Novel materials for high-performance solar cells

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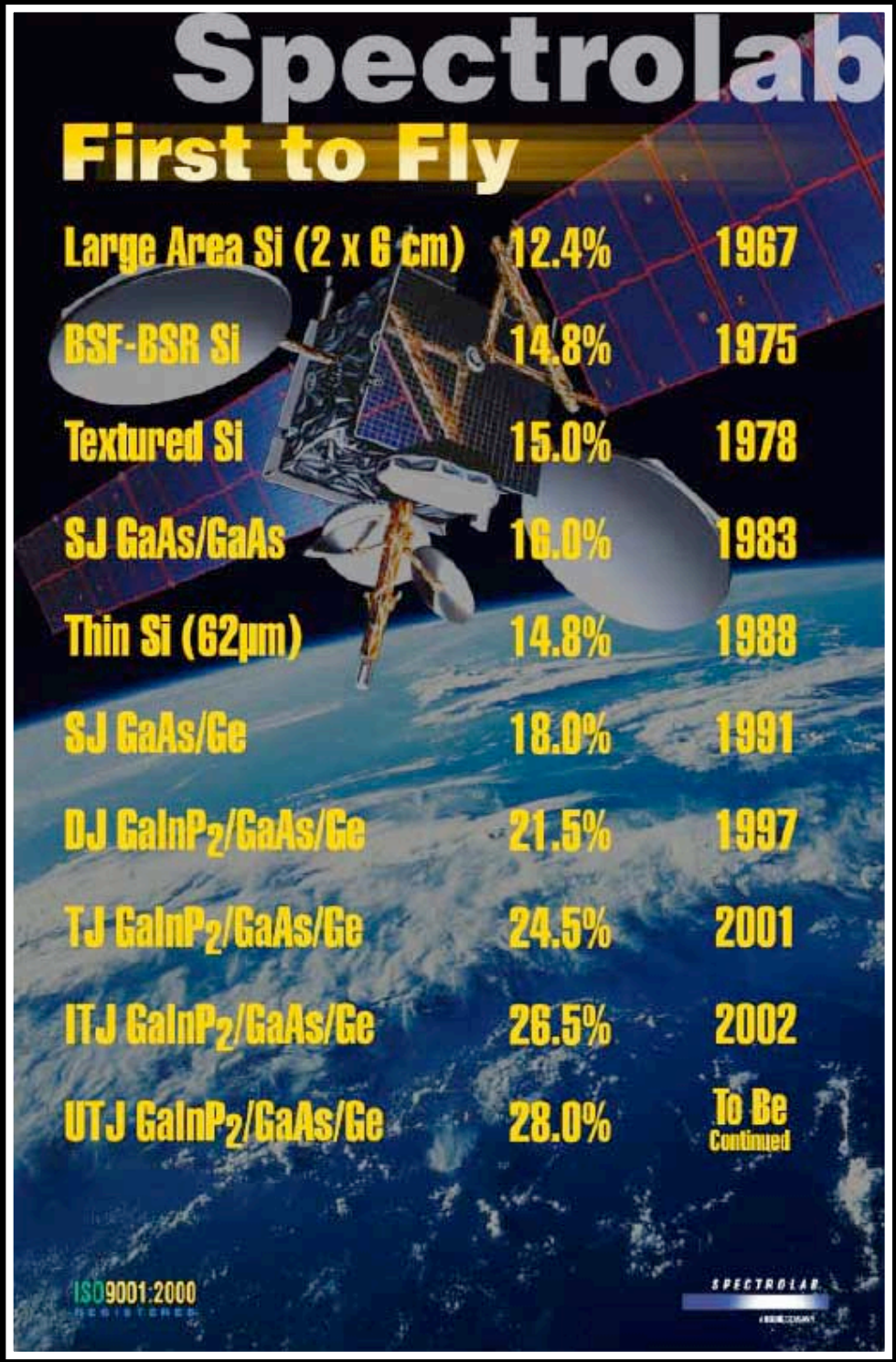
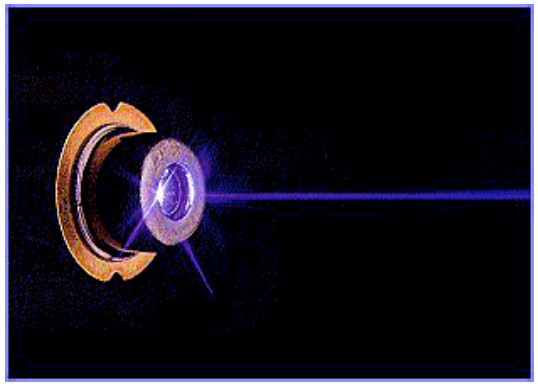
GaAs/Ge 19% eff.


GaInP2/GaAs/Ge ?

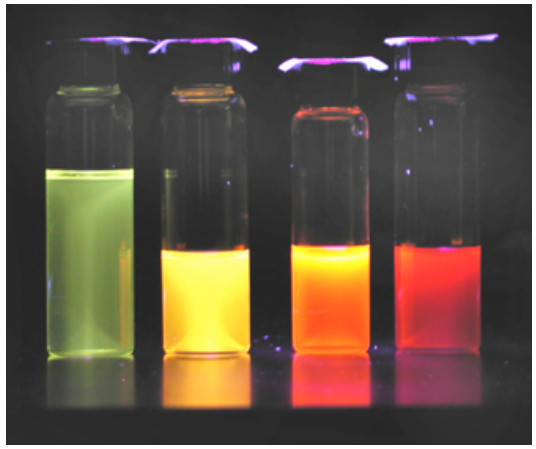

Spectrolab
First to Fly
Large Area Si (2 x 6 cm) 12.4% 1967
BSF-BSR Si 14.8% 1975
Textured Si 15.0% 1978
SJ GaAs/GaAs 16.0% 1983
Thin Si (62µm) 14.8% 1988
SJ GaAs/Ge 18.0% 1991
DJ GaInP2/GaAs/Ge 21.5% 1997
TJ GaInP2/GaAs/Ge 24.5% 2001
ITJ GaInP2/GaAs/Ge 26.5% 2002
UTJ GaInP2/GaAs/Ge 28.0% To Be Continued
ISO9001:2000
SPECTROLAB

Research directions

Higher efficiency: Nitride semiconductors



Lower cost: Nanostructured materials



This is the theorists viewpoint - packaging and manufacturing issues are very real and significantly contribute to total cost

Outline

1. Introduction

Photovoltaics

Efficiency & economy?

2. How can we model these systems?

Computational techniques

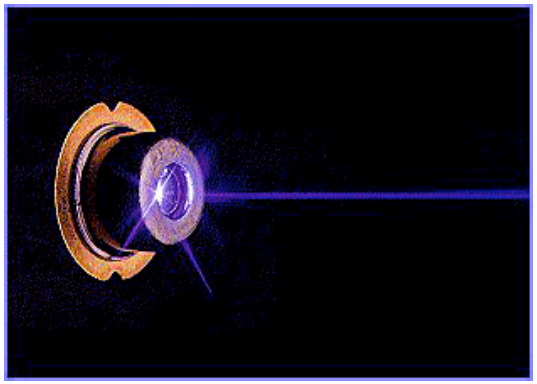
3. Nitride photovoltaic materials

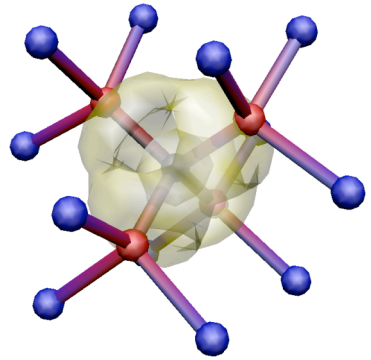
GaAsN (and GaPN)

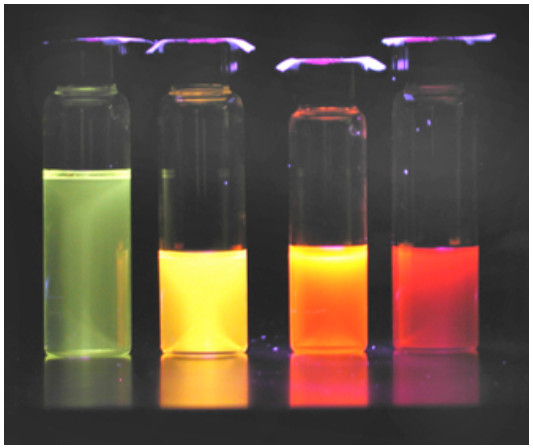
Band gap reduction. Localized states

4. Nanostructured materials

Cheap.Efficient?







Acknowledgements

National Renewable Energy Laboratory
Golden, Colorado

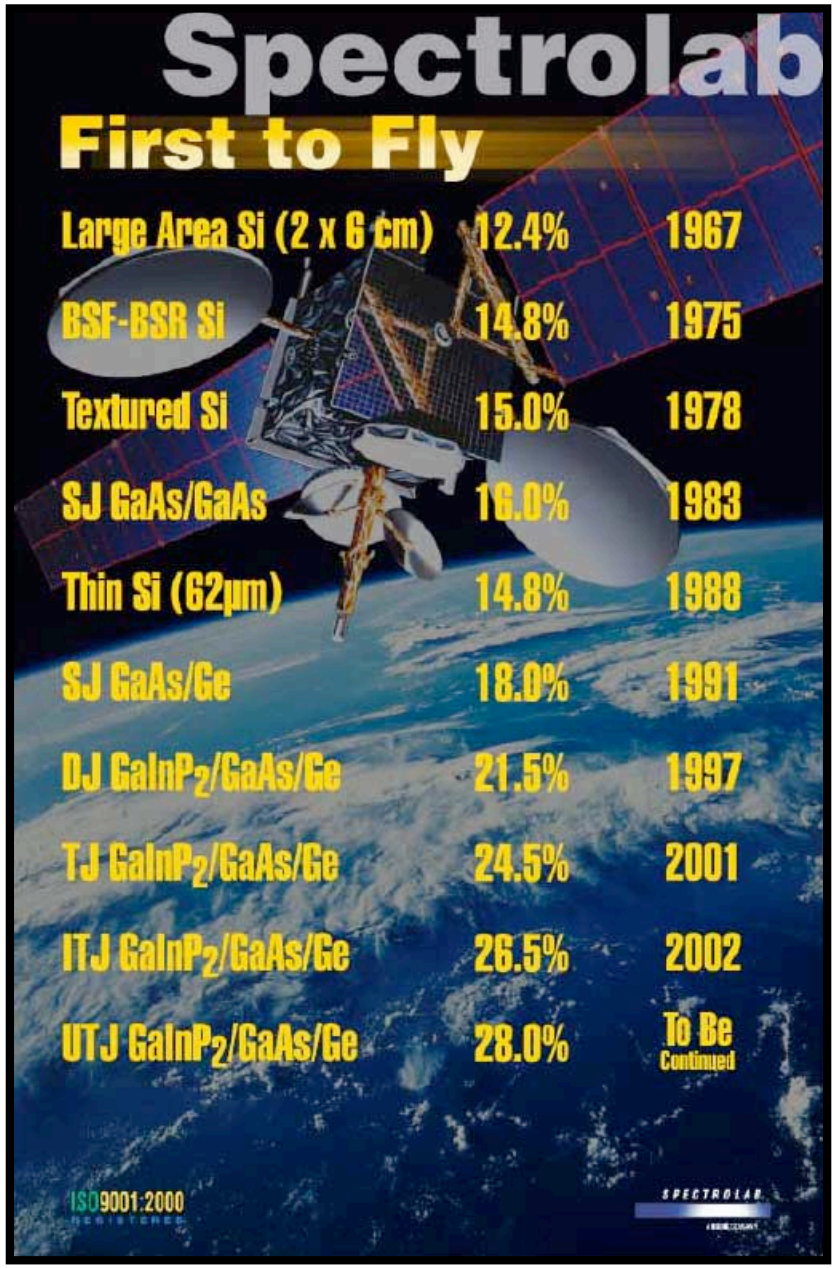
Alex Zunger

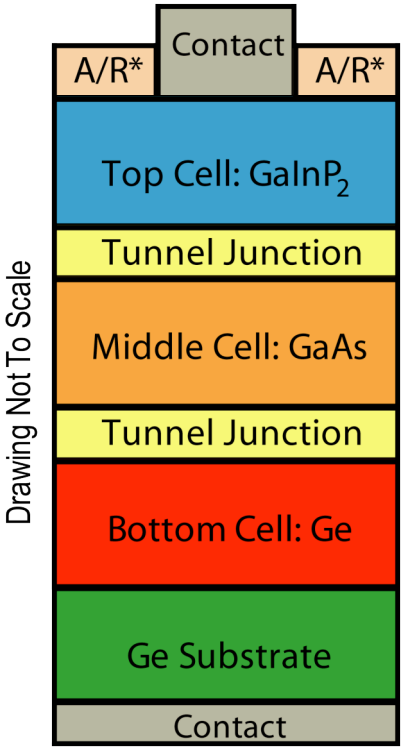
Lin-Wang Wang, Laurent Bellaiche, Tommi Mattila

Ongoing work (in II-VIs) with Clas Persson

U.S. Department of Energy
Office of Science
Basic Energy Sciences
Division of Materials Sciences

