QUANTUM THEORY GROUP:
FROM DISCOVERY TO INNOVATION

QNANO:
COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF SEMICONDUCTOR AND GRAPHENE NANOSTRUCTURES

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QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

CONTRIBUTIONS:

M.KORKUSINSKI (IMS)- TB, CI, QNANO, ALL
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O. VOZNYY (IMS) – AB-INTIO, NCs,PV

I.OZFIDAN,P.POTASZ.D.GUCLU - GRAPHENE

W.SHENG (IMS/FUDAN) – K*P, EBOM
S.J.SHENG (IMS/NCTU) – EFF.MASS, B, CI

QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

OUTLINE:

INTRODUCTION
ATOMIC STRUCTURE DEFINITION
STRAIN
ELECTRONIC STRUCTURE CALCULATION
- **TIGHT BINDING METHOD**
- **EFFECT OF STRAIN**
- **SURFACE PASSIVATION**
- **EXTERNAL FIELDS**

MANY-BODY EFFECTS
- **MULTI-EXCITON COMPLEXES**
- **CHARGED EXCITONS**

EXAMPLES:
- **InAs/GaAs SELF-ASSEMBLED DOTS**
- **CdSe NANOCRYSTAL**

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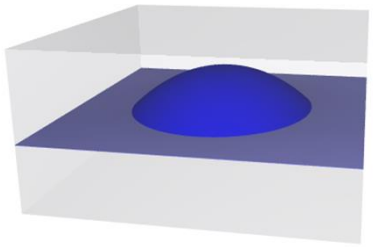
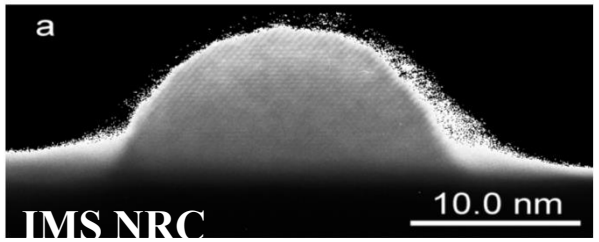
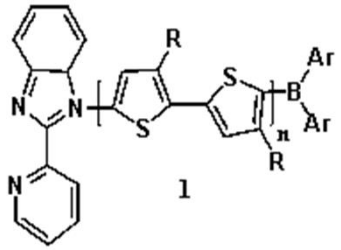
QNANO
SEMICONDUCTOR AND CARBON NANOSTRUCTURES

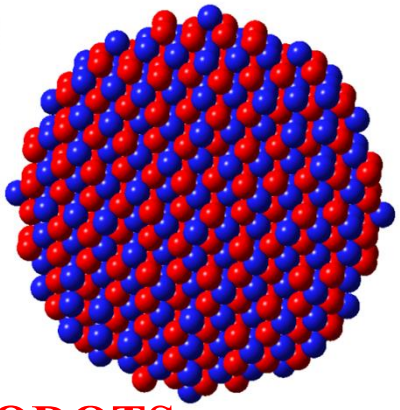
InAs/GaAs SELF-ASSEMBLED QDOTS: 2 MLN ATOMS, ~10^7 ELE.



