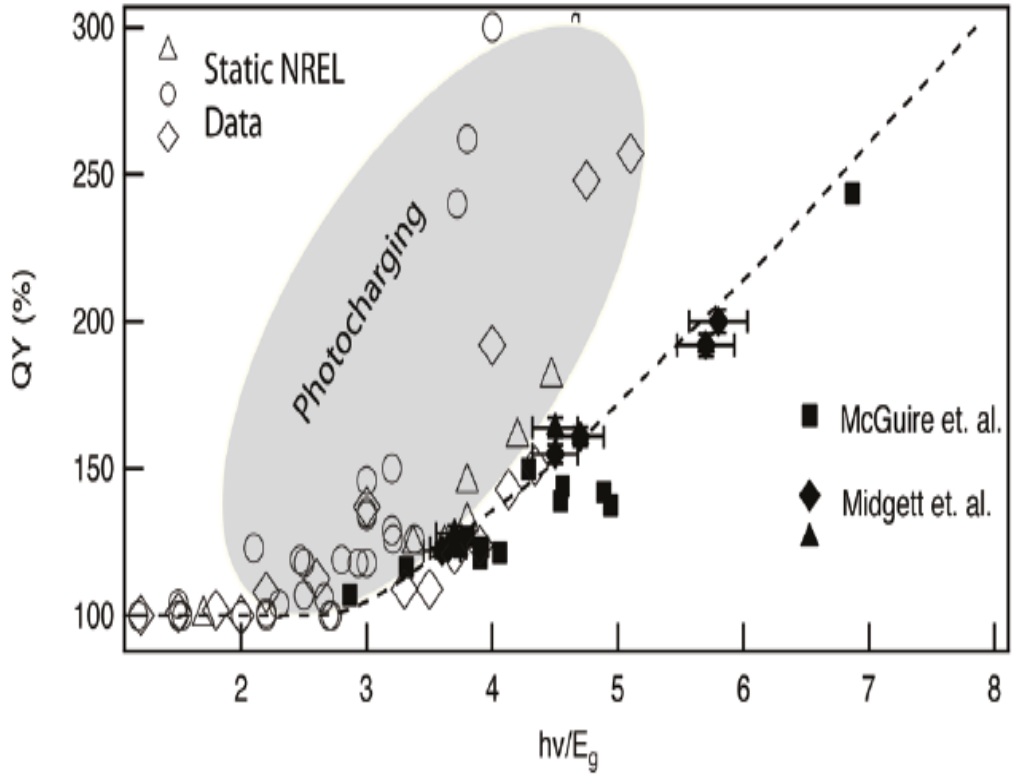
Perovskite NP PV is stable

Colloidal Nanoparticle Solar Cells are promising platform for the Full Spectrum Boost Project



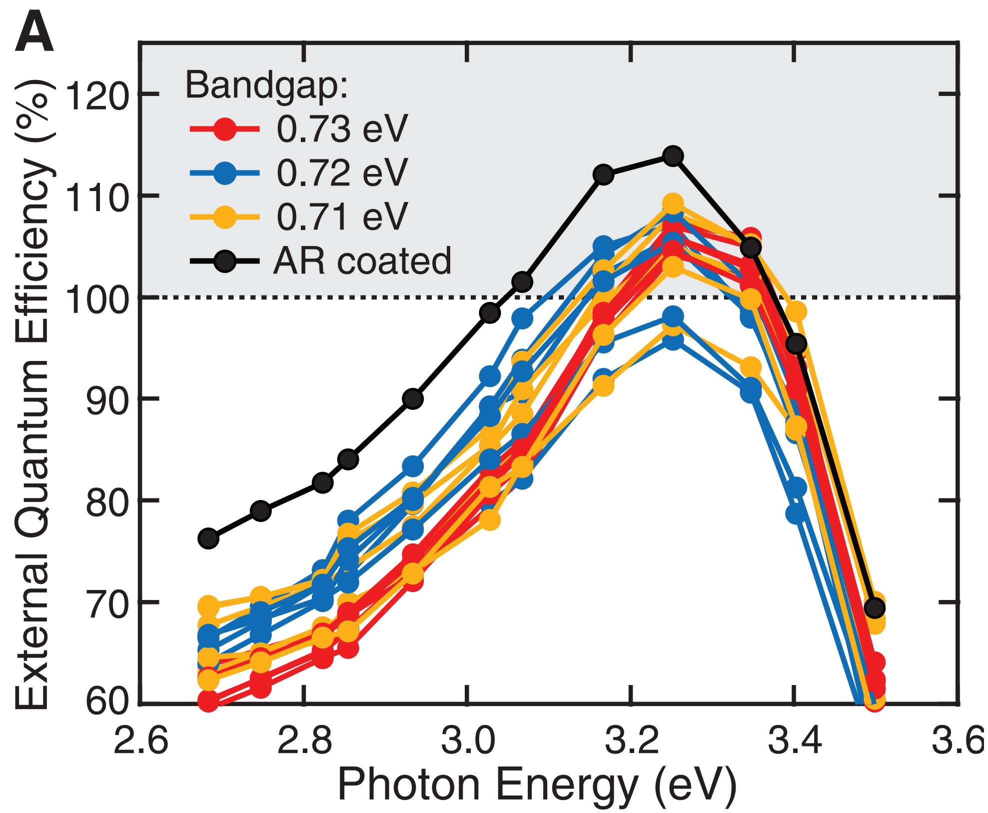


Carrier multiplication in Nanoparticles: Discovery, Status



Klimov (2004): Presence of CM in Nanoparticles proven

Beard (2011):
Report of consensus



Semonin et al (2012):
First working CM/MEG solar cell

QCD - The Quantum Confinement Dilemma in Nanoparticle Solar Cells

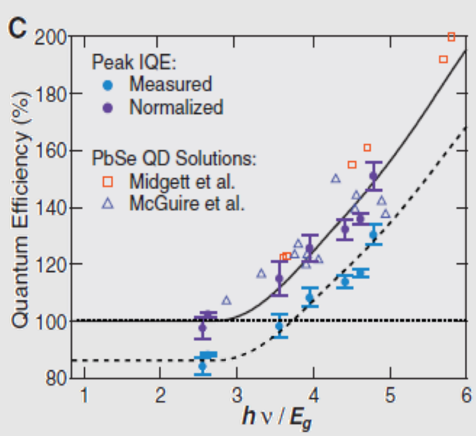
Positives of QC

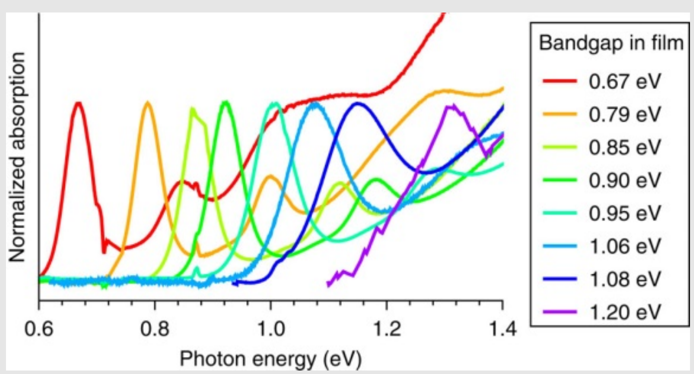
Negatives of QC

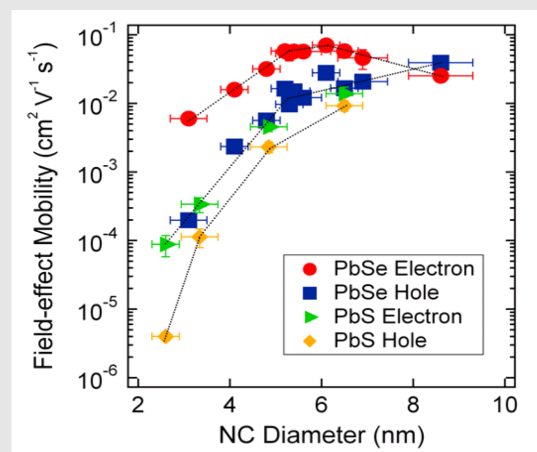
Enhances Coulomb interaction: Enhances CM