Sources of Improved Efficiency



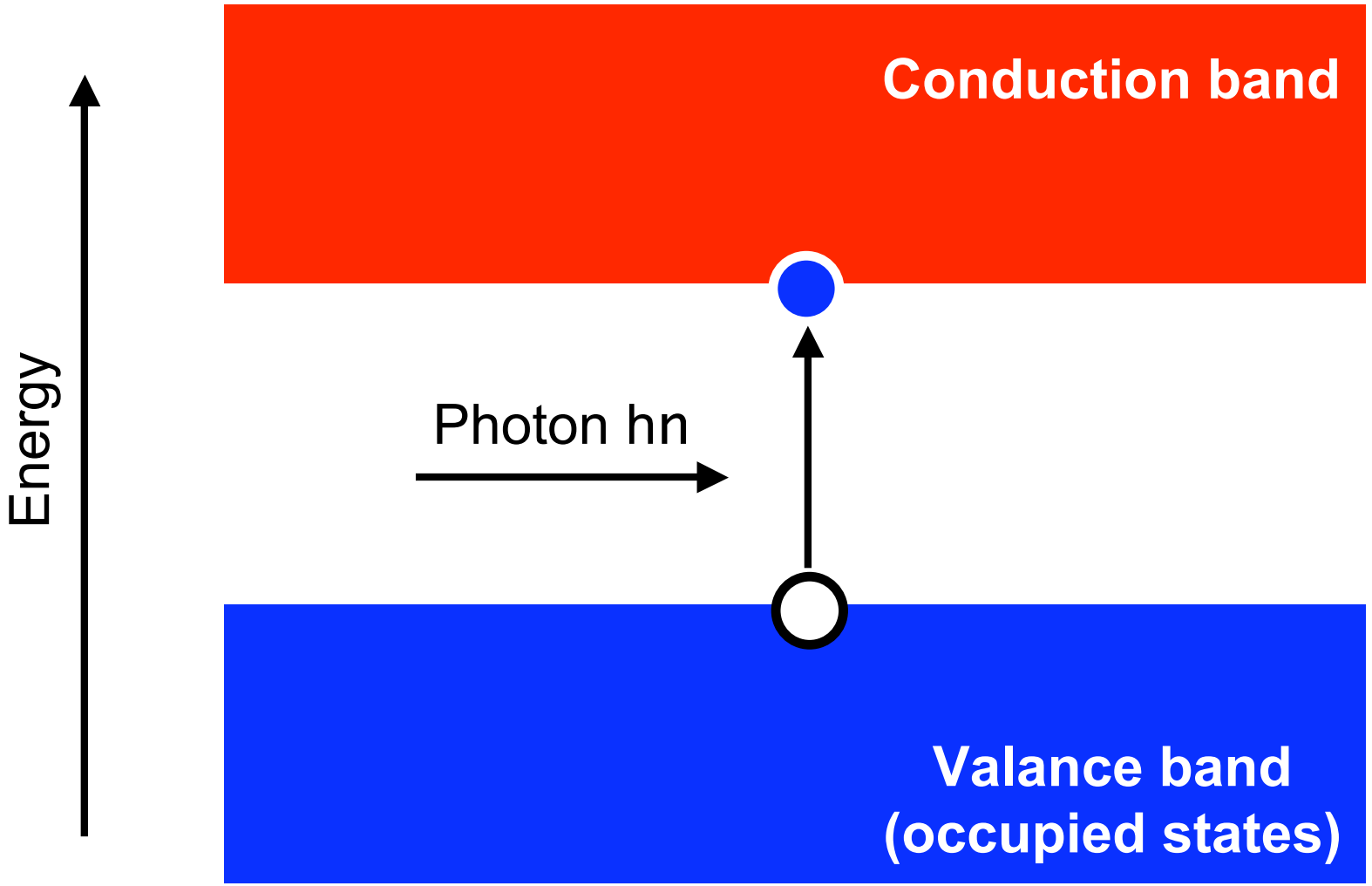


*A/R: Anti-Reflective Coating

1. Multiple materials(+junctions)
2. Junction optimisation

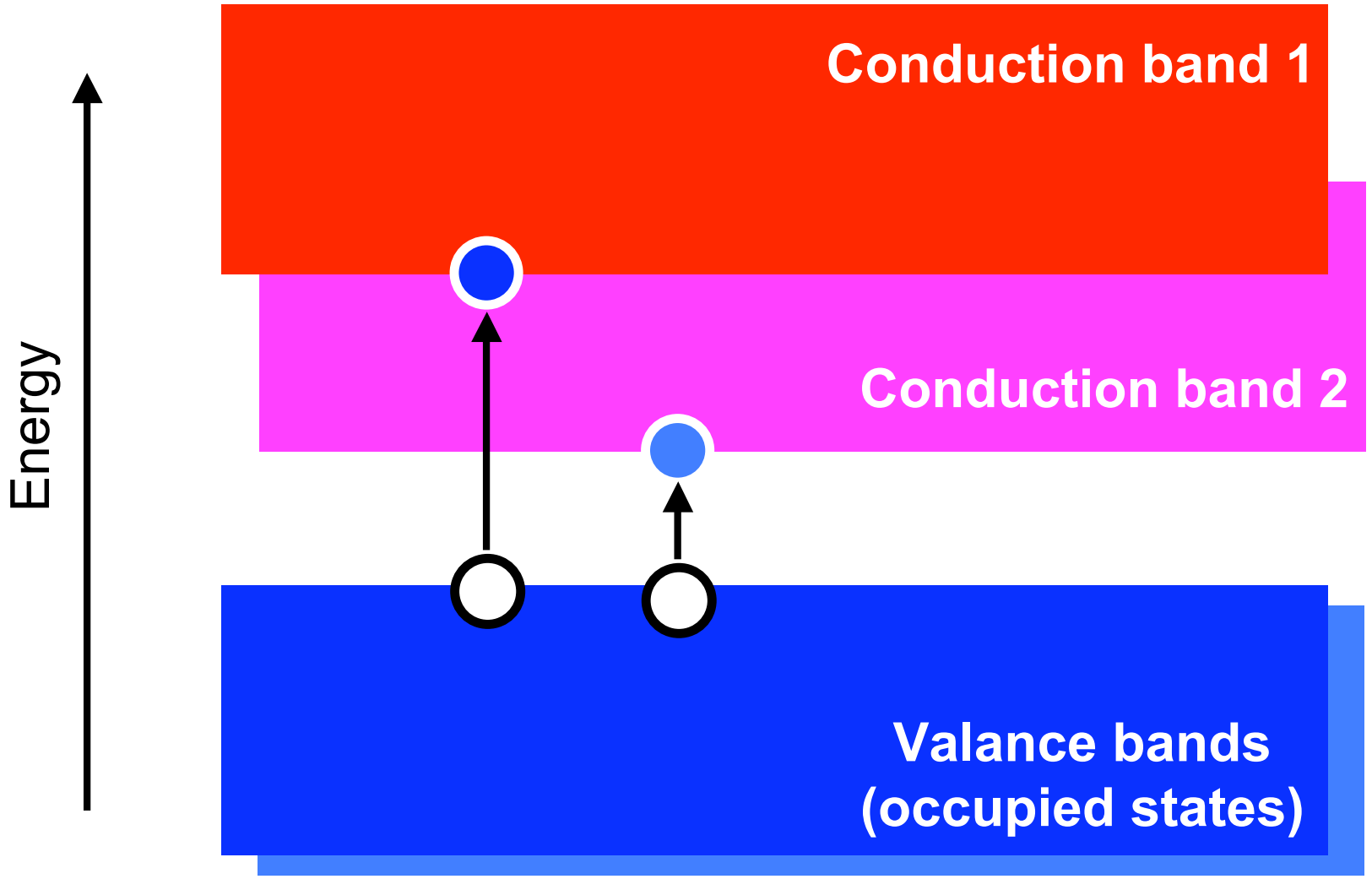
In this talk, I concentrate on (1)

Absorption in single material cells



Multi-junction solar cells

Use of multiple materials to harvest photons of different energies



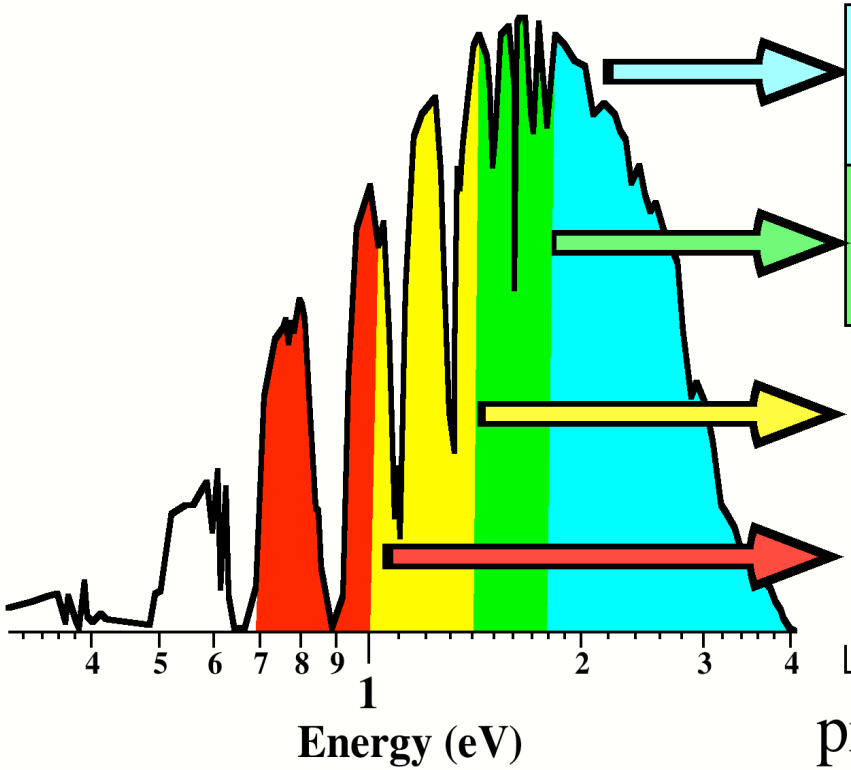
High Efficiency Multijunction Solar Cells

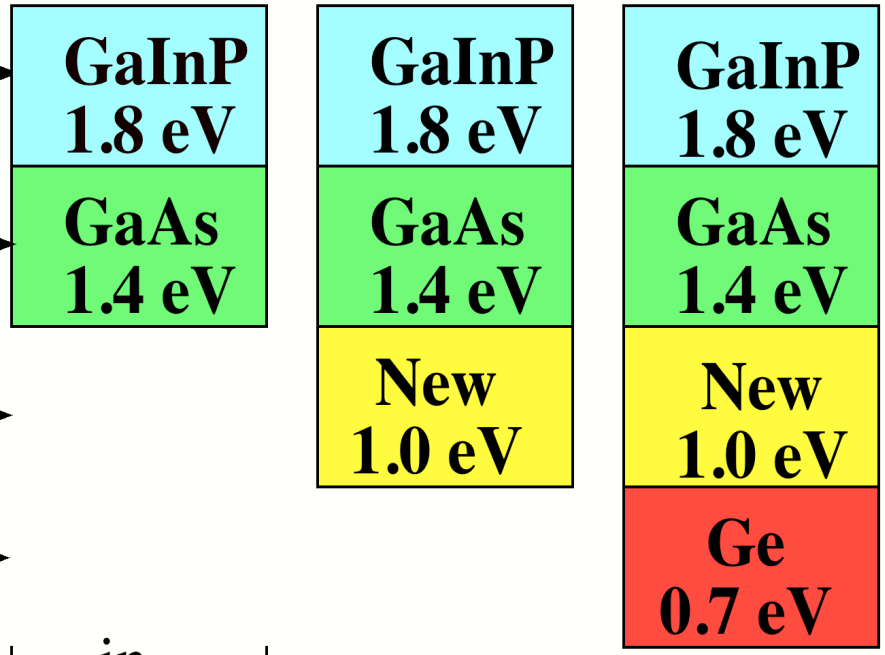
- Want 1 eV material lattice-matched to GaAs

Þ Try GaInNAs

Calculated efficiencies (ideal)