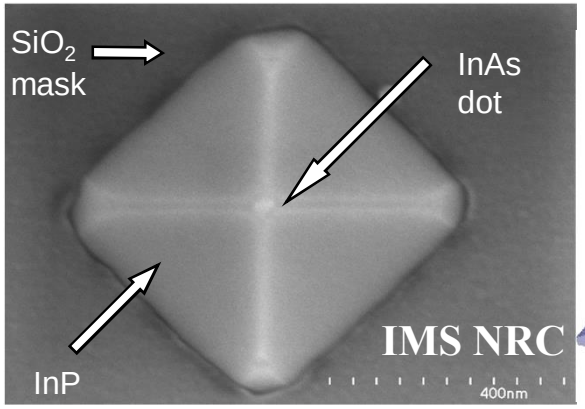


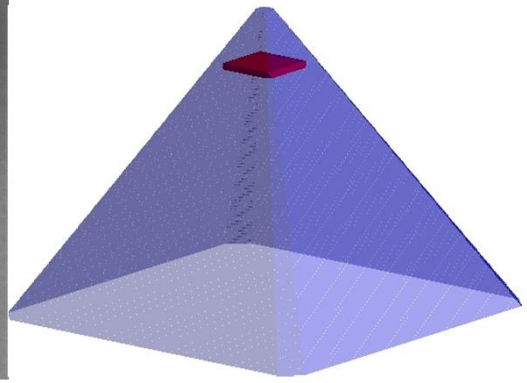
NANOCRYSTALS CdSe,PbS,.
~1000 ATOMS, ~10^4 ELE.
PLUS LIGANDS



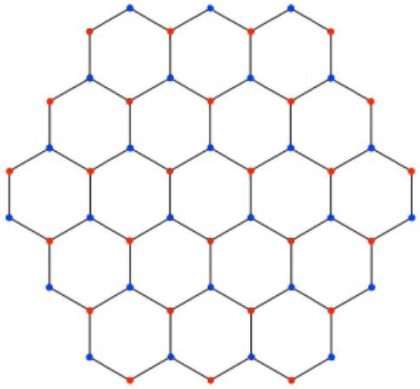


InAs/InP QDOTS ON PATTERNED SUBSTRATES: 10 MLN ATOMS, ~10^8 ELE.





GRAPHENE QDOTS: 100nm*100nm, ~10^6 ELE.



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ATOMISTIC THEORY OF QDOTS

NO EXACT SOLUTION TO THIS MANY BODY PROBLEM EXISTS

NO AB-INITIO APPROXIMATE SOLUTION EXISTS

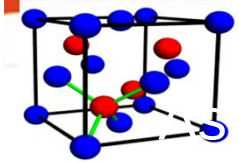
APPROXIMATE METHODS:

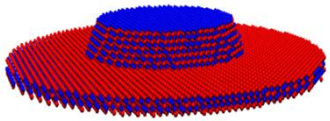
TIGHT BINDING APPROACH
Bryant et al.
Klimeck et al.
Whaley et al.
……

TB-DFT APPROACH
Frauenheim et al.

PSEUDOPOTENTIAL APPROACH
Zunger et al.

QNANO:ATOMISTIC THEORY OF QDOTS





QNANO M.Korkusinski, M.Zielinski, PH

Multi-scale

Model structure → atomistic strain → m* / k*p / Atomistic EBOM / Atomistic Tight Binding sp3d5,… → CI / CI+HF / DFT / DFT+CI → High Excitation PL / Single photon gun / Solar cells

Shape, composition ~ 10^9 atoms → Mechanical ~ 10^9 atoms → Electronic ~10^6 atoms → Optical ~ 10 quasipaticles

M.Zielinski,M.Korkusinski,PH,JAPL2009,PRB2010

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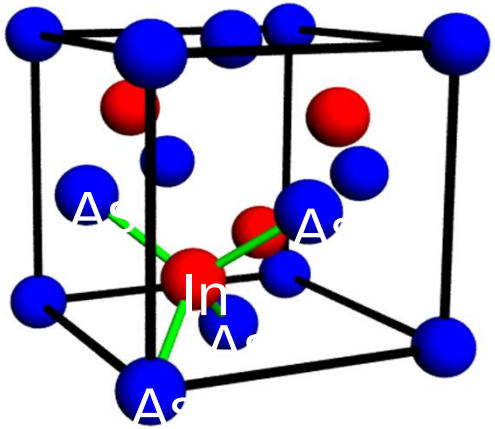
QNANO-ATOMISTIC THEORY OF QDOTS

QNANO:

- **MATERIALS:InAs,GaAs,InP,CdSe,PbSe,C,ZnTe,…)**
- **BULK ELECTRONIC STRUCTURE**
- **MILLION ATOM QDOTS**
- **SPECIFIC CRYSTAL LATTICES**
- **INTERFACES**
- **STRAIN – MULTIPLE SCALES**
- **SPIN ORBIT COUPLING**
- **ATOMISTIC DISORDER**
- **EXCITON FINE STRUCTURE**
- **POLARIZATION OF LIGHT**
- **MULTI-EXCITON COMPLEXES**
- **MAGNETIC FIELD**
- **MAGNETIC IMPURITIES**
- **……**