Widens gap: Absorption is pushed out of solar spectrum

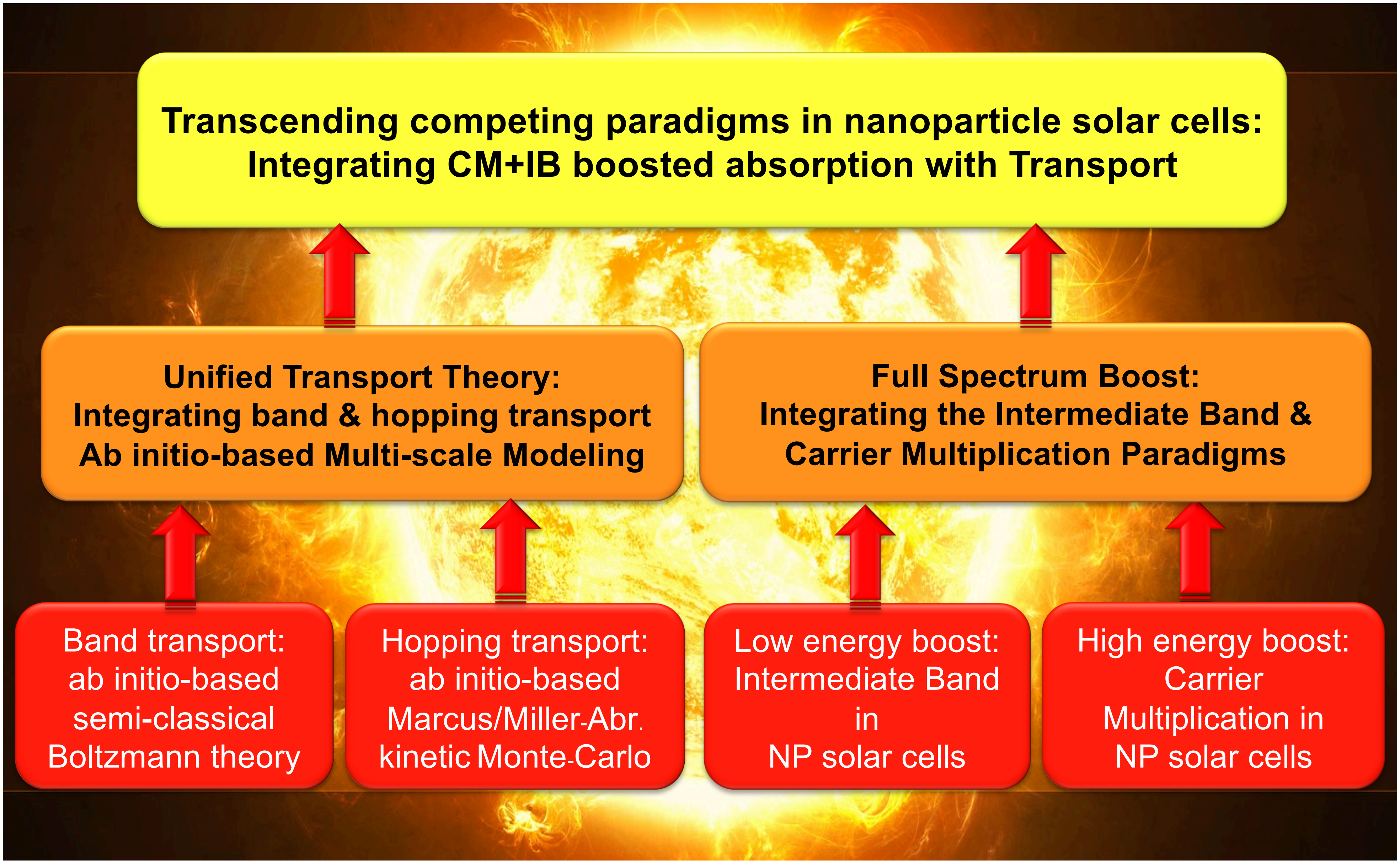
Localizes charges: Hinders transport



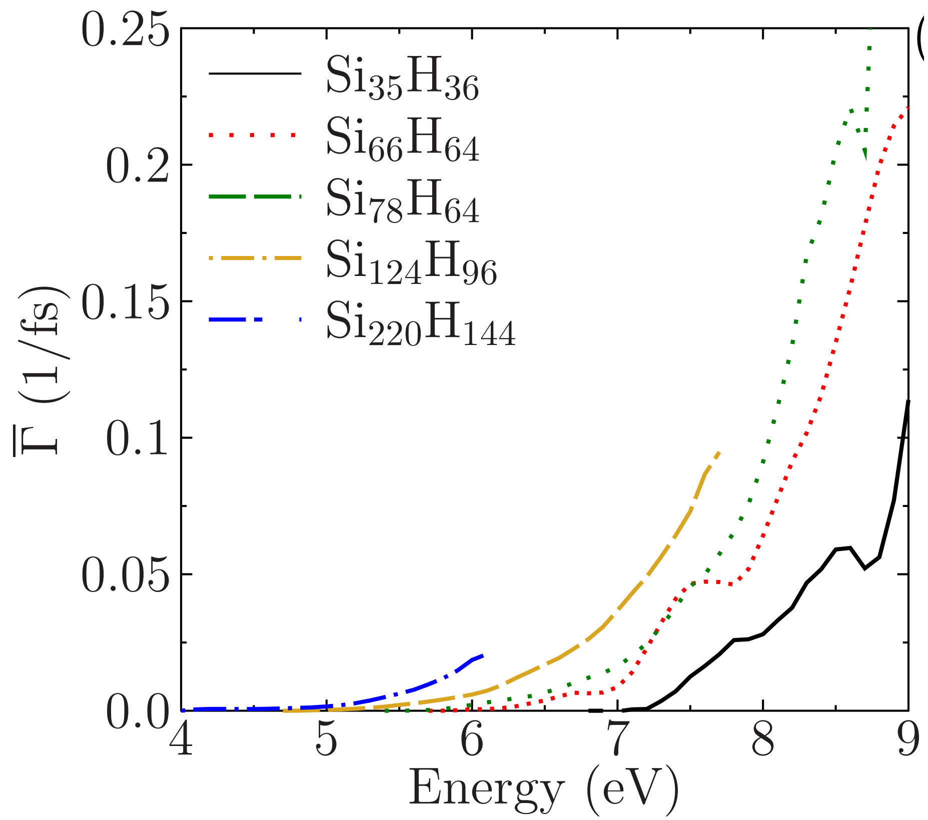


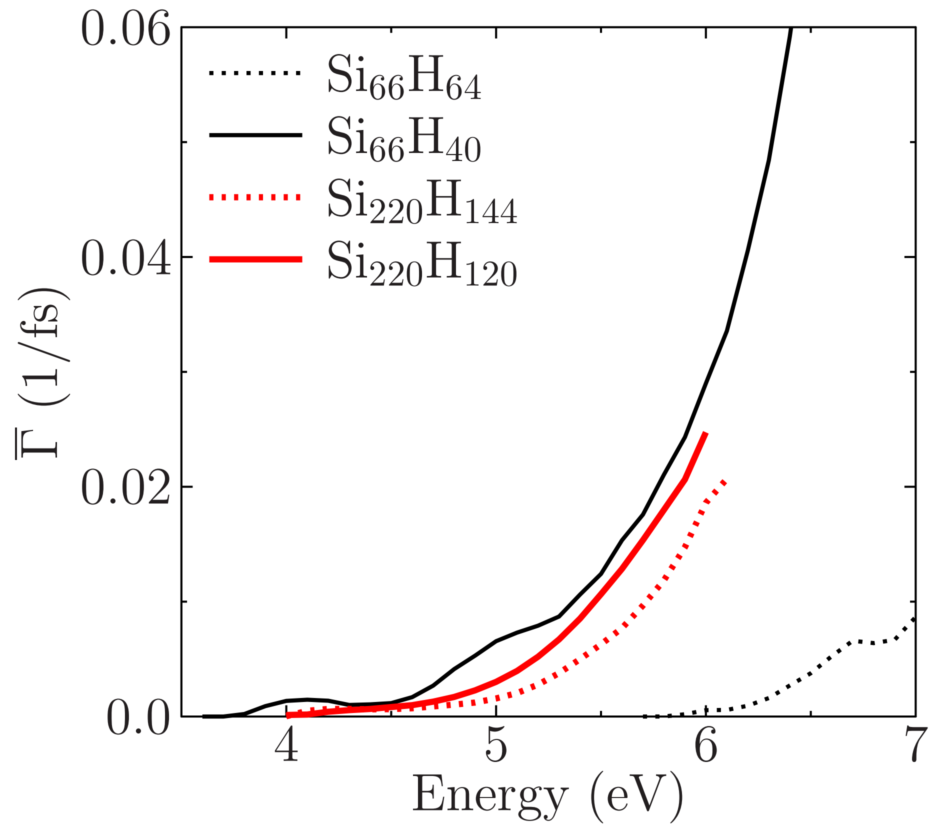


The Full Spectrum Boost Project:
Path towards synergetic 55%



1.a Compensate Gap-Enhancement without Reducing Coulomb Strength: Reconstruction



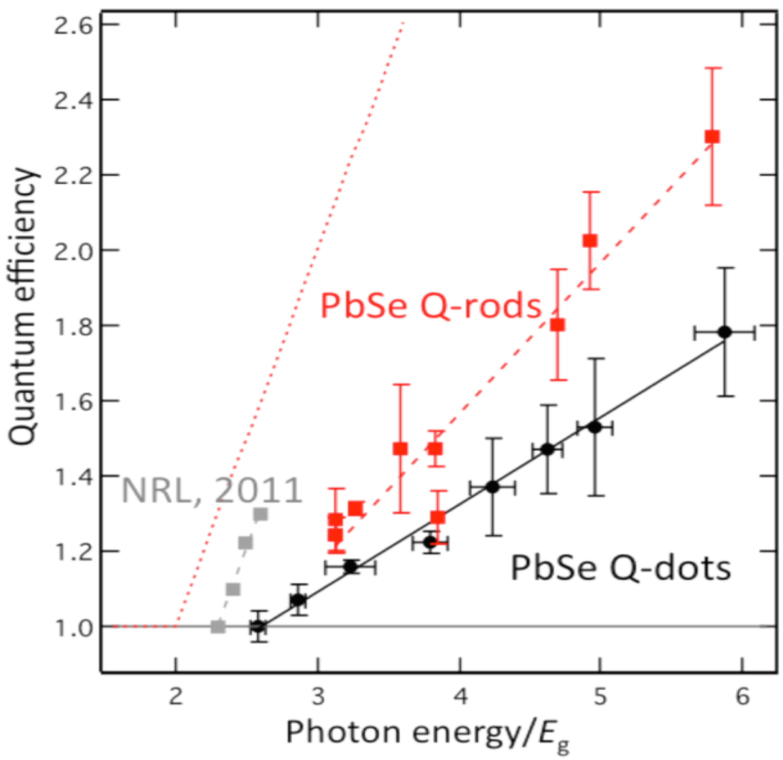


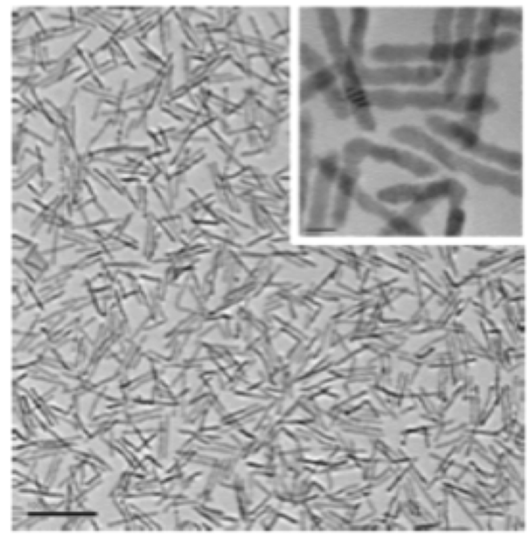