	500X		
AM1.5D:	36%	47%	52%
one sun AM0:	31%	38%	41%





in production

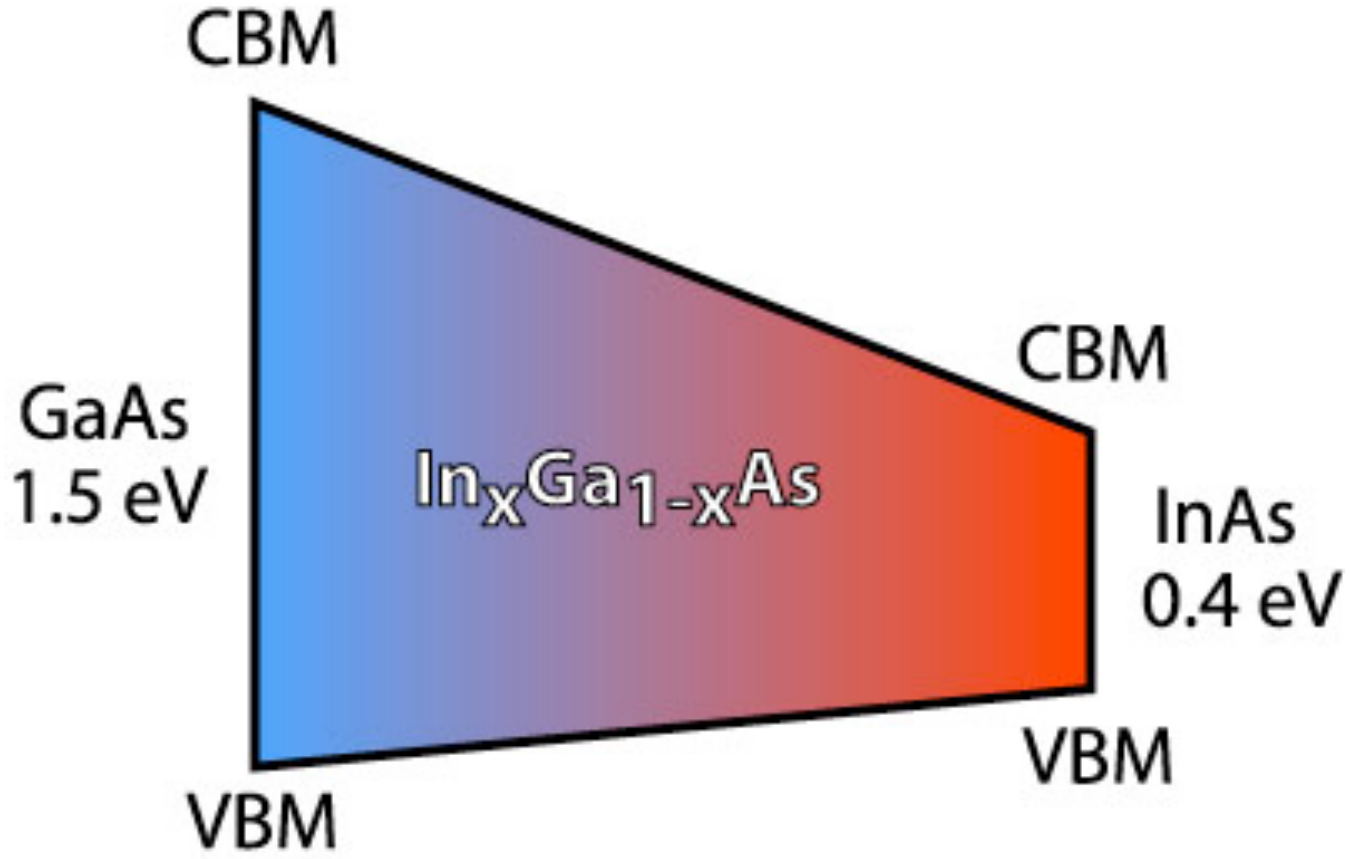
future generation

National Renewable Energy Laboratory

Aim

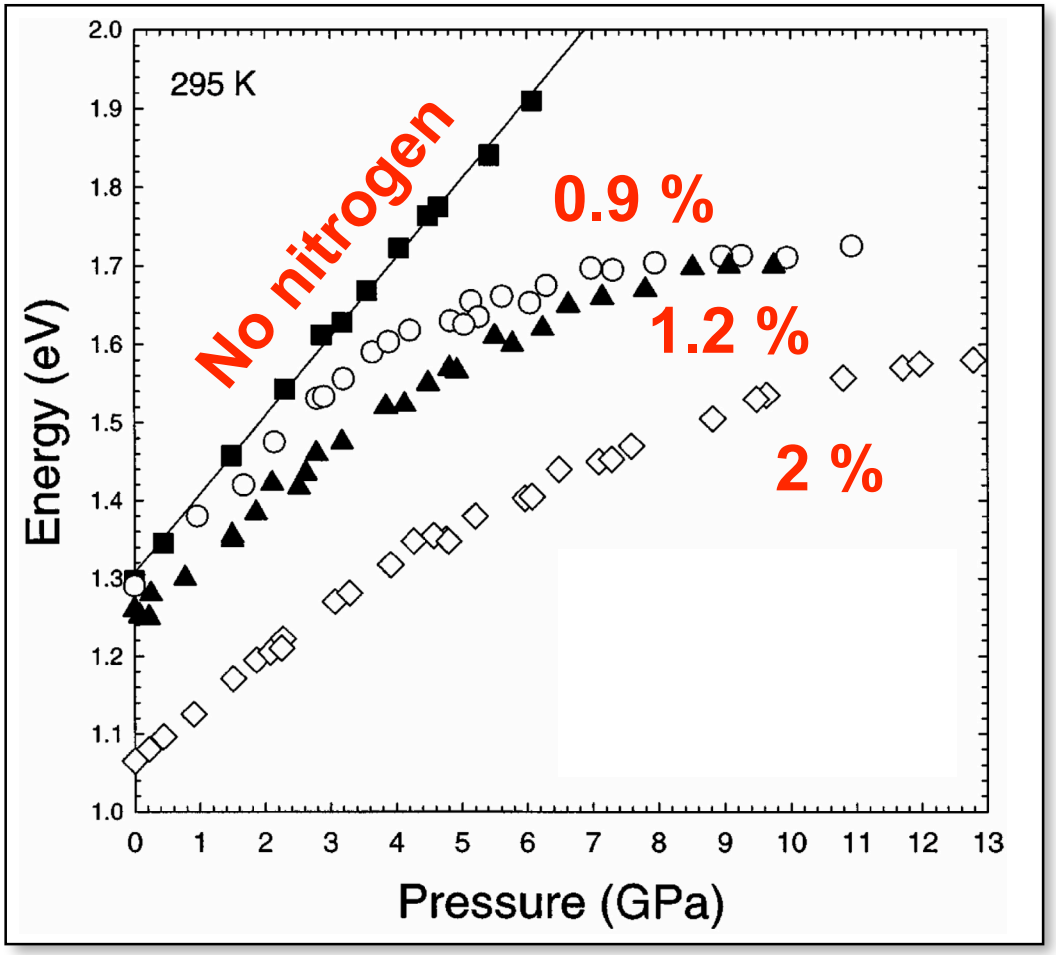
Find a 1eV band gap material that is near lattice matched to GaAs

Isostructural semiconductor alloying



Properties approx. a linear combination of the components

Anomaly #1: Band gap reduction in GaAsN

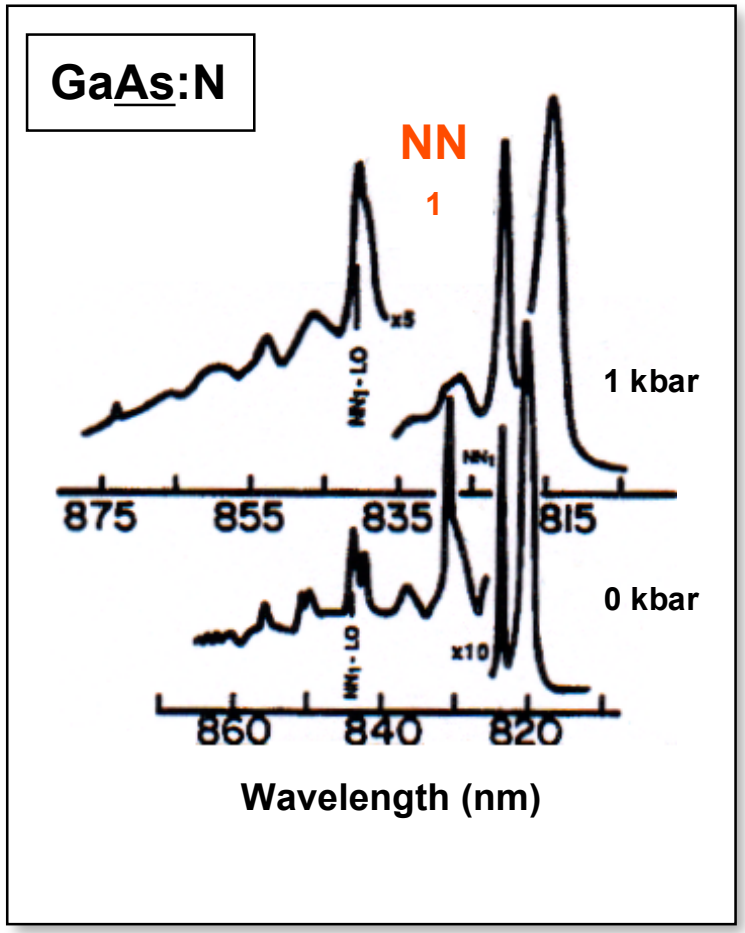


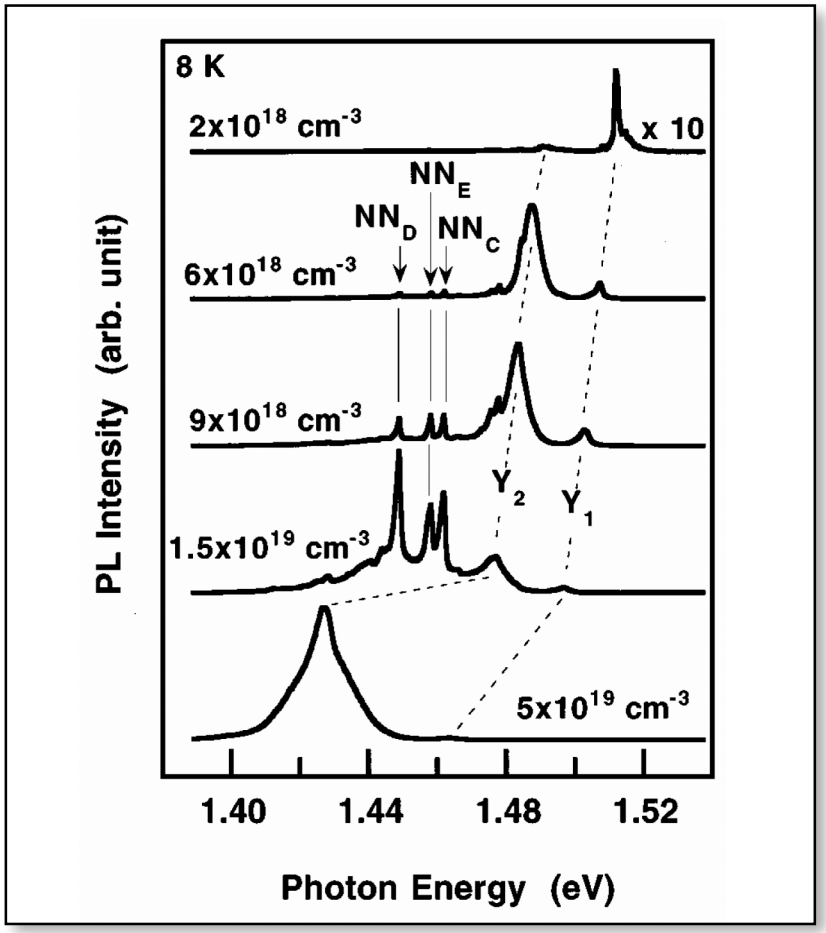
Band gaps
GaAs ~1.5 eV
GaN ~3.5 eV

Shan *et al.* Phys. Rev. Lett. **82** 1221 (1999)

Band gap reduced by ~120meV per % nitrogen!

Anomaly #2: Dilute Nitrogen in GaAs





Liu, Pistol and Samuelson. Appl. Phys. Lett. **56** 1451 (1990)

T. Makimoto *et al.* Appl. Phys. Lett. **70** 2984 (1997)

Many sharp lines seen in emission!

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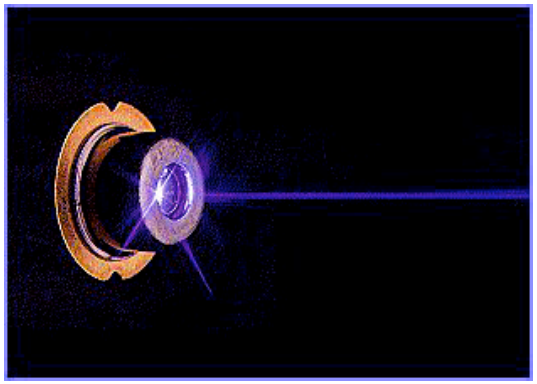
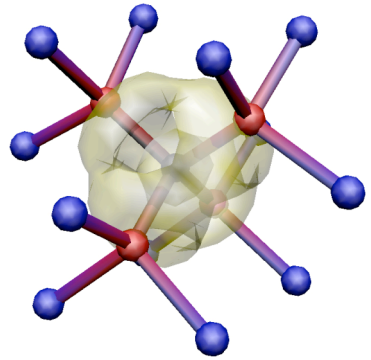
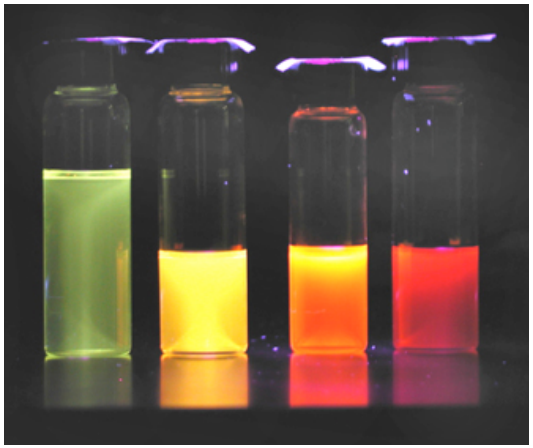
Cheap.Efficient?







Computational modeling

Conventional “off the shelf” first-principles LDA-DFT cannot be applied

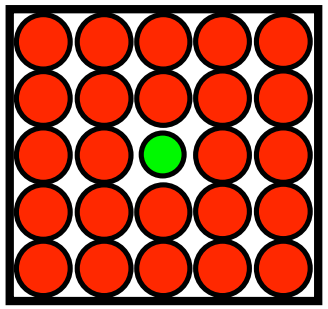
- The band gaps are wrong (1eV+ errors)
- System size is limited (10^2 vs 10^4-10^6 atoms).