OTHER WORK: tb:BRYANT,KLIMECK,…..,
pseudopotential: ZUNGER,…

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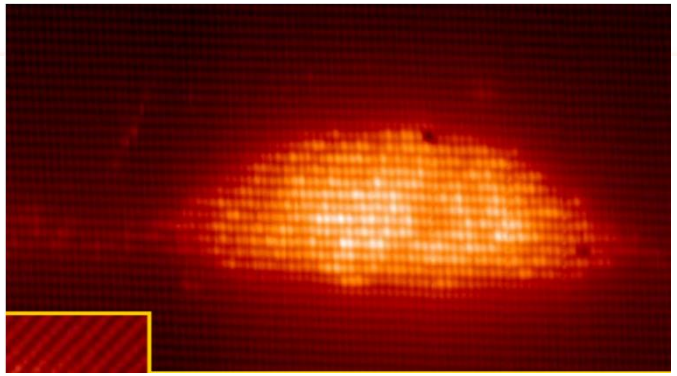
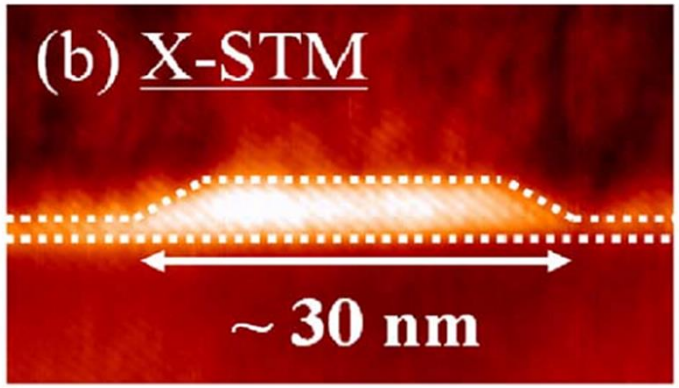
REFERENCES

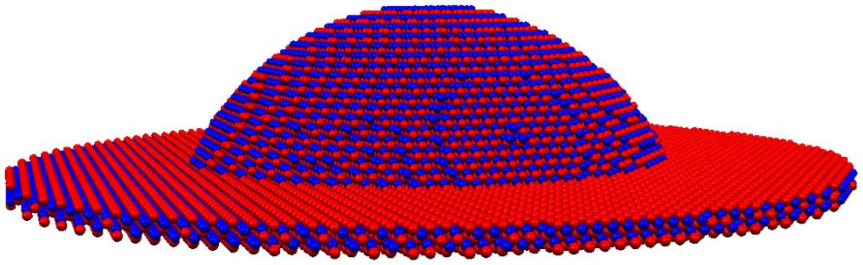
QNANO: BUILDING QUANTUM DOT WITH ATOMS

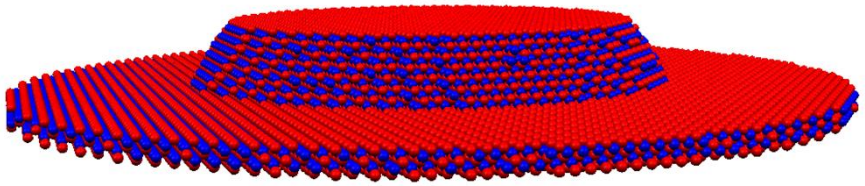
P. Koenraadôs group X-STM



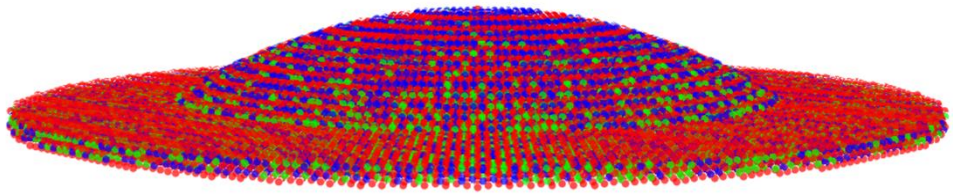


P. Koenraadôs group X-STM





Alloy (vertical gradient)