Quantum confinement enhances the gap in unreconstructed NPs

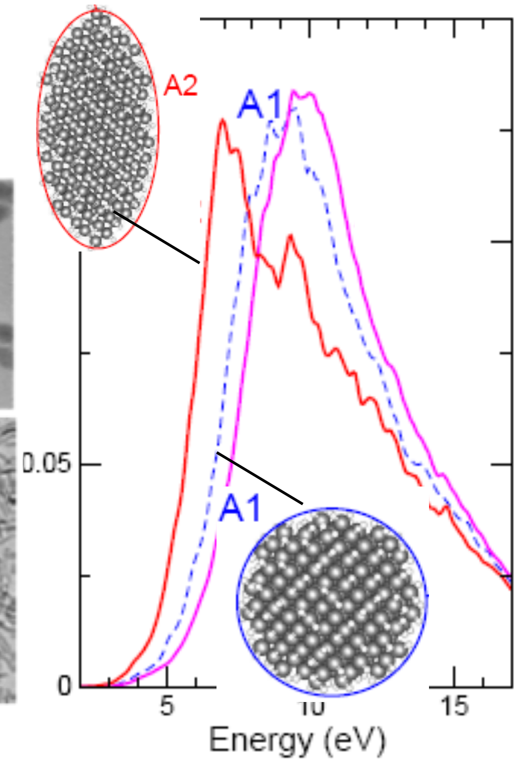
Reconstruction
- compensates gap enhancement
- preserves enhanced Coulomb/MEG

Voros, Galli, GTZ
Phys. Rev. B, 2013

1.b Reduce Gap by Lowering NP Symmetry: More Allowed Transitions







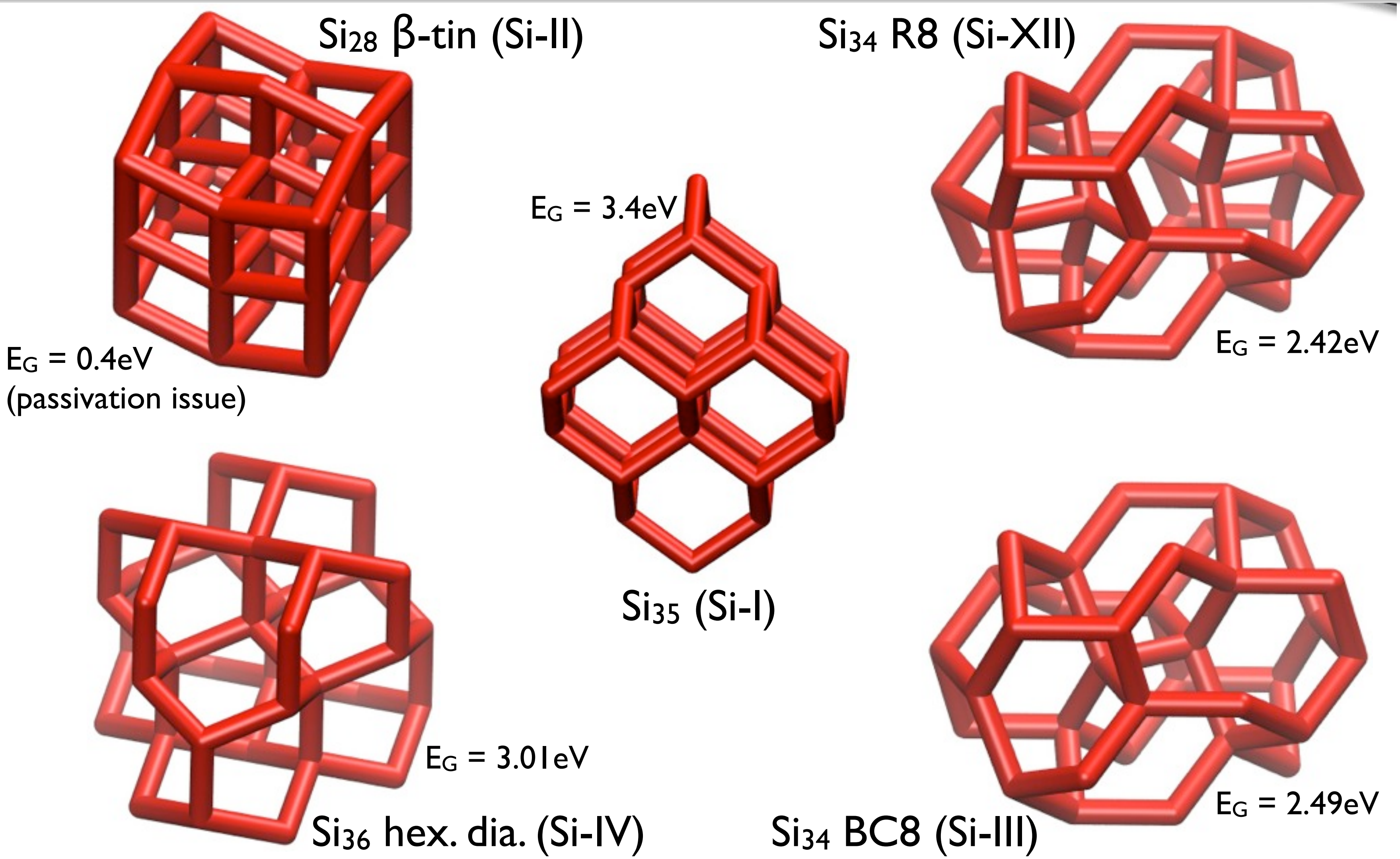
Many transitions forbidden by symmetry-driven selection rules
Lowering symmetry of nanoparticles allows more transitions:

Nanorods: lower CM onset energy; enhanced CM at higher energy

Klimov, Cui

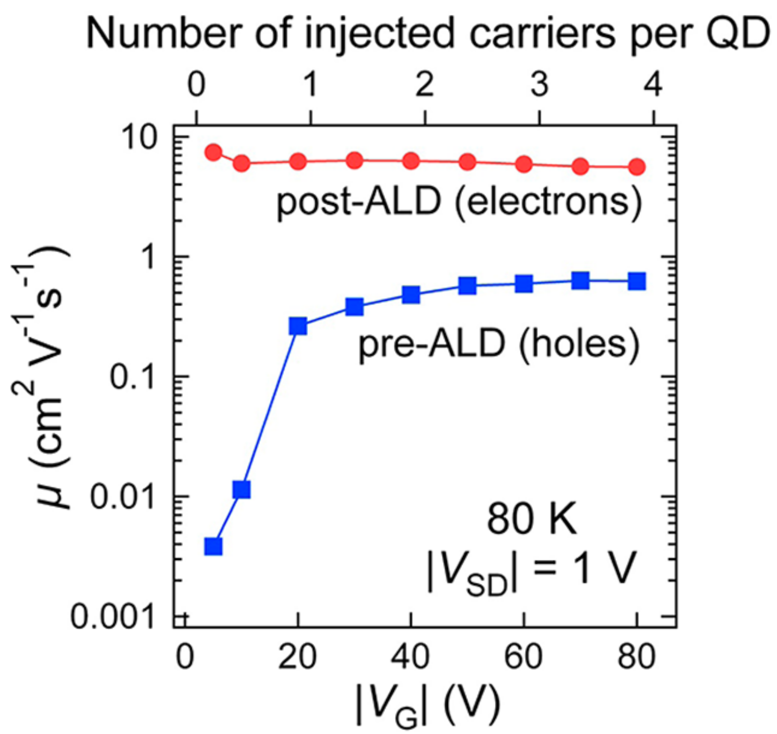
Gali, Kaxiras, Zimanyi, Meng, Phys. Rev. B 2010

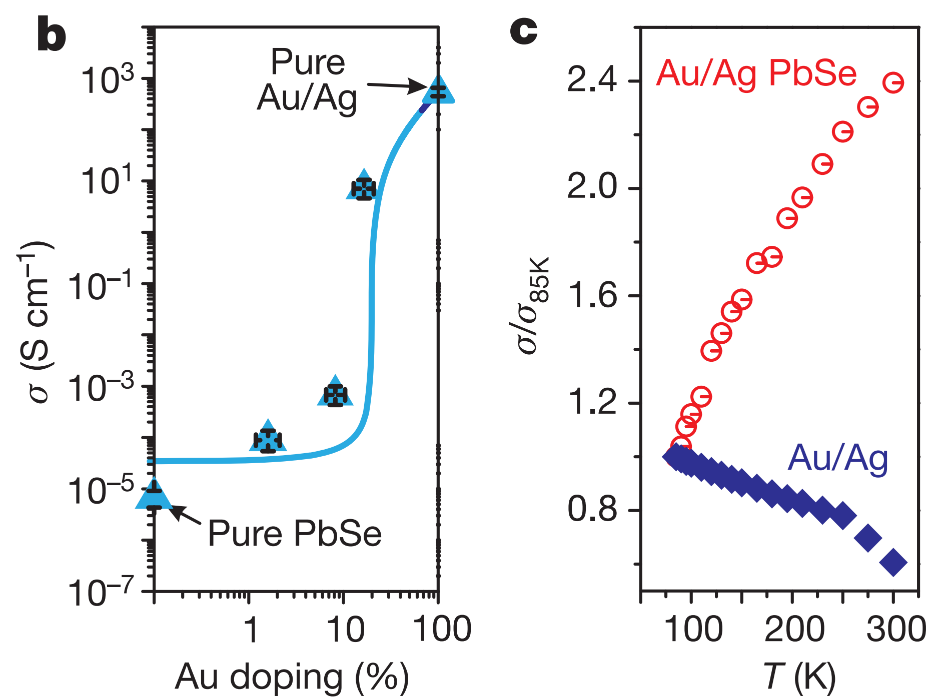
1.c Reduce Gap by using Bulk-Gapless Phases: Exotic Core Phase Si/Ge NPs



Wippermann, Voros, Gali, Rocca, Zimanyi, Galli Phys. Rev. Lett. **110**, 046804 (2013)

2. Boosting carrier extraction by driving CNP solids through Metal-Insulator Transition





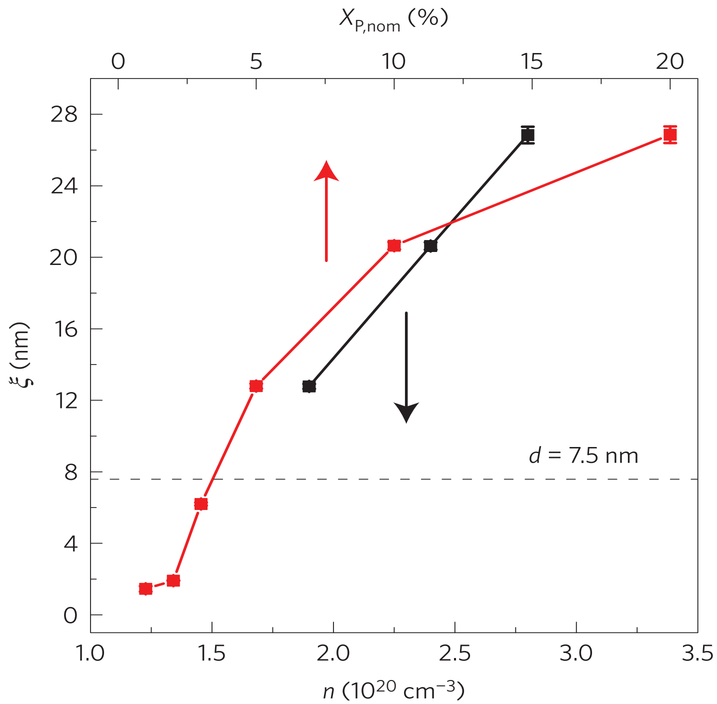
PbSe NP film - Atomic Layer Deposition:
Mobility exhibits MIT

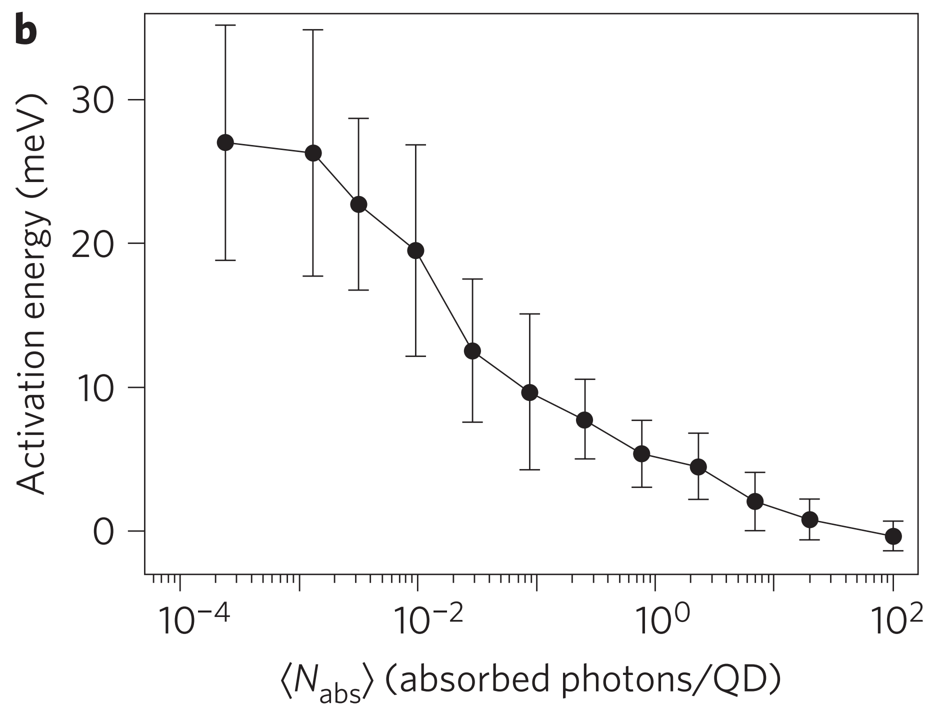
Law group
Nature, **524**, 450 (2015)

PbSe NP film - Au/Ag CNPs substitution:
Mobility exhibits MIT

Kagan, Murray group
Nature, **524**, 450 (2015)