Choose:

1. Empirical pseudopotential method for potential (accuracy)
2. Folded spectrum method for eigenstates (size)

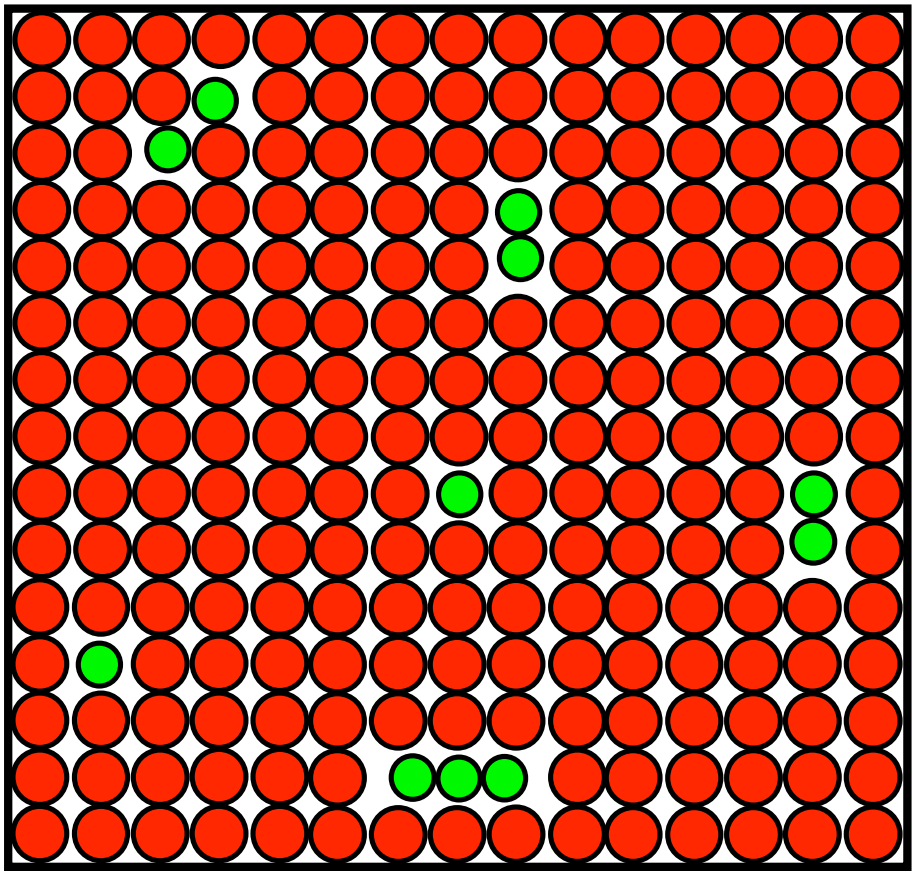
These same methods will also be used for quantum dots

Large supercell modeling of alloys



Small Supercell Approach

Large Supercell Approach



- Use large supercells (10^3-10^6 atoms) containing many nitrogens
- Statistically average properties of many random configurations
- Use Valence Force Field for structural relaxation
- Use Empirical Pseudopotential Method for wavefunctions

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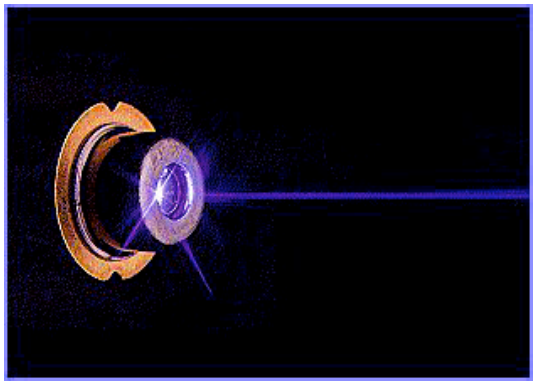
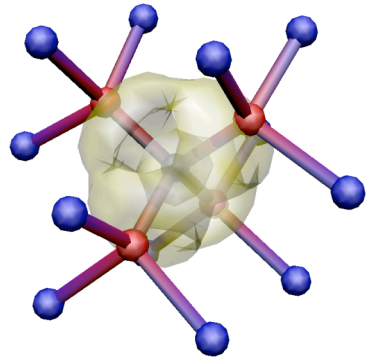
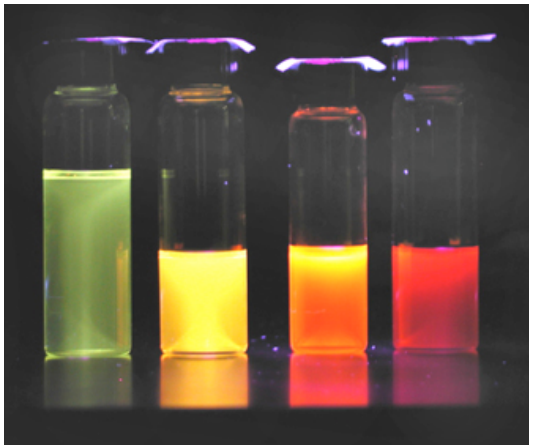




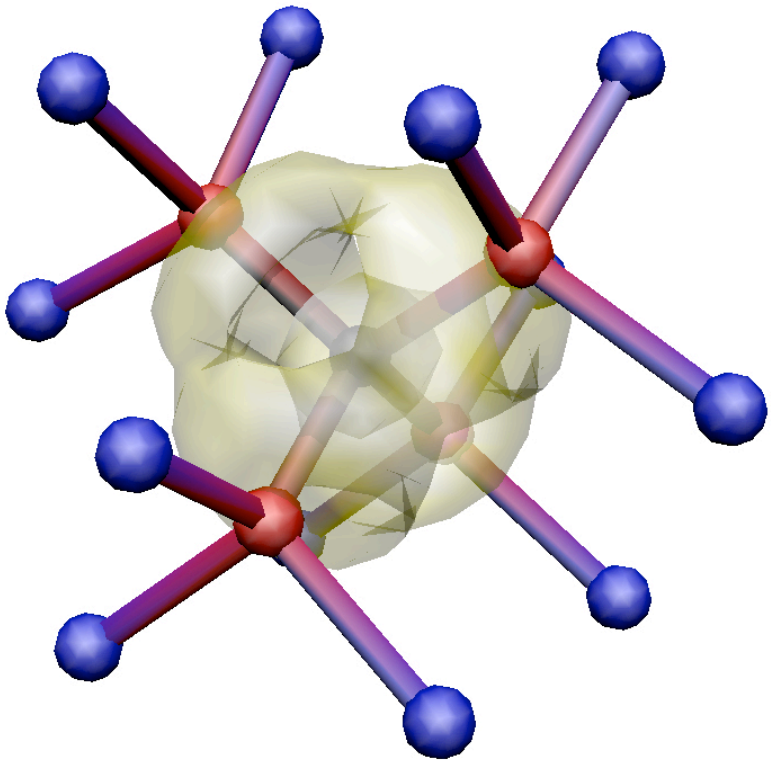


N in GaAs, GaP

I will discuss three cases:

1. **Isolated Nitrogen**
2. Pairs and clusters
3. Well-developed alloys

GaP:N

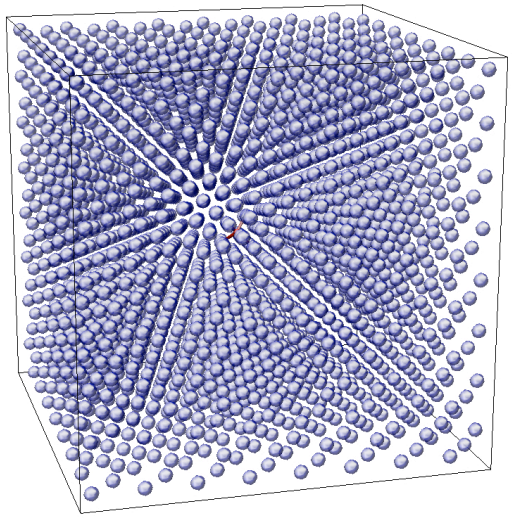


Nitrogen localized a_1(N)

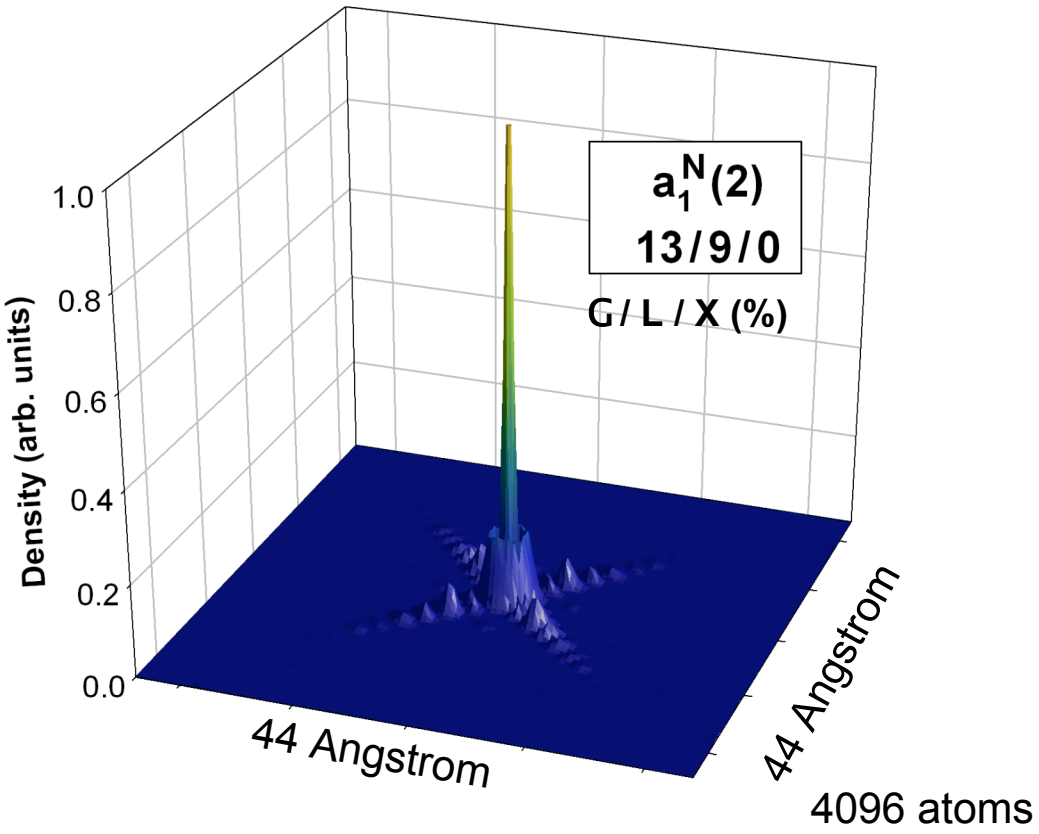
In GaP:N (0.01%):

Level ~30 meV below CBM
Introduces G character -
"direct gap"

Delocalized wavefunction



Localized Level in GaAs:N



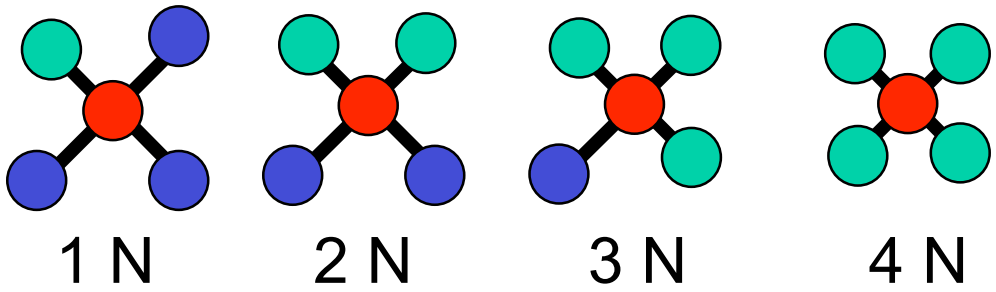
Nitrogen localized level ~ 150 meV inside conduction band

N in GaAs, GaP

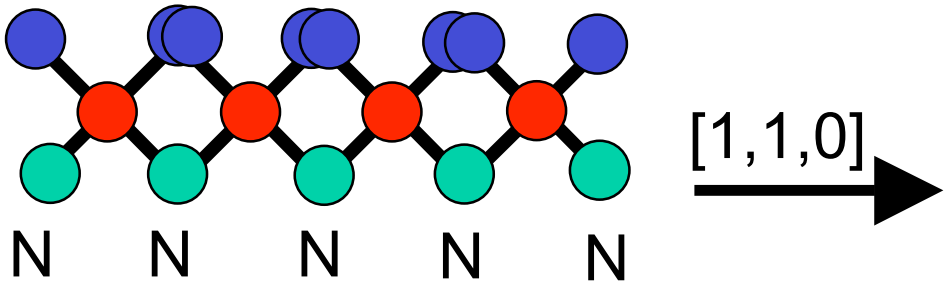
1. Isolated Nitrogen
2. **Pairs and clusters**
3. Well-developed alloys