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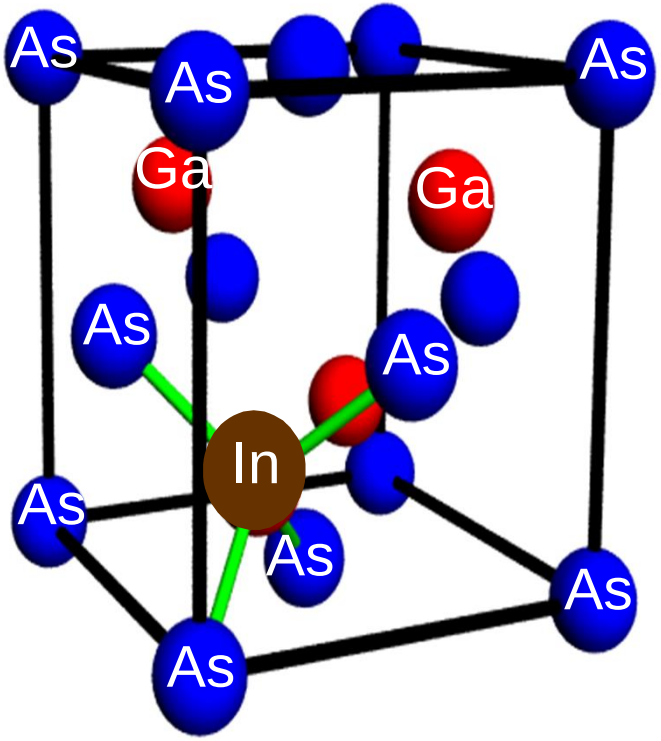
QNANO: BUILDING QUANTUM DOT WITH ATOMS

Zinc blend lattice



Build GaAs layer

Replace Ga with In
Put InAs
On GaAs
Lattice

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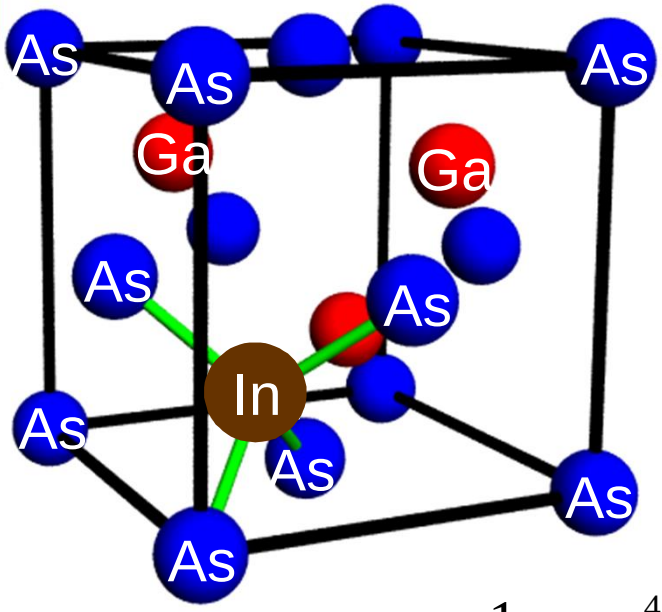
QNANO: ATOMISTIC CALCULATION OF STRAIN



MINIMIZE TOTAL ELASTIC ENERGY
FIND POSITION OF ATOMS

$$E_{TOT} = E_{TOT}(\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3, \ldots\ldots, \mathbf{R}_N)$$

VALENCE FORCE FIELD:

$$E_{TOT} = \frac{1}{2}\sum_{i}\sum_{j=1}^{4} A_{ij}\left(\left(\mathbf{R}_i - \mathbf{R}_j\right)^2 - \left(d_{ij}^0\right)^2\right)^2$$

$$+\sum_{i}\sum_{j=1}^{3}\sum_{k=j+1}^{4} B_{ijk}\left(\left(\mathbf{R}_j - \mathbf{R}_i\right)\left(\mathbf{R}_k - \mathbf{R}_i\right) - \cos\theta d_{ij}^0 d_{ik}^0\right)^2$$