Metal-Insulator Transition in CNP solids





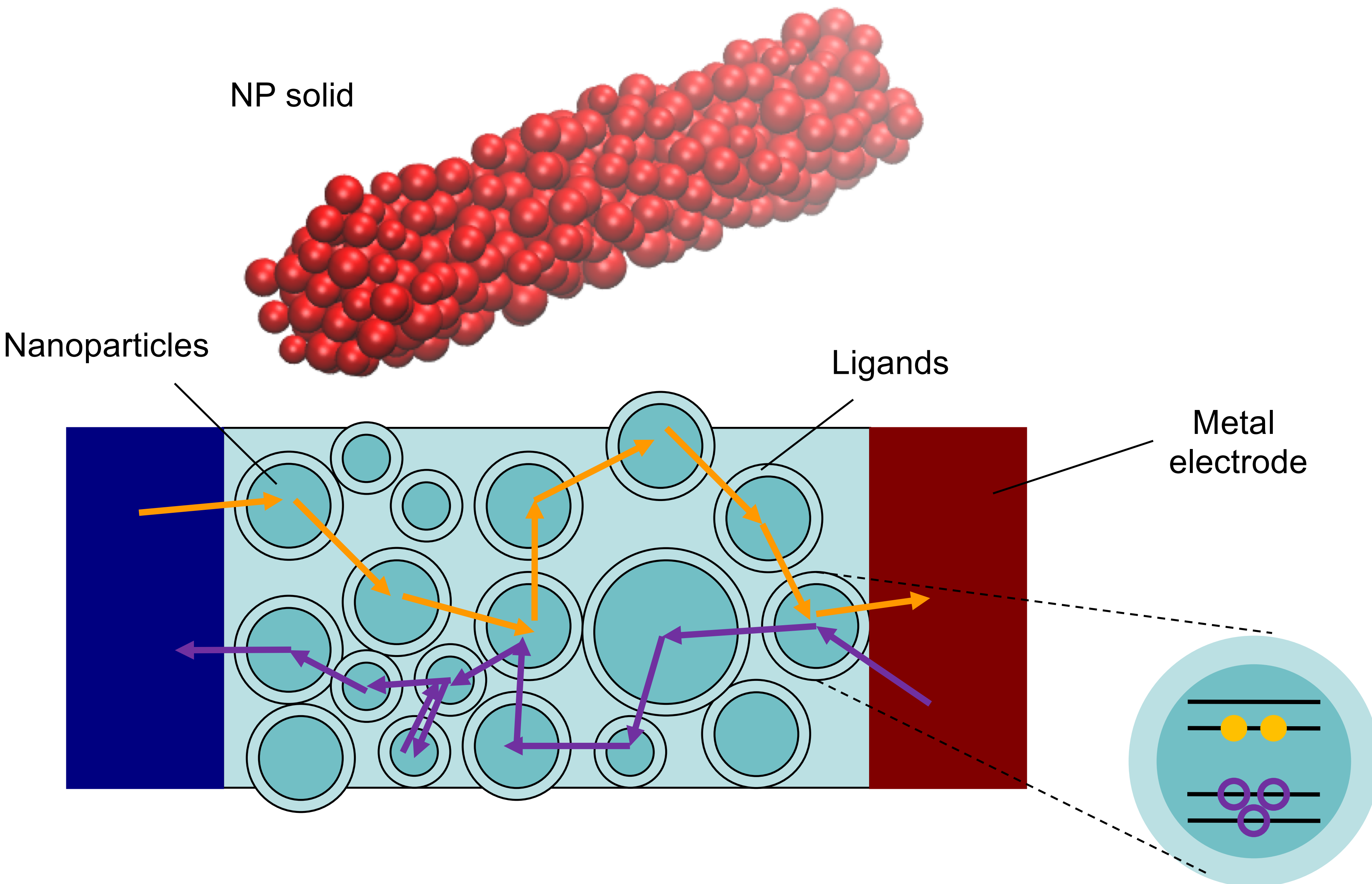
P doping of Si NPs:
Localization length exceeds CNP diameter

Kortshagen, Shklovski
Nature Materials, **11**, 299 (2015)

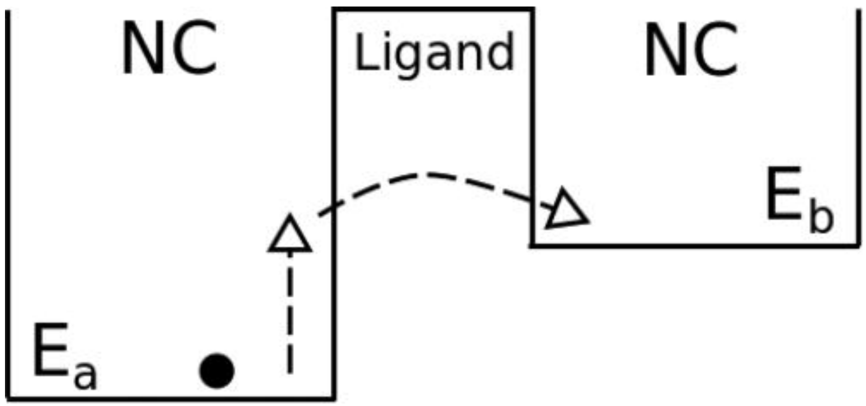
Photo-doping of PbSe CNPs:
Activation energy goes to zero

Van der Zant, Siebbeles group
Nature Nanotech, **6**, 733 (2011)

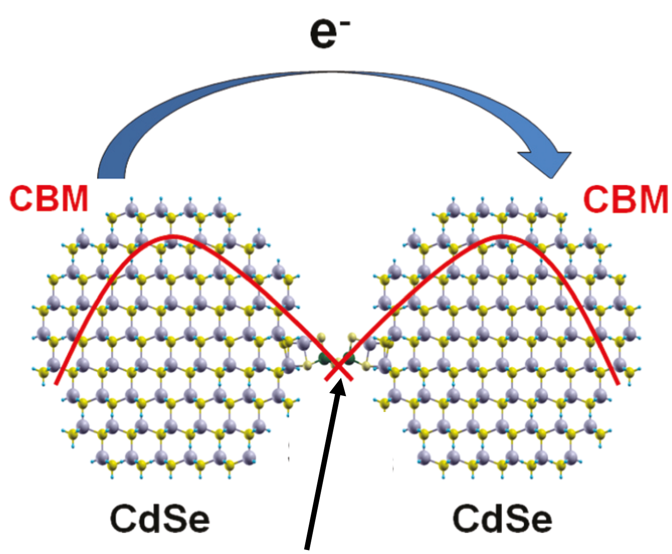
HiNTS: Hierarchical Nanoparticle Transport Simulator with Kinetic Monte Carlo



Approaching the Metal-Insulator Transition from the Hopping regime: "Overlap Energy"



$(E_b\text{-}E_a)$ > Overlap Energy (OE):
Thermally activated hopping transition



Overlap Energy (OE)

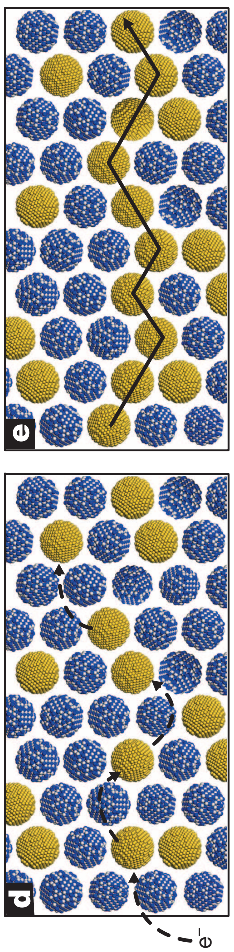
$(E_b\text{-}E_a)$ < Overlap Energy (OE): Metallic, non-activated quantum transition

Qu, Voros, Zimanyi, Sci. Rep. 2017

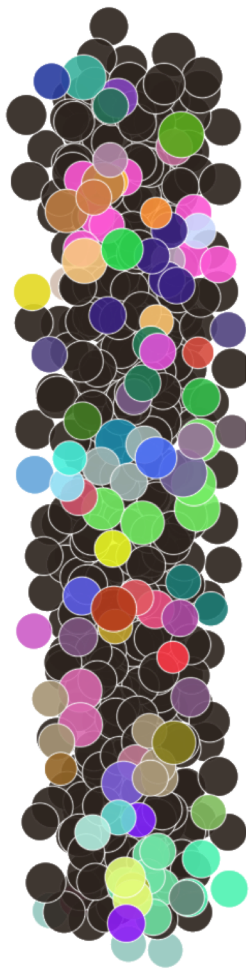
Metal-Insulator Transition: Nanoparticles with metallic couplings percolate