N Clusters in GaAs, GaP

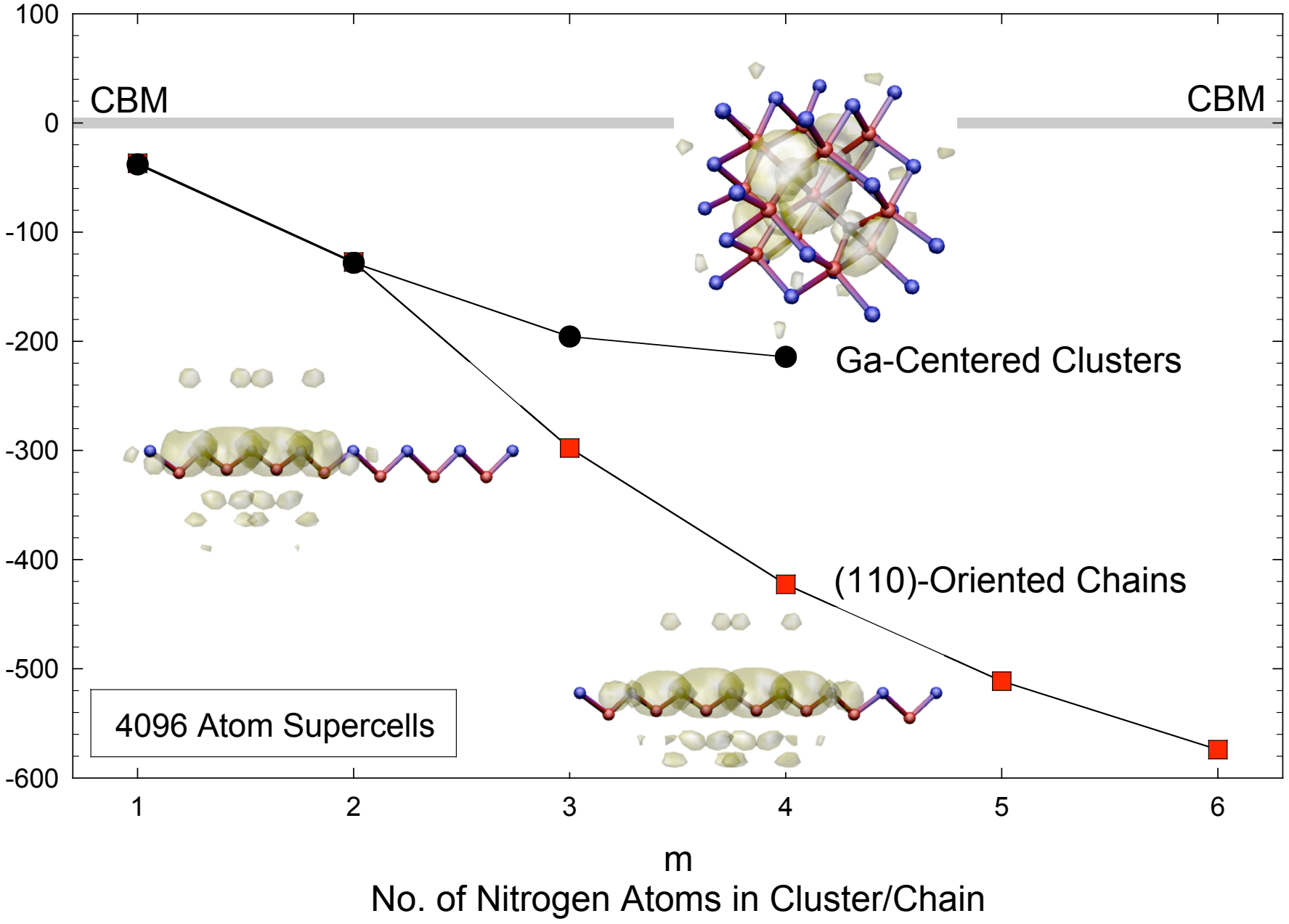
1. $Ga(P_mN_{4-m})$ Clusters



2. [1,1,0]-Oriented Nitrogen Chains

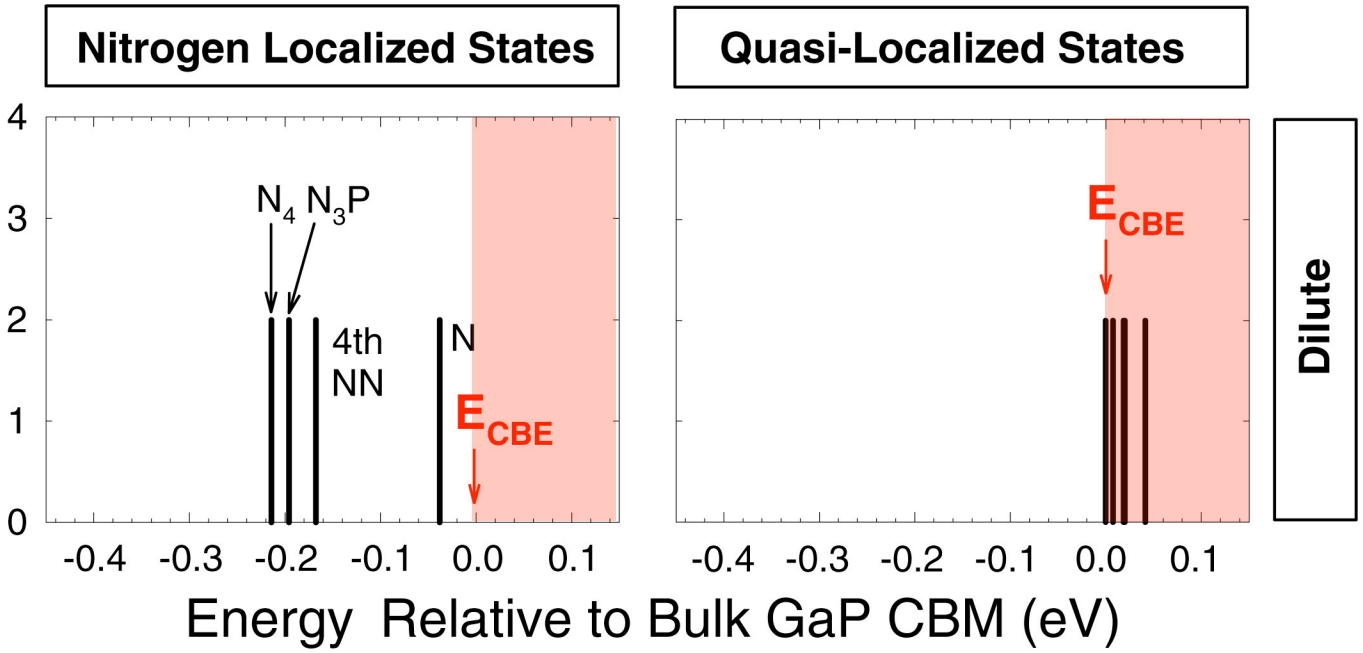


Energy levels of Clusters and Chains in GaP

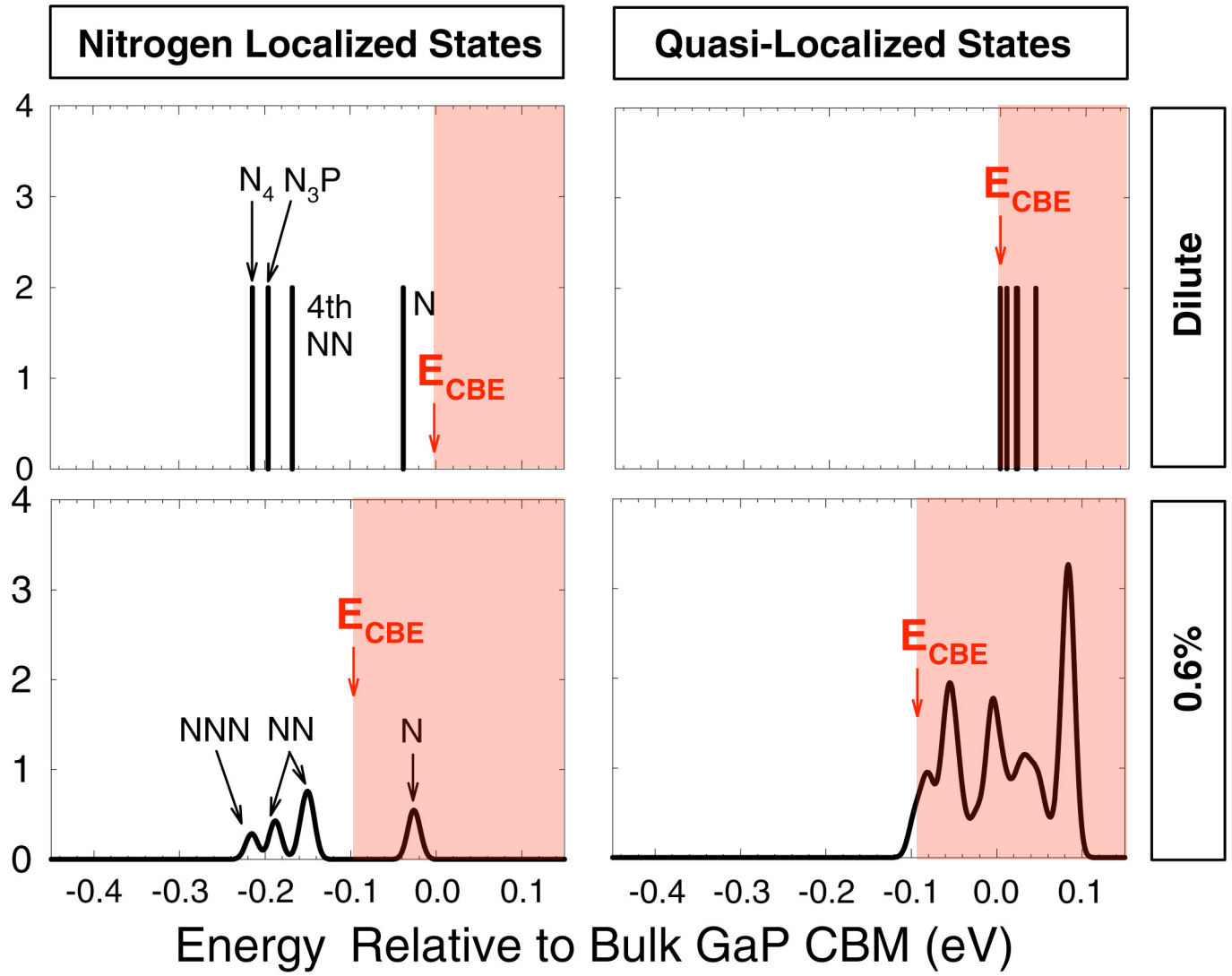


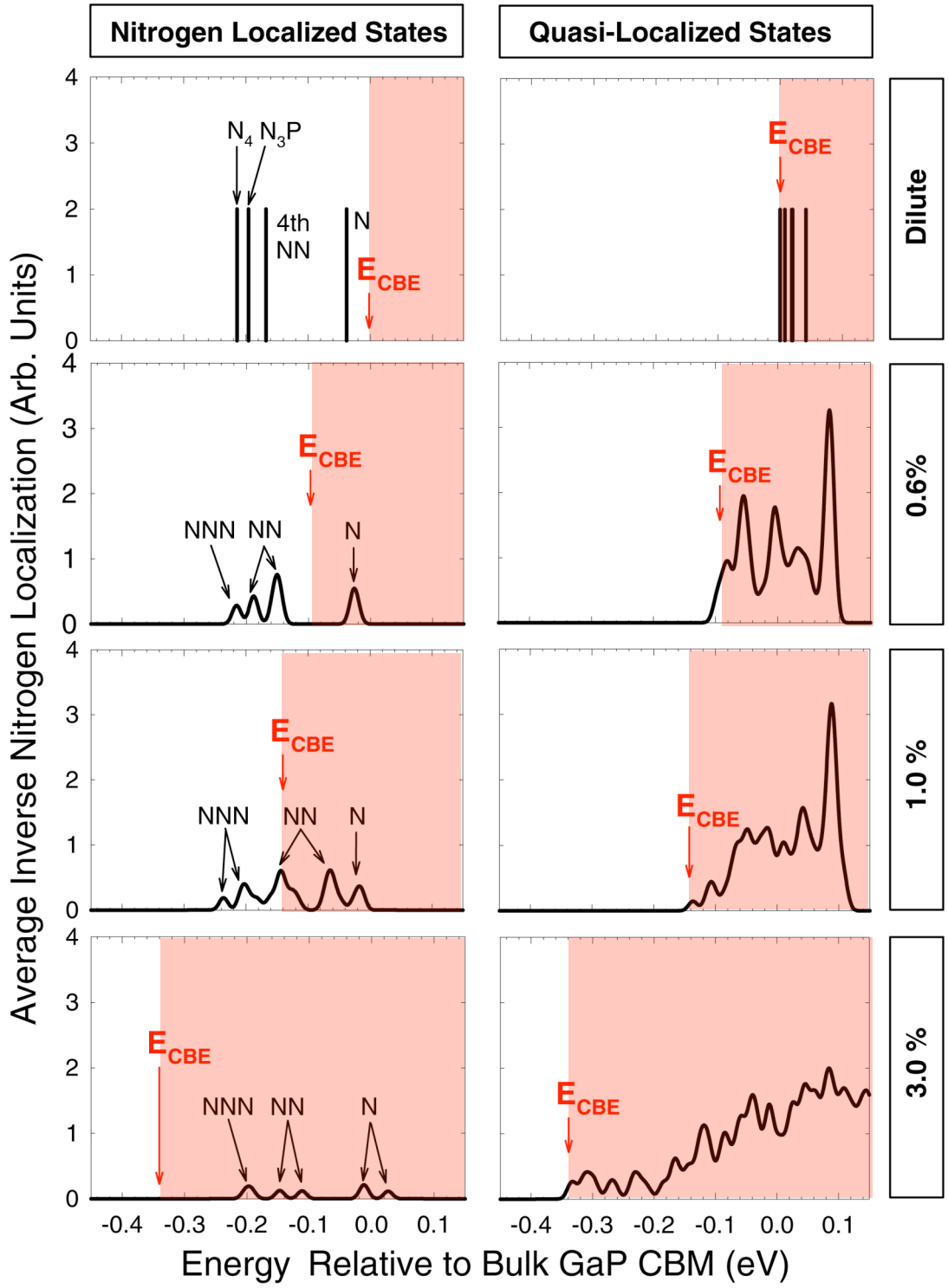
N in GaAs, GaP

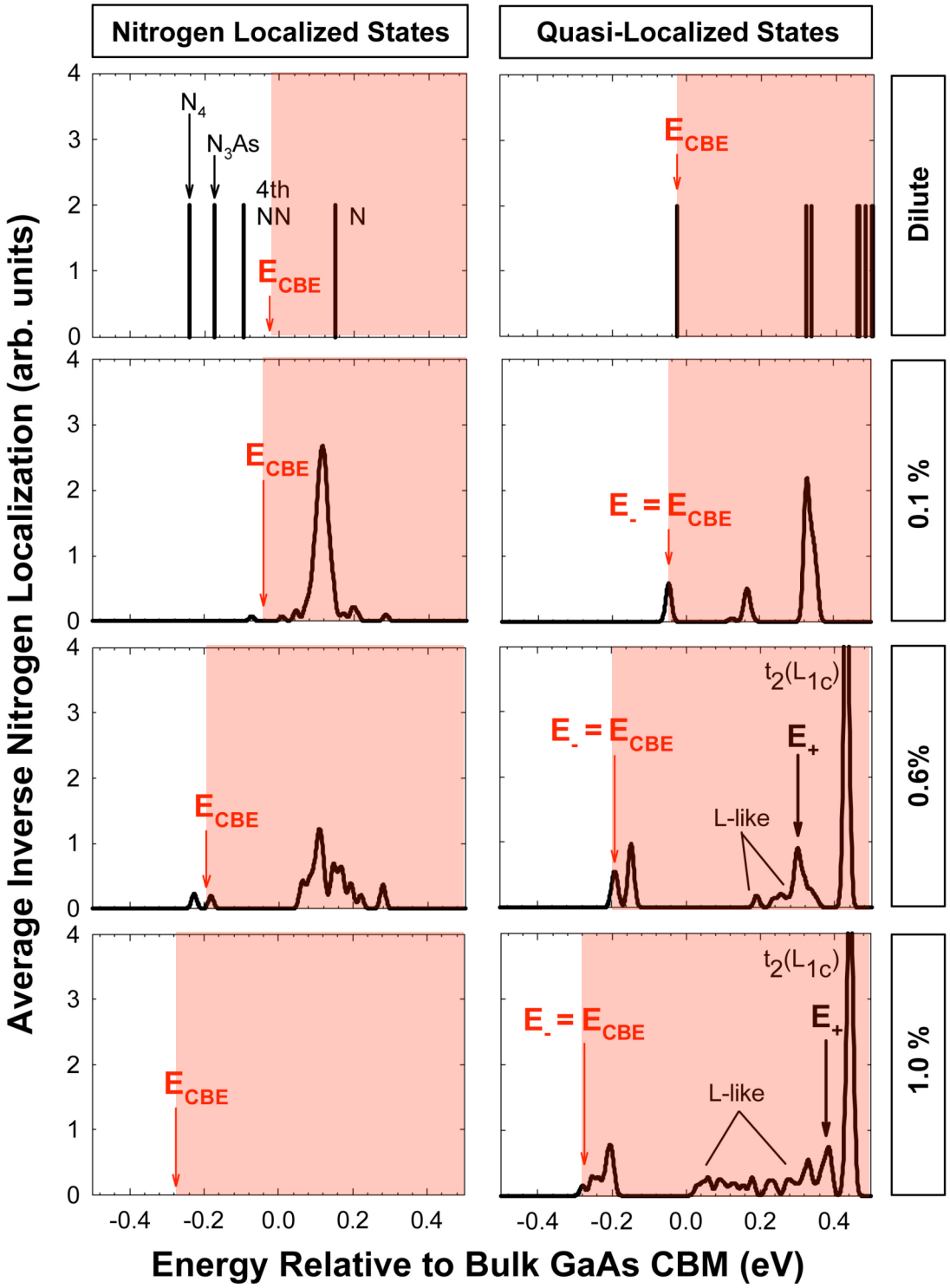
1. Isolated Nitrogen
2. Pairs and clusters
3. **Well-developed alloys**



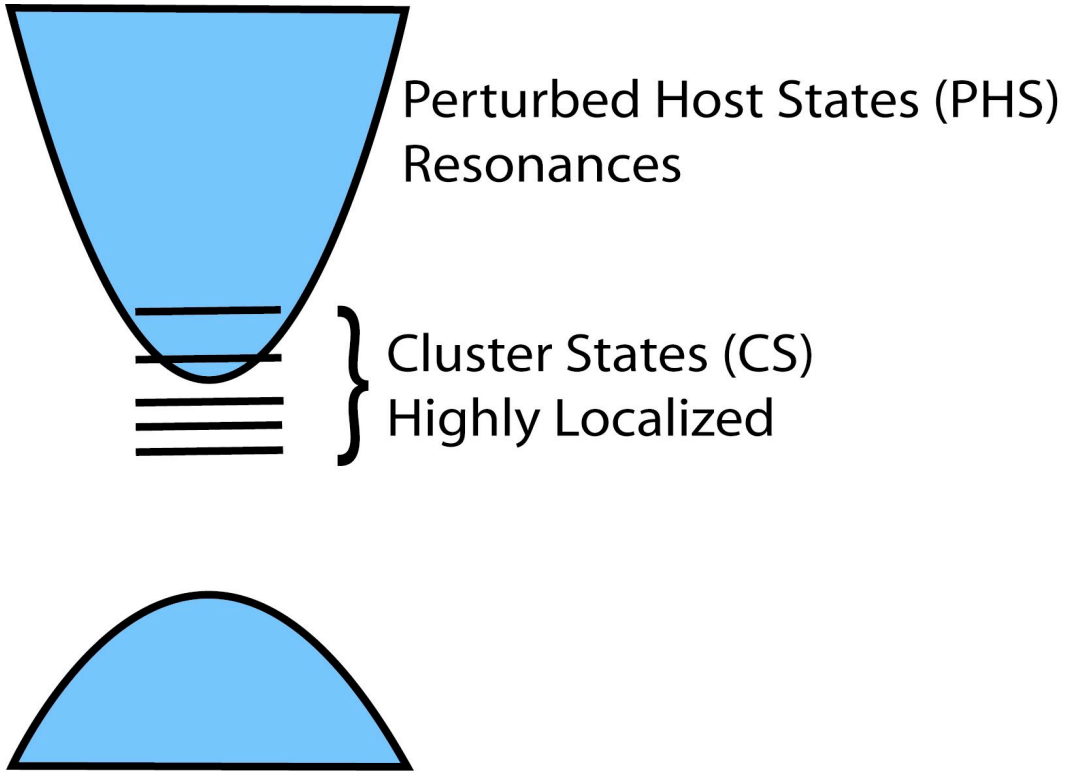
E_{CBE} = Delocalized Conduction Band Edge


Nitrogen Localized States
Quasi-Localized States
Dilute
0.6%
N4
N3P
4th NN
N
ECBE
NNN
NN
0
1
2
3
4
-0.4
-0.3
-0.2
-0.1
0.0
0.1
Energy Relative to Bulk GaP CBM (eV)


Nitrogen Localized States
Quasi-Localized States