10^8 atoms = 300.000.000 variables

OPTIMAL DISPLACEMENT FIELD FOUND WITH CONJUGATED-GRADIENT METHOD (P. Keating, A. Zunger, C. Pryor,…)

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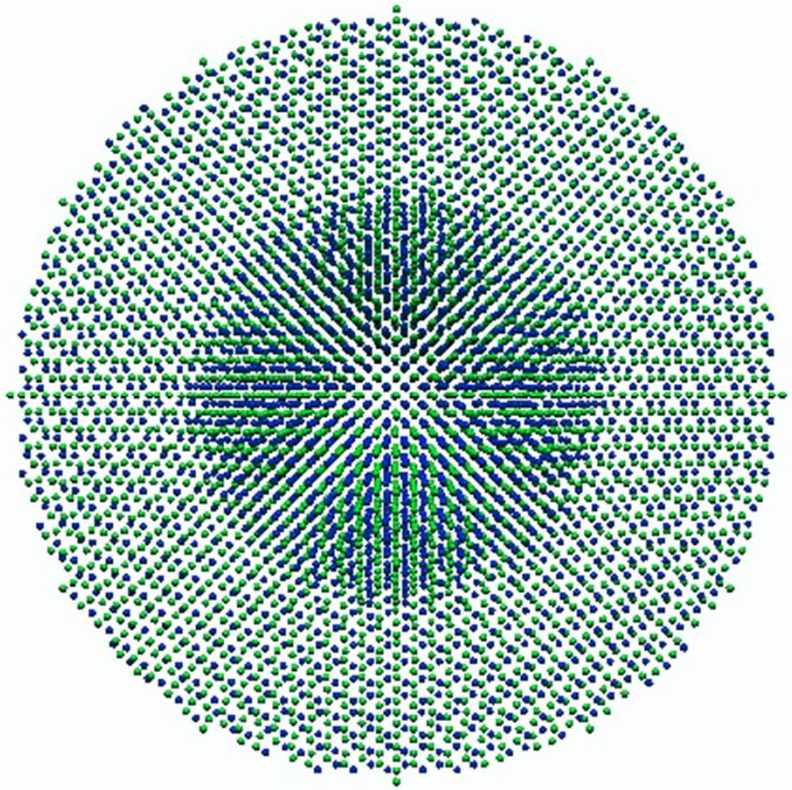
QNANO: ATOMISTIC CALCULATION OF STRAIN

In – blue, As - green



M.Zielinski

STRAIN RELAXED STRUCTURE

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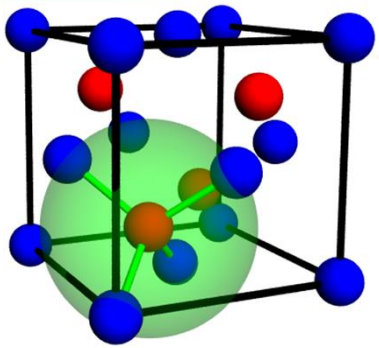
TIGHT BINDING APPROACH



Quasi-electron

$$\left[-\nabla^2/2 + V_{ion}(r) + V_{Hartree}(r) + \Sigma(r, E_l)\right]\varphi_l(r) = E_l\varphi_l(r)$$

LCAO APPROACH

$$\varphi_l(r) = \sum_{R=1}^{N}\sum_{\alpha=1}^{20}\phi_{l,\alpha}(R)u_\alpha(r-R)$$