PbSe NP film: Au/Ag CNPs substituted

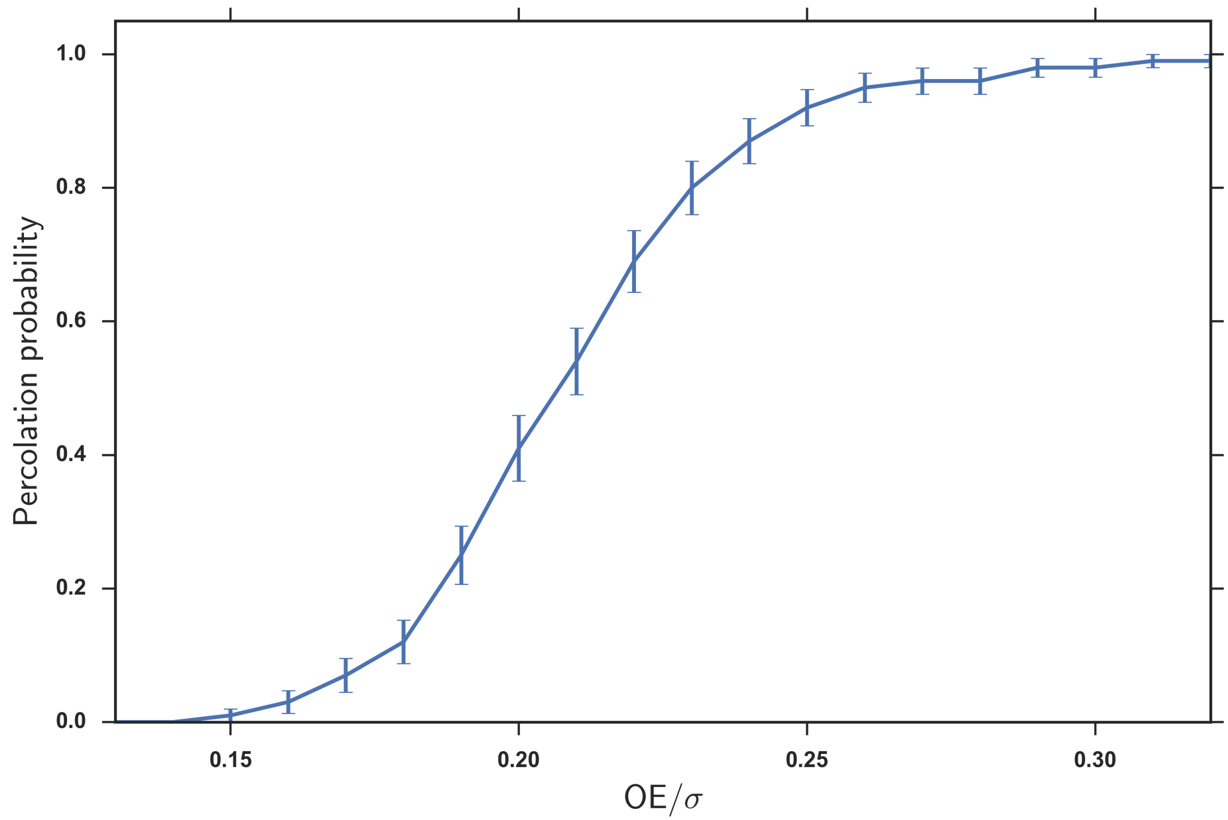
Kagan, Murray group
Nature, **524**, 450 (2015)



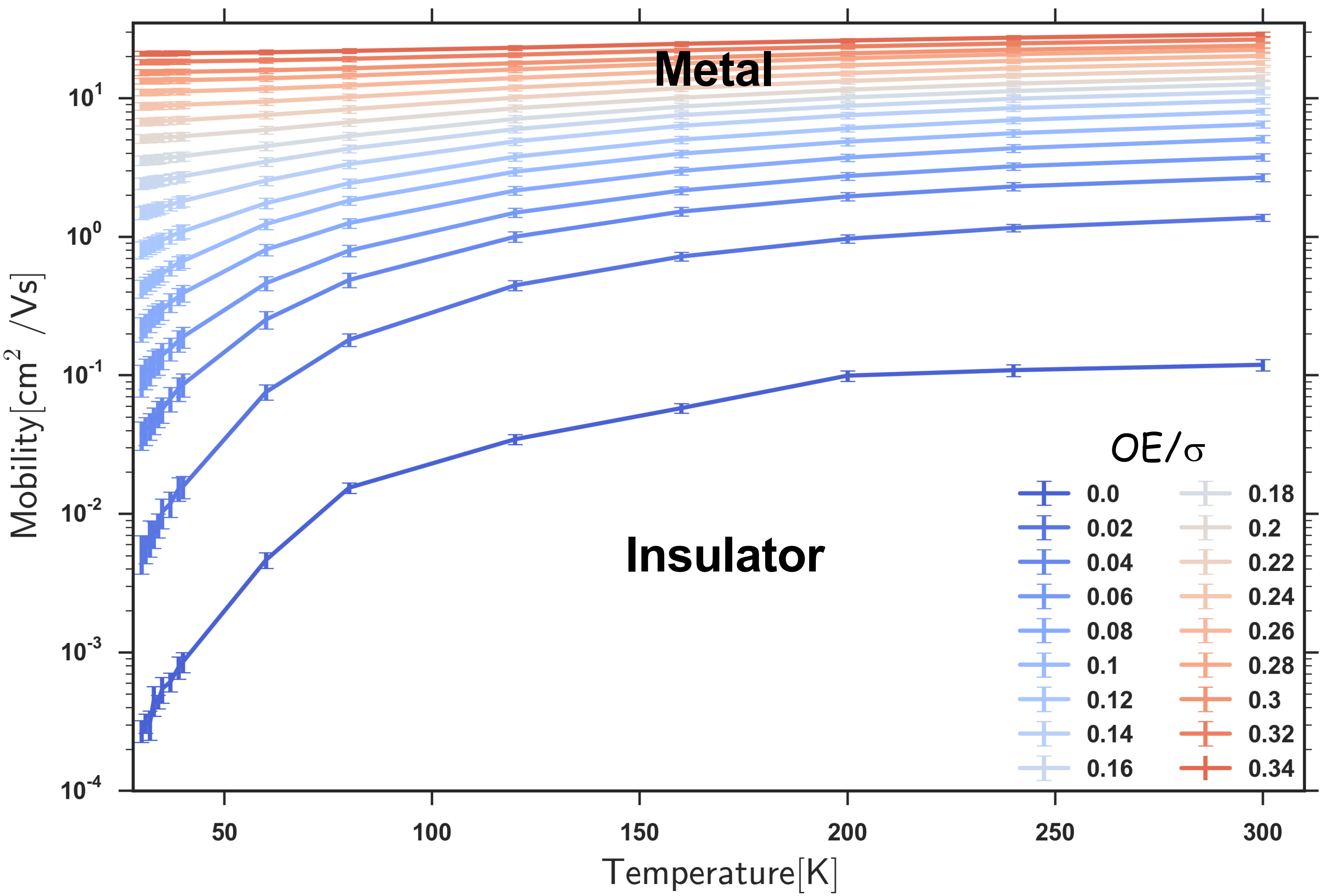
CNPs connected by metallic transitions percolate