Dilute
0.6%
1.0 %
3.0 %
N4 N3P
4th NN
N
ECBE
NNN
NN
Average Inverse Nitrogen Localization (Arb. Units)
Energy Relative to Bulk GaP CBM (eV)
0
1
2
3
4
-0.4
-0.3
-0.2
-0.1
0.0
0.1


Nitrogen Localized States
Quasi-Localized States
Dilute
0.1 %
0.6%
1.0 %
N4
N3As
4th NN
N
ECBE
E- = ECBE
E+
t2(L1c)
L-like
Average Inverse Nitrogen Localization (arb. units)
Energy Relative to Bulk GaAs CBM (eV)
0
1
2
3
4
-0.4
-0.2
0.0
0.2
0.4

Two types of state observed



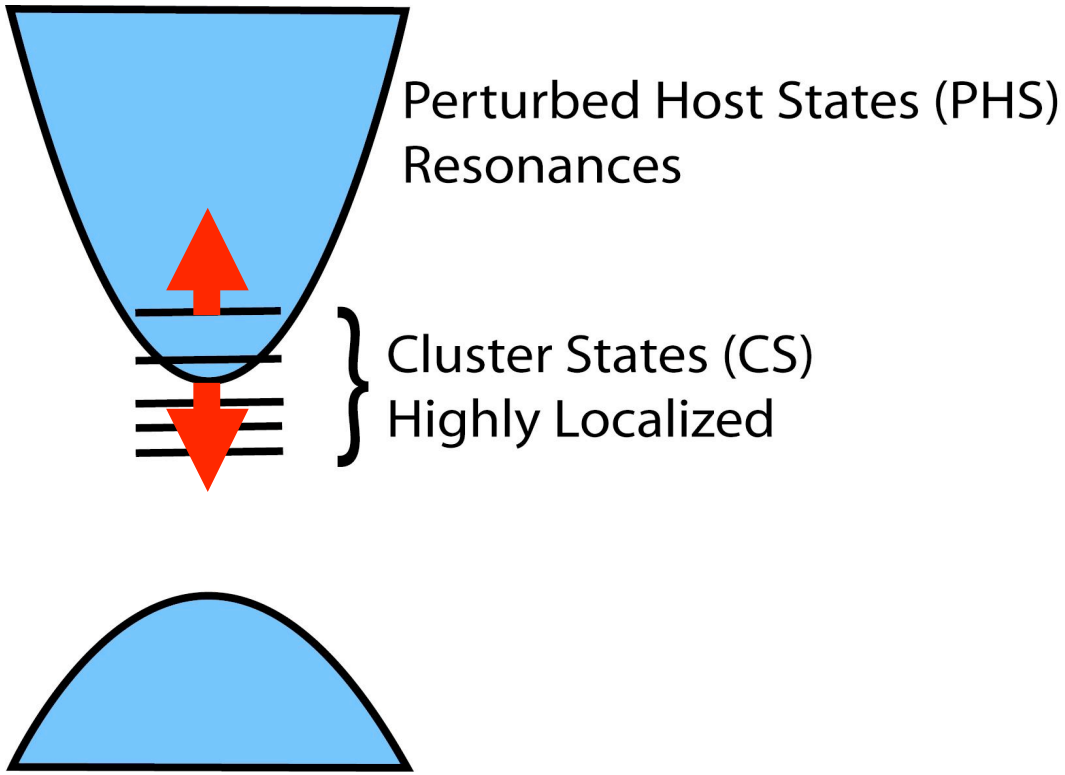
Dilute Limit: PHS in conduction band and pair/cluster CS in gap

Intermediate Range: CS do not move
PHS plunge down in energy

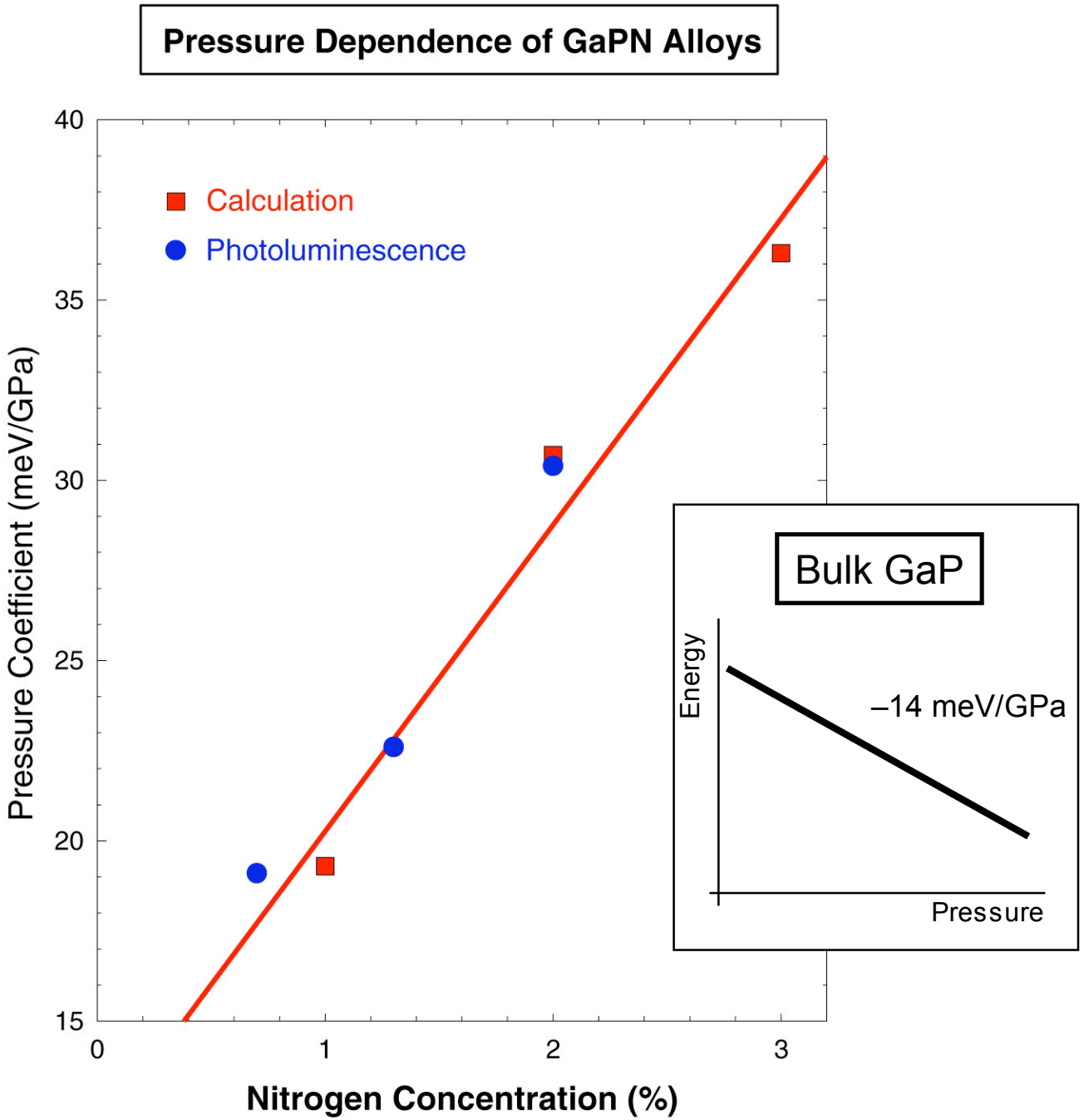
Amalgamation Point: Lowest energy PHS just below CS