Sp3d5s*
Slater-Koster
orbitals

We don't really know electronic density
nor V_h and V_{xc} ! Parametrize matrix elements

$$< u_b(R') \mid H \mid u_\alpha(R) >$$

Tight binding Hamiltonian

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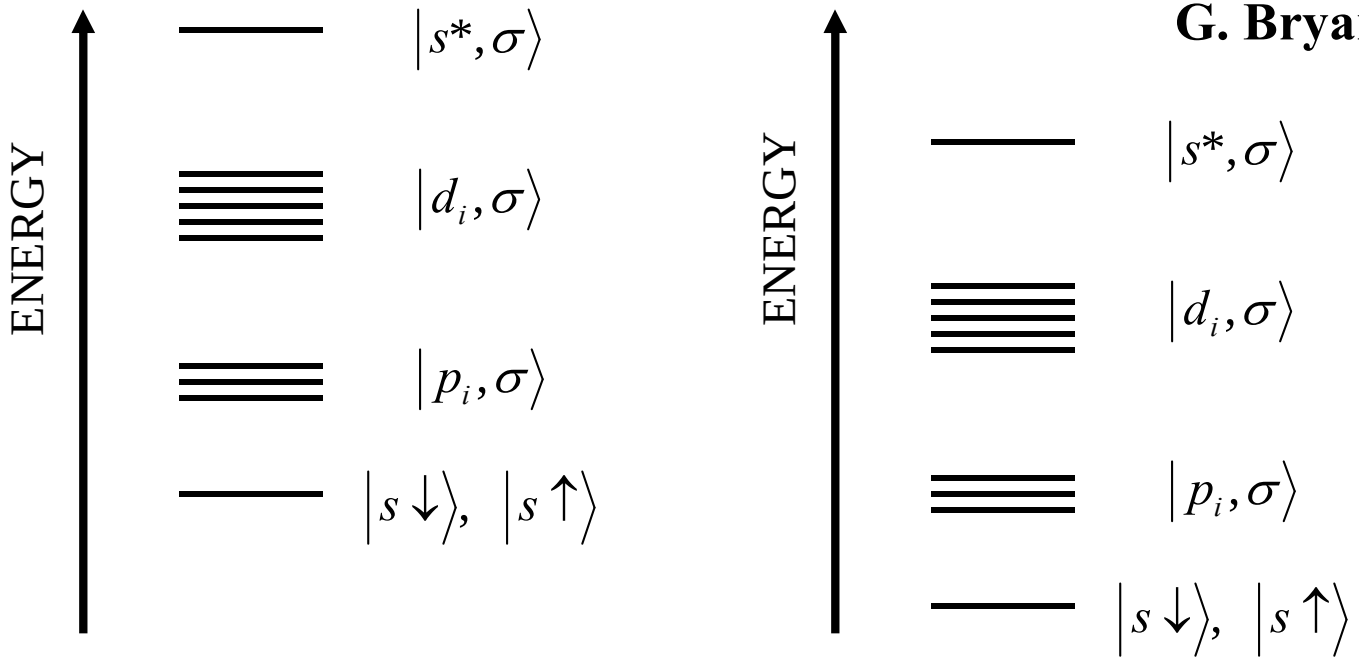
ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING APPROACH - ORBITALS