Percolation probability as the function of OE/σ

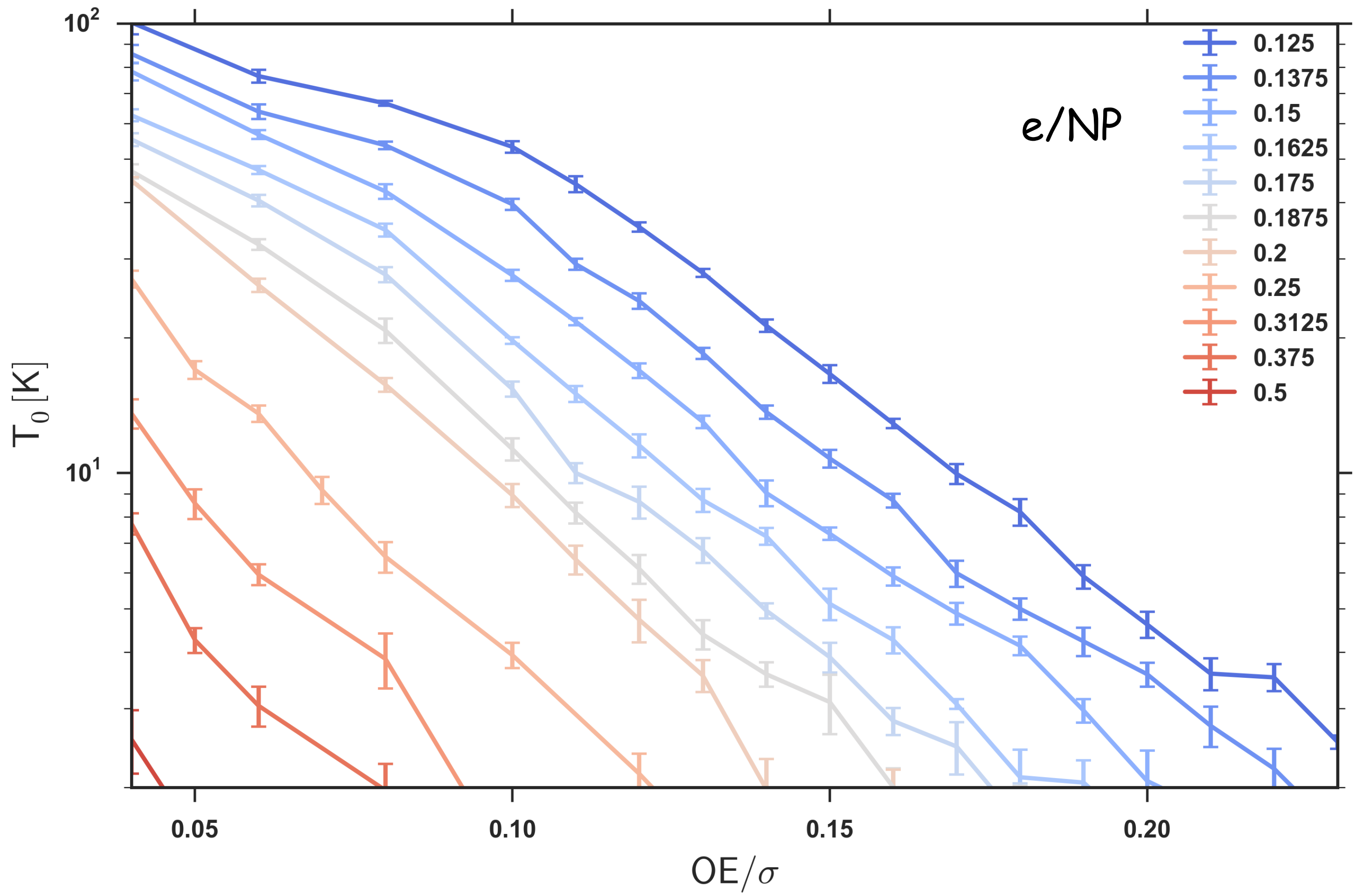


Mobility exhibits Metal-insulator Transition

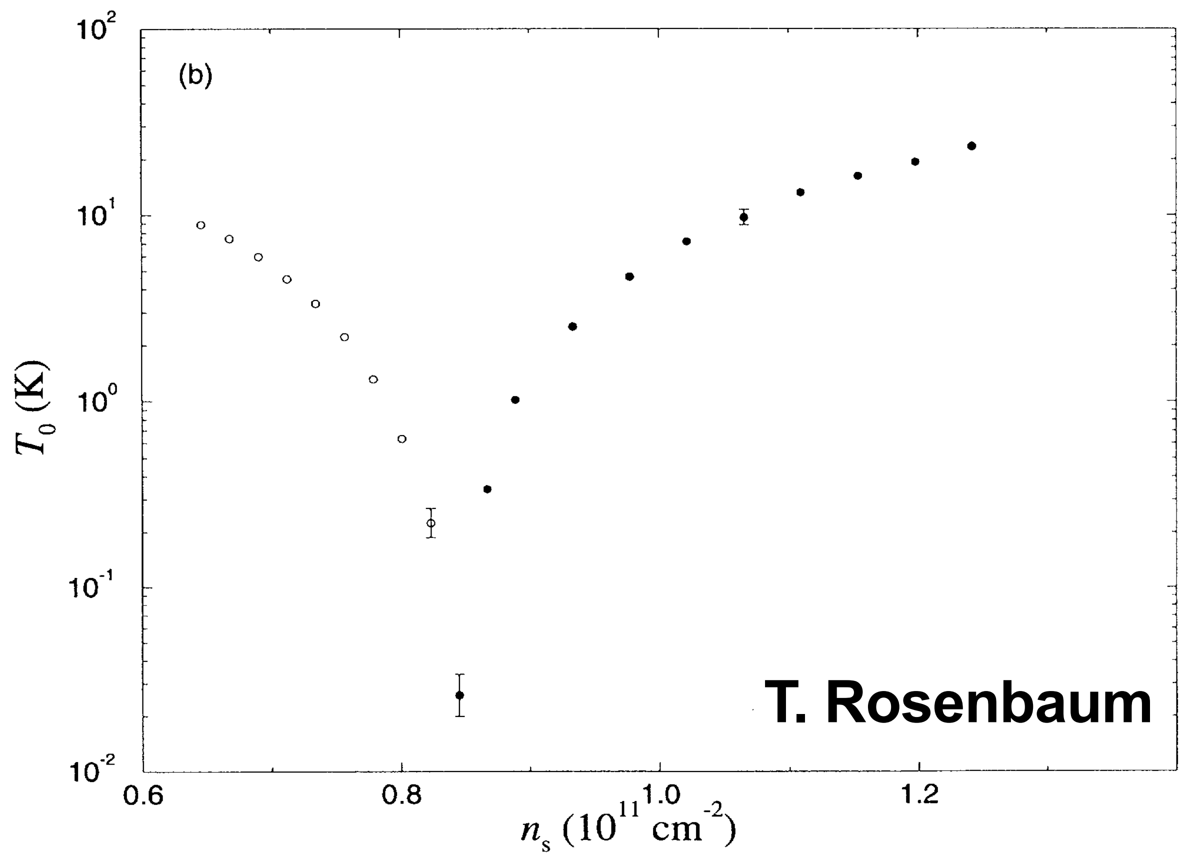


Collapse of effective gap T_0 indicates MIT

Effective gap T_0 as a function of OE/σ (Overlap energy/width of site energy distribution), for different e/NP densities



Possible interpretation:
MIT as a Quantum Phase Transition



$\sigma(T) \sim \exp(-T_0/T)$

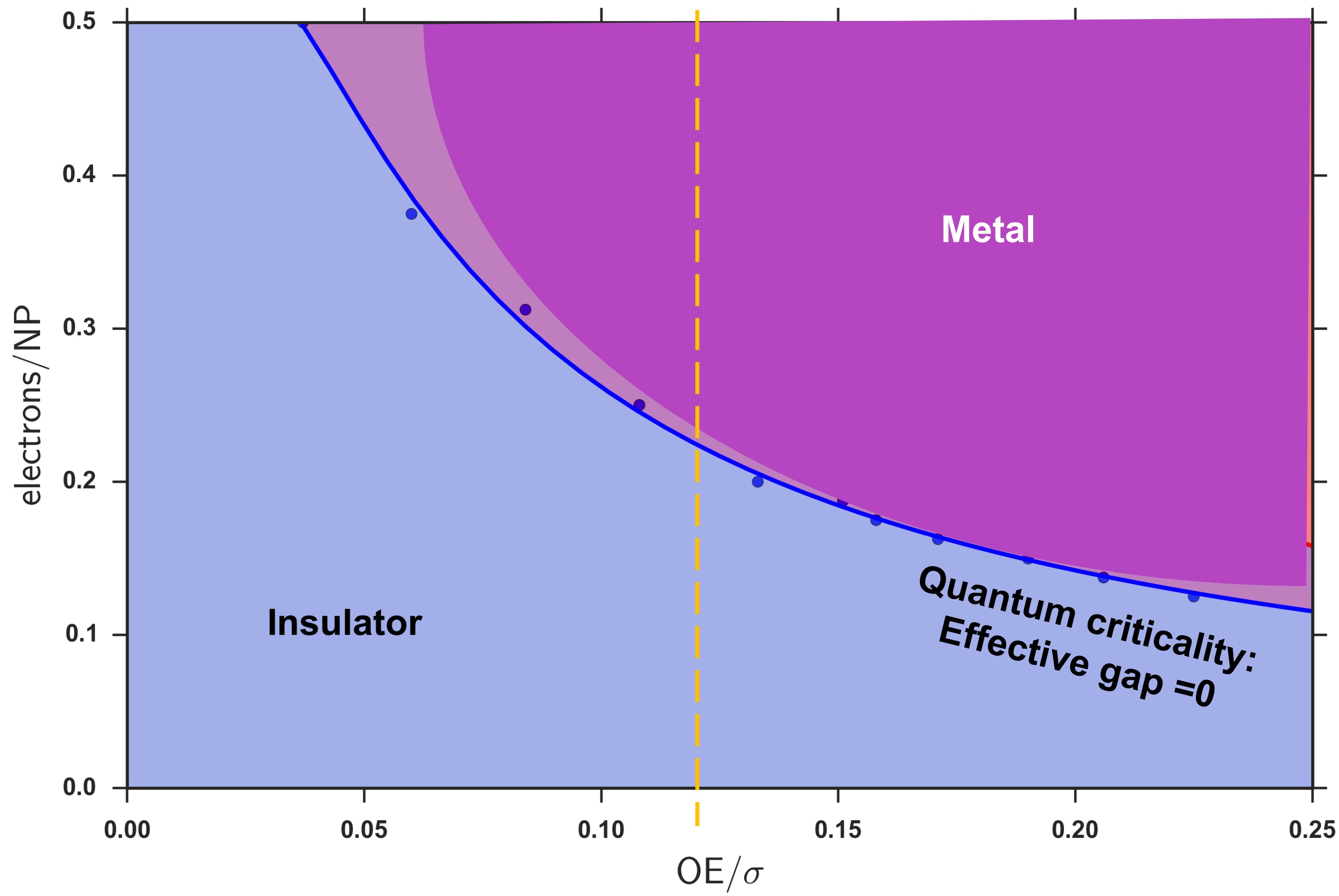
Gap T_0 (in exponential) is critical:

$T_0 \sim (n-n_c)^\beta$

S. Sachdev

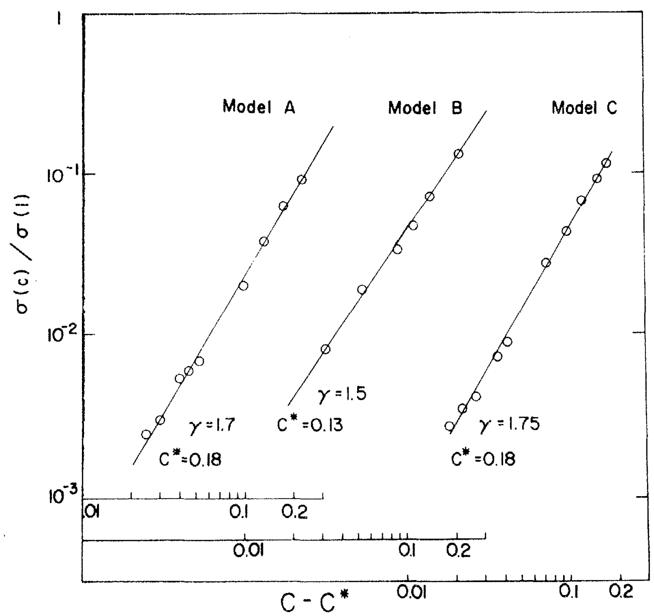
MPA Fisher

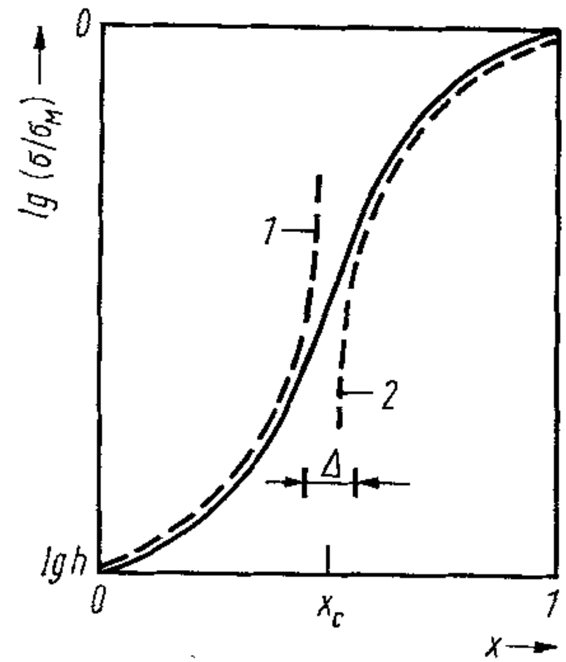
Gap goes to zero before percolation completed?



Geometric Percolation
transition onset

Alternative: MIT as a Quantum Percolation transition





One component system
Mobility σ is critical:
$\sigma \quad \sim (c-c^*)^\gamma$

Webman et al, PRB, 11, 2885 (1975)

Two component system:
Mobility has critical crossover:
$\sigma \quad \sim (\sigma_i/\sigma_m)^s\, \phi[(x-x_c)(\sigma_i/\sigma_m)^m]$

Efros, Shklovskii, Phys.Stat.Sol. 76,475 (1976)

Quantum vs. Percolation: formal difference

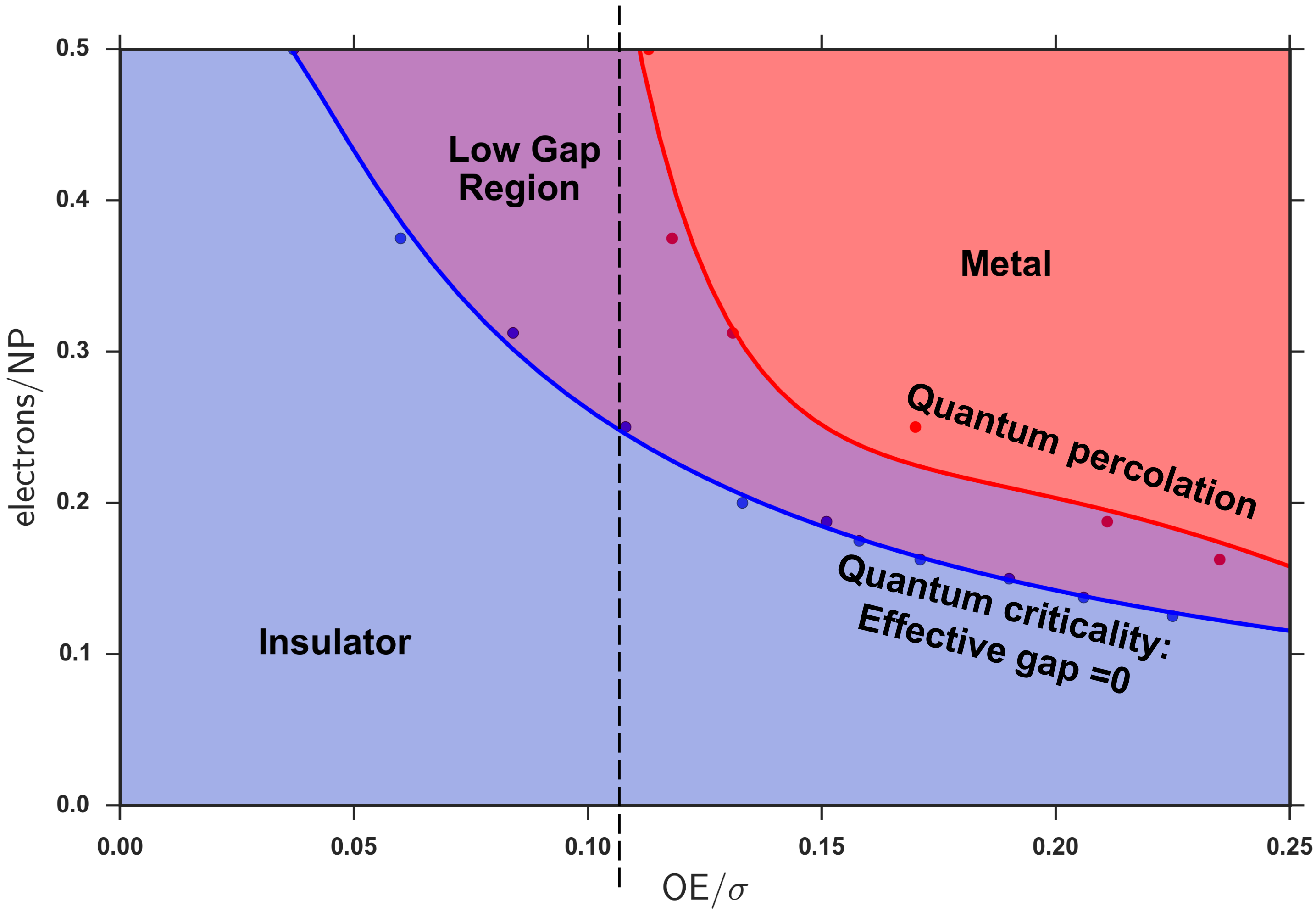
Quantum critical:
Criticality in exponent:
average gap experienced by electrons goes to zero

$$\sigma_{crit}(x,T) = e^{-T_0(x_c-x)^{\gamma}/T}$$

Quantum percolation:
Criticality in pre-exponent:
average number of hopping steps in conducting path goes to zero, gap remains finite

$$\sigma_{crit}(x,T) = \frac{\sigma_{non-crit}}{1+a(x_c-x)e^{T_0/T}}$$

Metal-Insulator Transition in NP FETs: Quantum Criticality vs. Quantum Percolation



Geometric Percolation transition onset

The quantum criticality & the quantum percolation theories yield different phase boundaries

Only the quantum percolation picture is consistent with the geometric percolation of metallic bonds.

Qu, Voros, Zimanyi, Sci. Rep. 2017