Band gap reduction

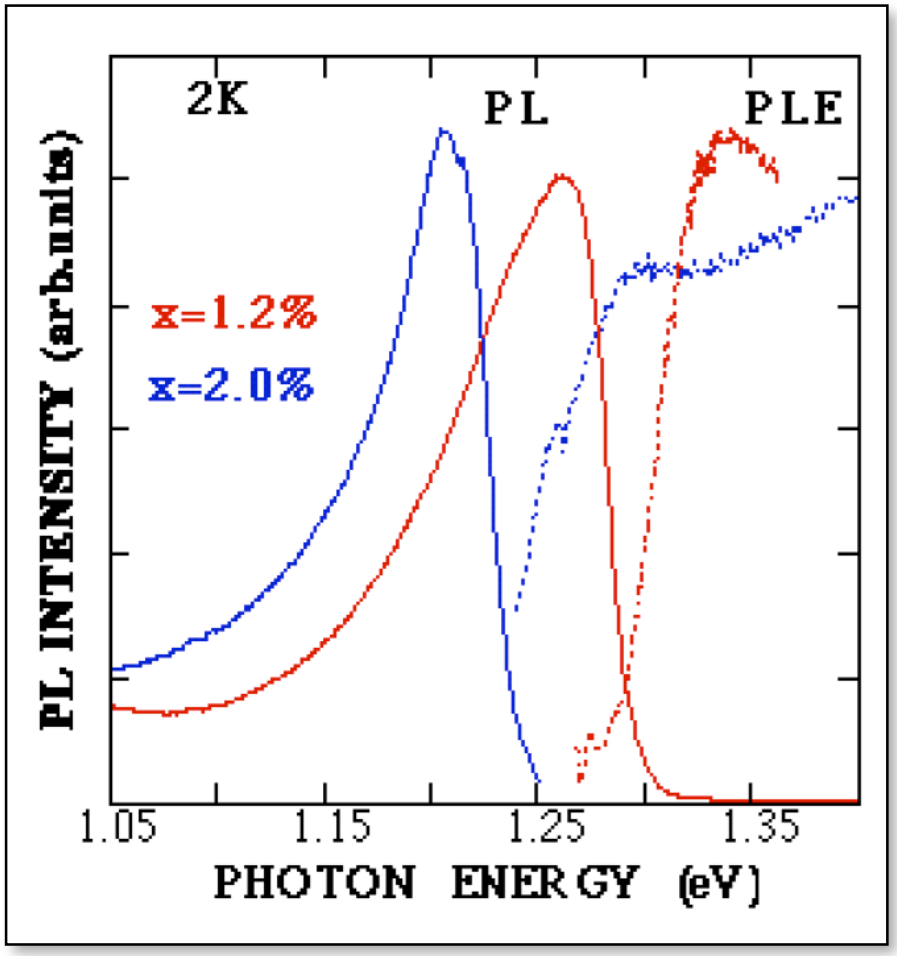
Anticrossing/repulsion between band edge and localized states drives band gap down



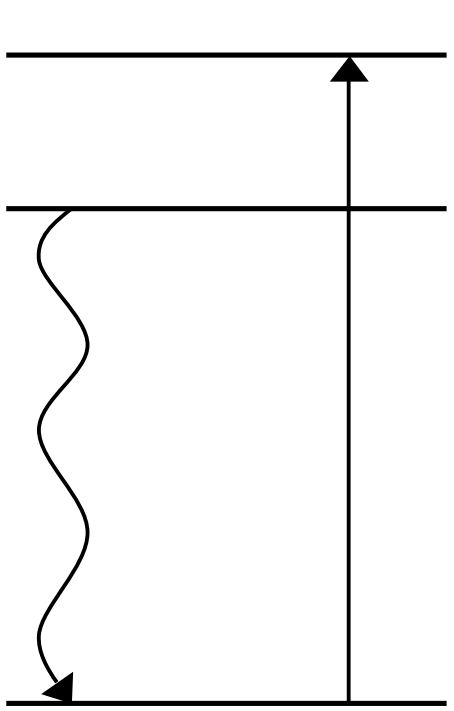
The origin of the strong repulsion is still not fully understood


Pressure Dependence of GaPN Alloys
Calculation
Photoluminescence
Pressure Coefficient (meV/GPa)
Nitrogen Concentration (%)
40
35
30
25
20
15
0
1
2
3
Bulk GaP
Energy
–14 meV/GPa
Pressure

Red Shift of PL *vs* PLE



I. A. Buyanova *et al.* MRS IJNSR **6** 2 (2001)



- Emission from localized minority states

- Absorption to majority states

Summary

1. **Nitrogen clusters create localized electronic states**
   Large band gap bowing results: a way of accessing new optical regions
2. **Applies to other III-Vs: InAsN, GaAsSbN…**
   also O in II-VIs - a general mechanism
3. **But carrier lifetimes are limited (intrinsic? extrinsic?)**

Kent & Zunger Phys. Rev. Lett. **86** 2613 (2001)

Kent & Zunger Phys. Rev. B **64** 5208 (2001)
Kent & Zunger Appl. Phys. Lett. **79** 2339(2001)

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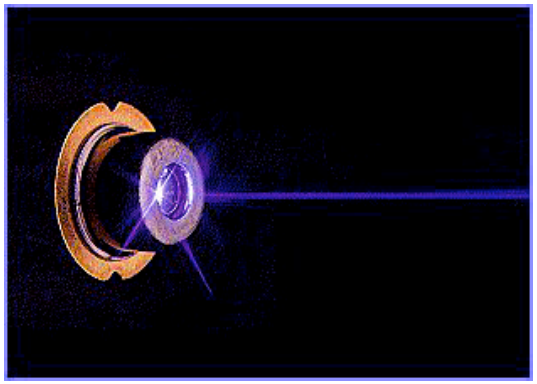
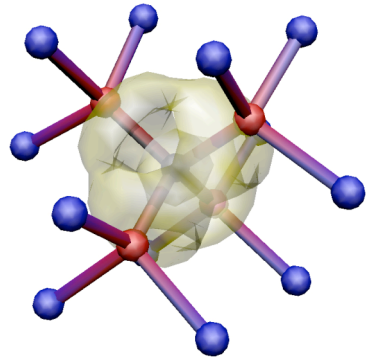
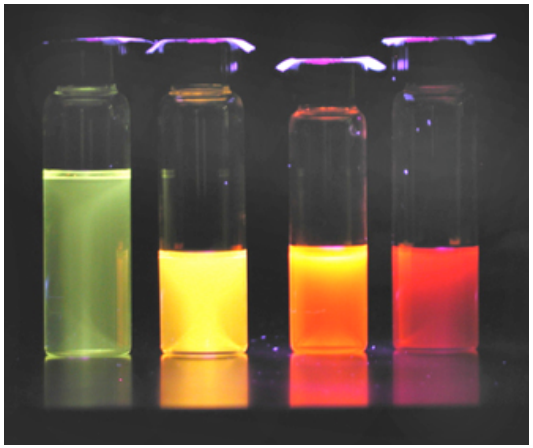
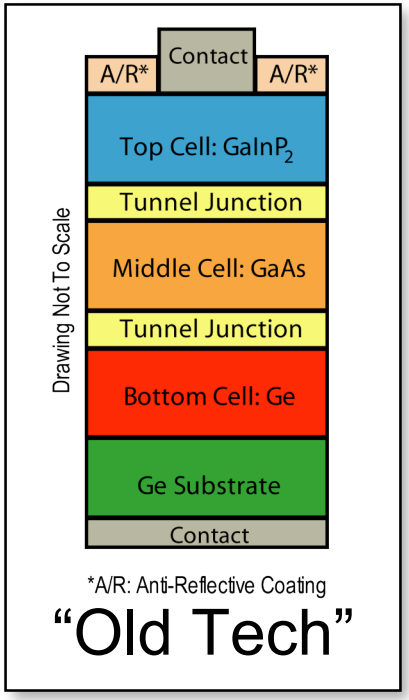


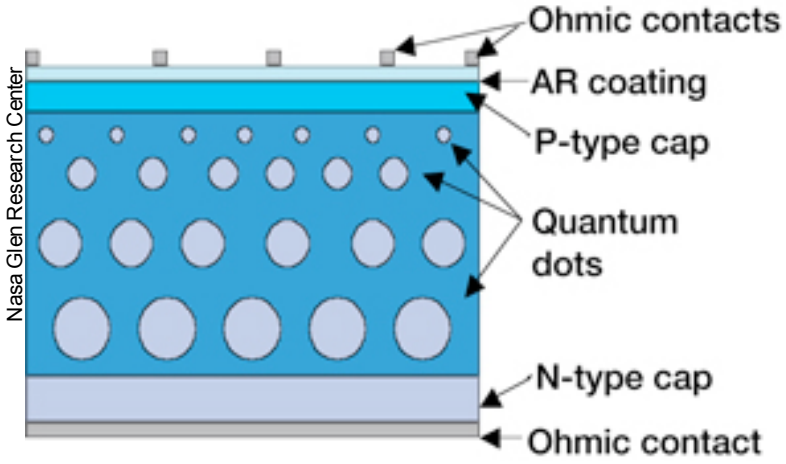




A new kind of photovoltaic cell



"Old Tech"

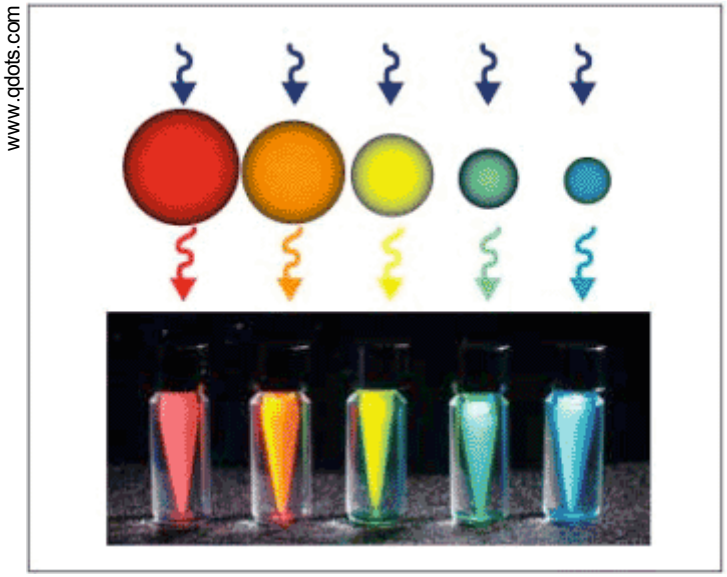


Separates absorption and transport

What to use for absorption?
Suggestion: Colloidal quantum dots (+others)

Current efficiencies are e.g. 2% (Alivisatos)
High efficiencies promised by simple theories
Many claims, press releases, companies

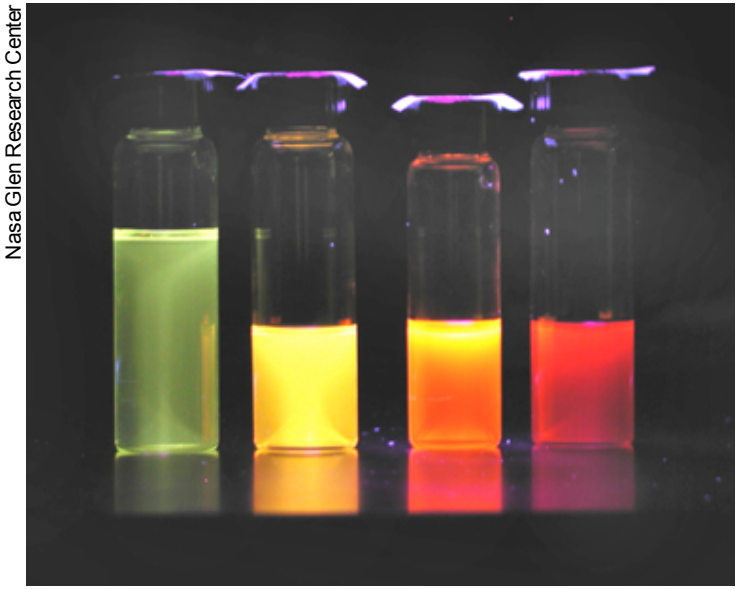
Colloidal quantum dots

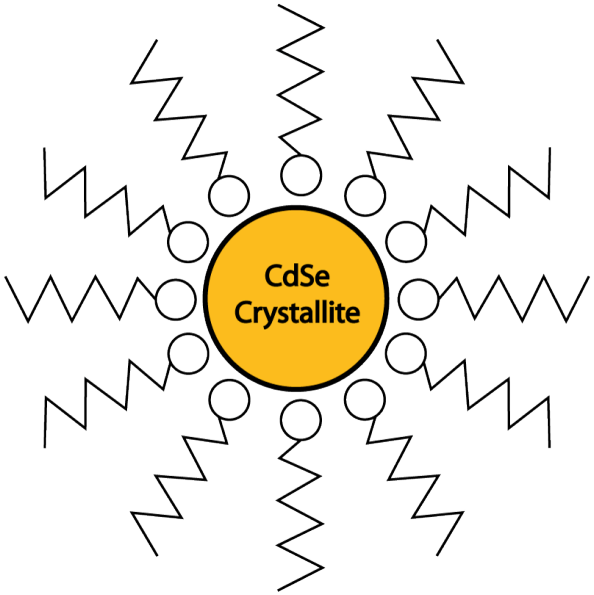


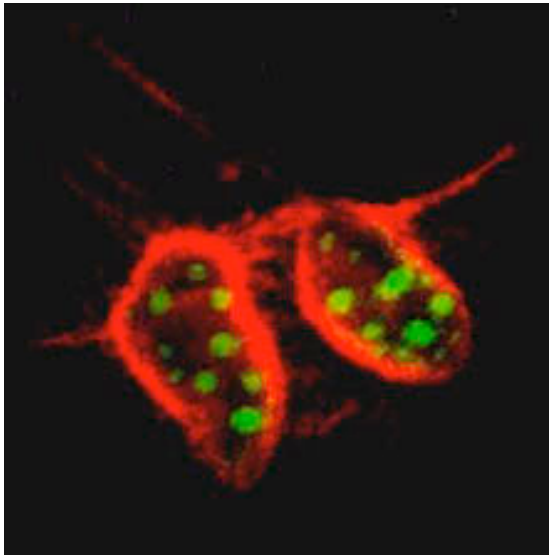
Few 1000 atoms of e.g. CdSe
Bawendi, Alivisatos, Klimov etc. late 1990s+
(Many developments in 1980s)

Exploit quantum confinement.
Continuously tunable band gap

Reasonable control over size,
shape (spheres, rods,…)

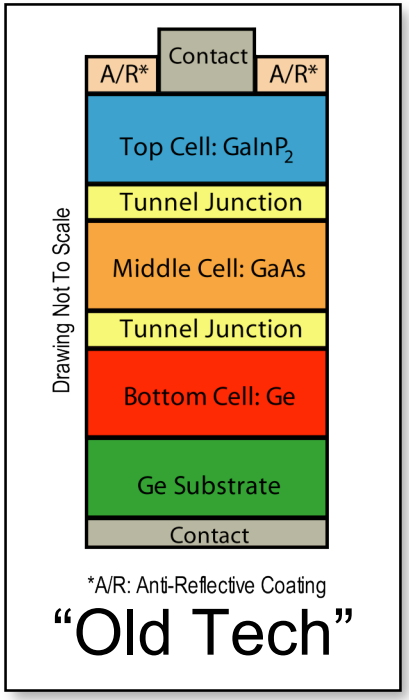




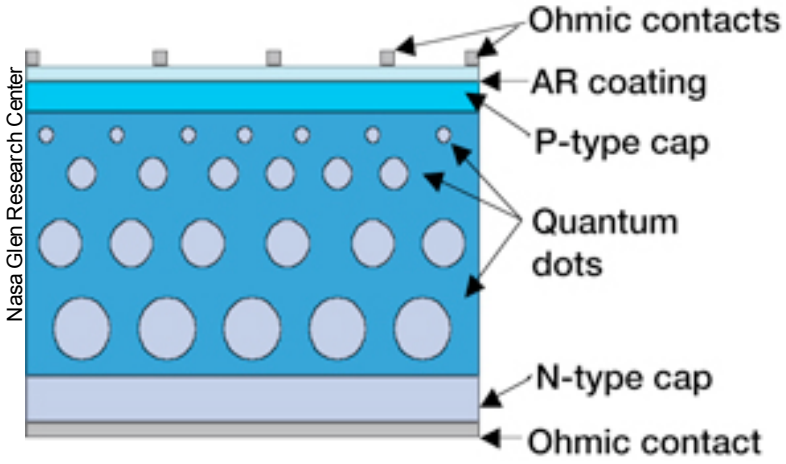


www.qdots.com

A new kind of photovoltaic cell



"Old Tech"



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“There is *plenty* of room at the bottom”

Richard Feynman

(APS meeting 1959)

“For a successful technology, reality must take precedence over public relations, for nature cannot be fooled.”

Richard Feynman
(Rogers Commission 1986)

Many questions

What is “optimal”? Realistically?

Influence of size, shape, composition on dot levels?

What is the role of the “host matrix”? Interface?

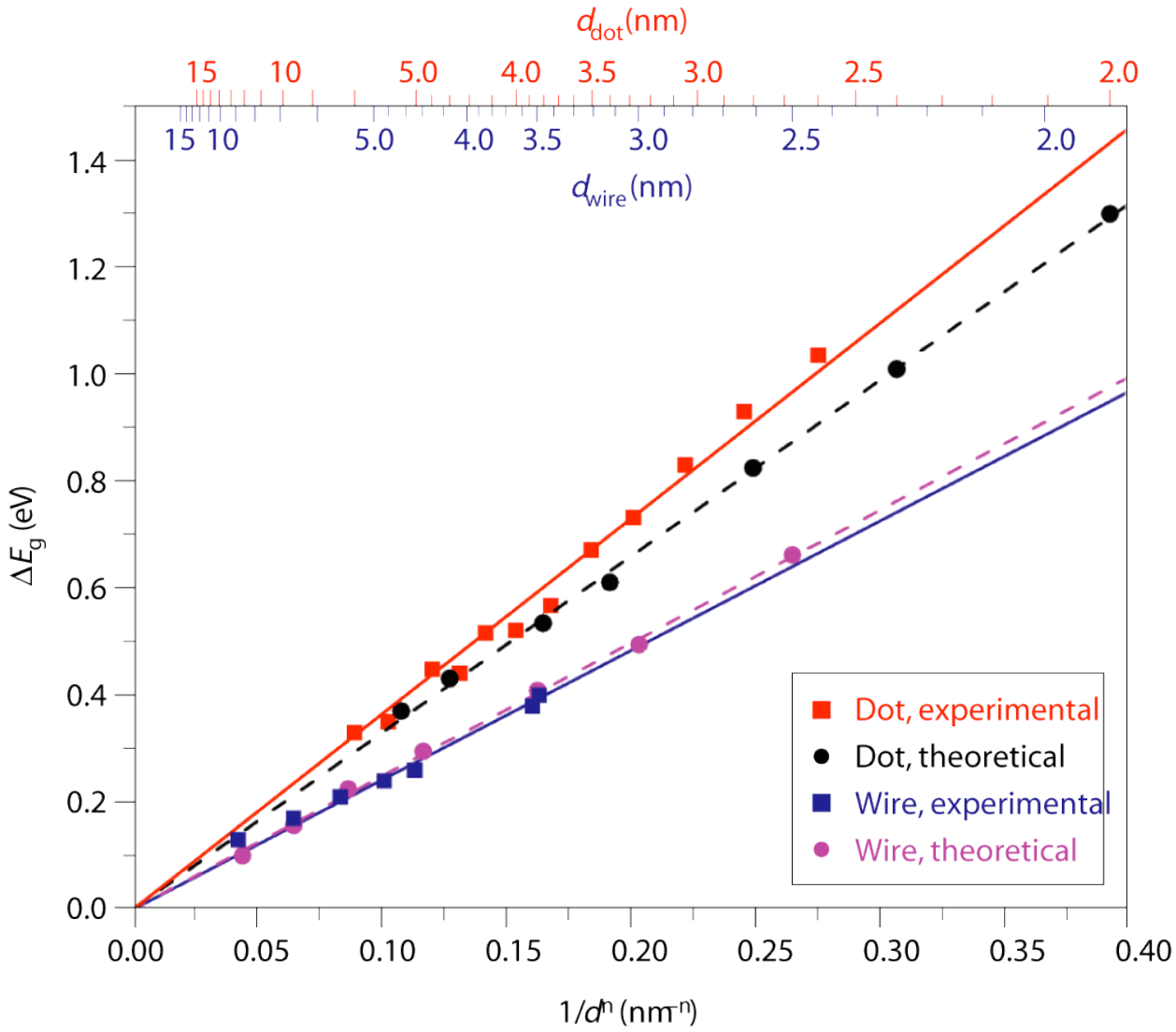
How are carriers transferred?

How are carriers “killed”?

…

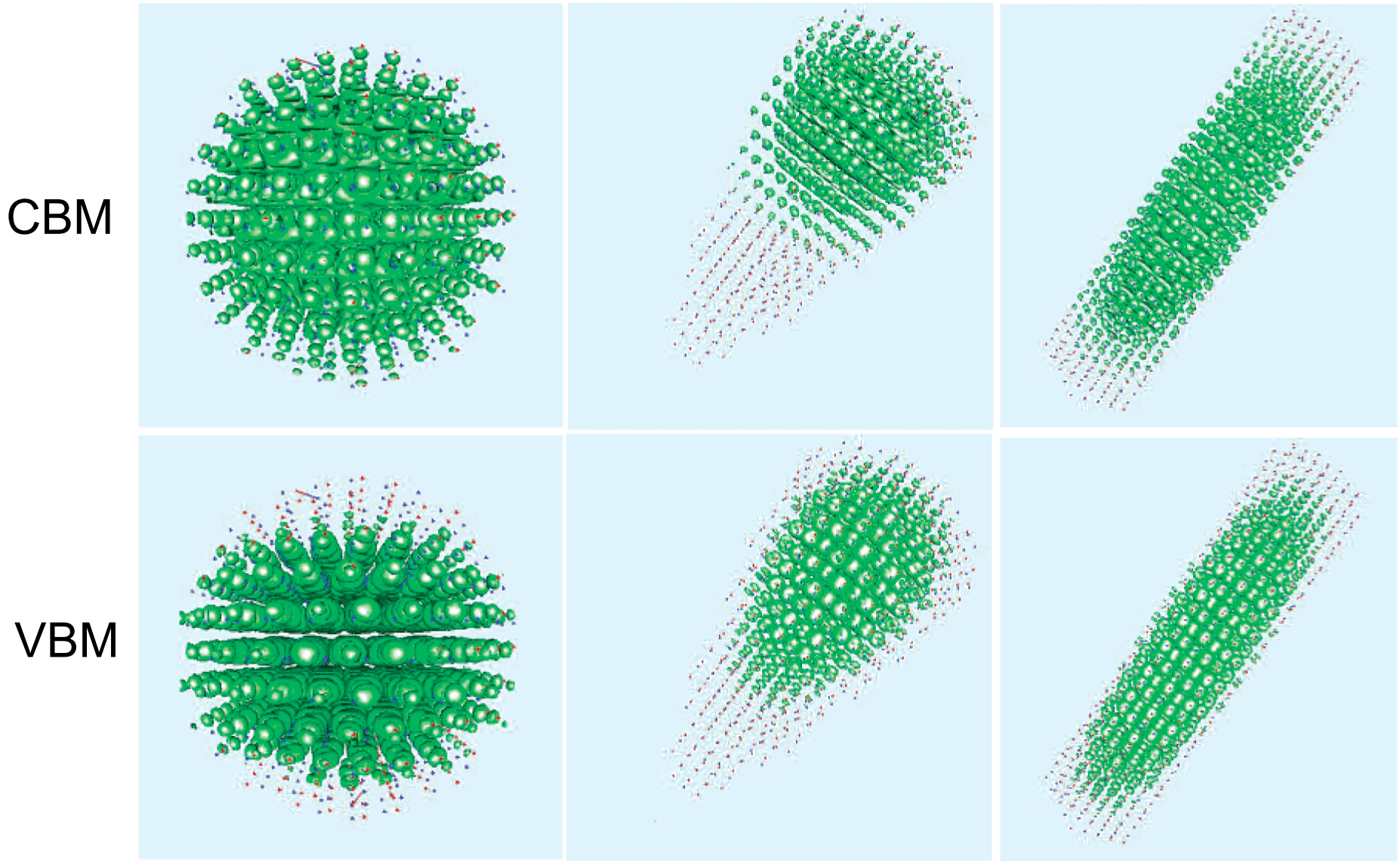
Here, focus on the third question.

Quantum confinement in InP dots, wires



Li & Wang Nature Materials **2** 517 (2003)

Shape effects



~300 meV variation in gap (and offsets) with shape

Summary

Shape strongly influences absorption energies of colloidal “dots”

Reasonable agreement with experiment for few nm sized dots

Next step -

Evaluating different hosts, interfaces. Basic transport modeling.

Conclusions

Efficiency improvements in photovoltaics are ongoing

Computational modeling is a useful tool for understanding optical properties

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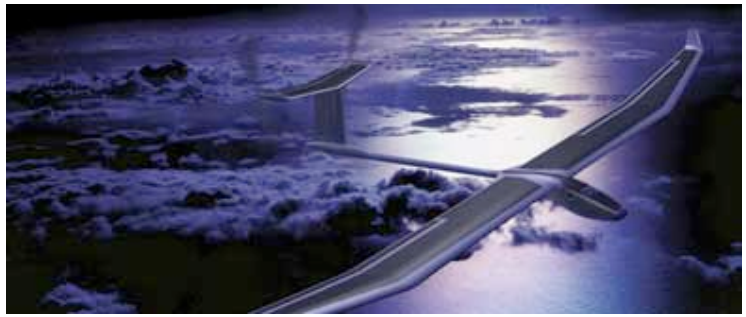

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