In CORES FROZEN As

J. Slater and G. Koster,
G. Klimeck,
T. Boykin,
G. Bryant



BASIS ORBITALS
FOR THE VALENCE ELECTRON

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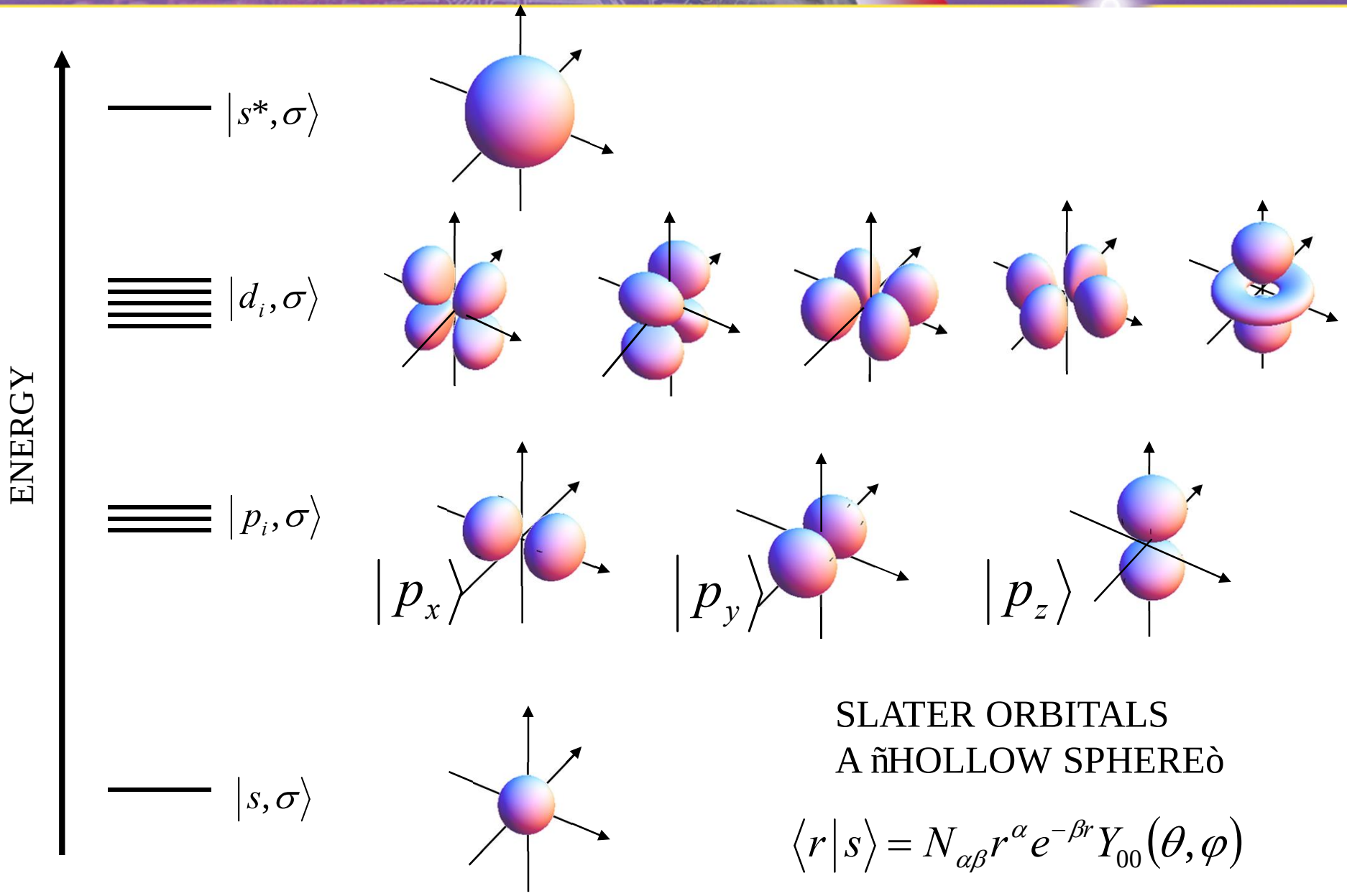
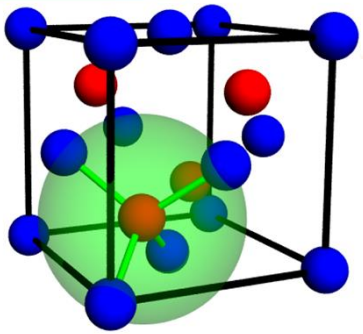
ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING APPROACH - ORBITALS



SLATER ORBITALS
A ñHOLLOW SPHEREò

$$\langle r|s\rangle = N_{\alpha\beta} r^{\alpha} e^{-\beta r} Y_{00}(\theta,\varphi)$$

ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING HAMILTONIAN



$$< u_b(R') \mid H \mid u_\alpha(R) >$$

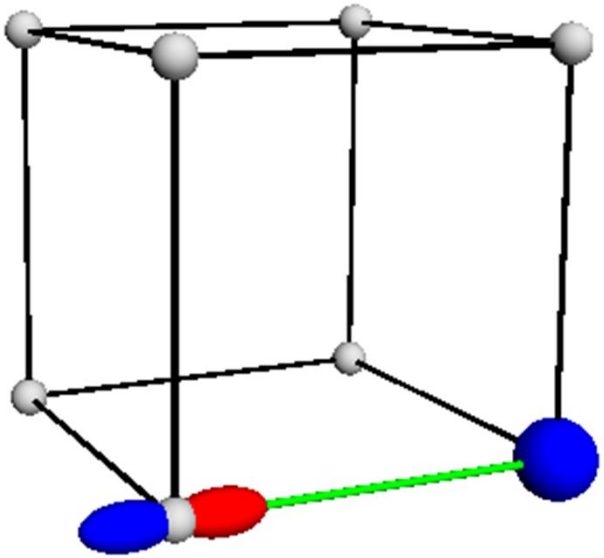
$$\hat{H} = \sum_{atoms\,R} \sum_{\substack{\alpha=1 \\ bands}}^{20} \varepsilon_{R\alpha} c^{+}_{R\alpha} c_{R\alpha} + \sum_{atoms\,R} \sum_{\substack{\alpha=1 \\ bands}}^{20} \sum_{\substack{\alpha' \neq \alpha \\ bands}}^{20} \lambda^{SO}_{R\alpha\alpha'} c^{+}_{R\alpha} c_{R\alpha'}$$

$$+ \sum_{atoms\,R} \sum_{atoms\,R'=1}^{4nn} \sum_{\substack{\alpha=1 \\ bands}}^{20} \sum_{\substack{\alpha'=1 \\ bands}}^{20} t_{R\alpha,R'\alpha'} c^{+}_{R\alpha} c_{R'\alpha'}$$

TIGHT-BINDING PARAMETRIZATION
WITH 1st NEAREST NEIGHBORS

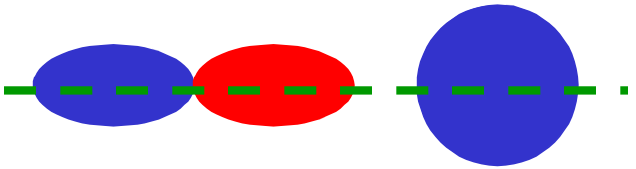
PROBLEM:
100 PARAMETERS!

ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING MATRIX ELEMENTS

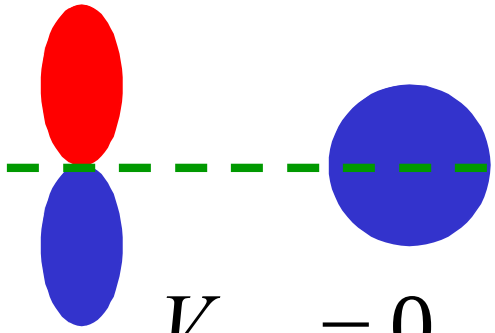


$$t_{i,j} \approx V_{sa,pc\sigma}$$

CASE OF SIMPLE CUBIC LATTICE



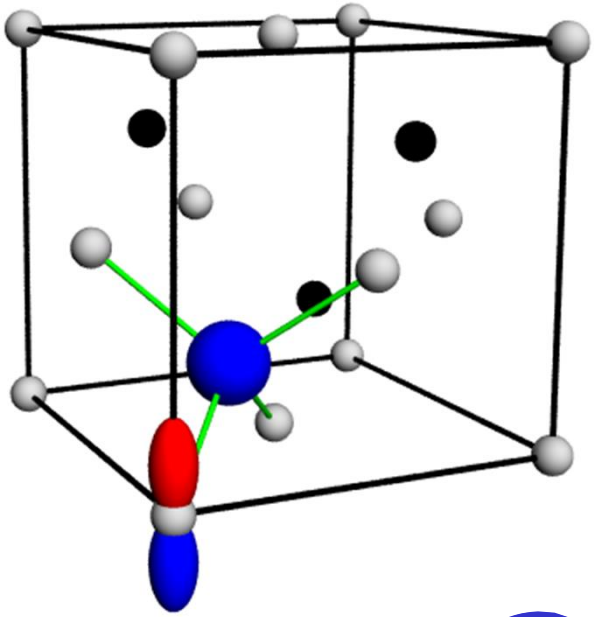
$$V_{sp\sigma} \neq 0$$

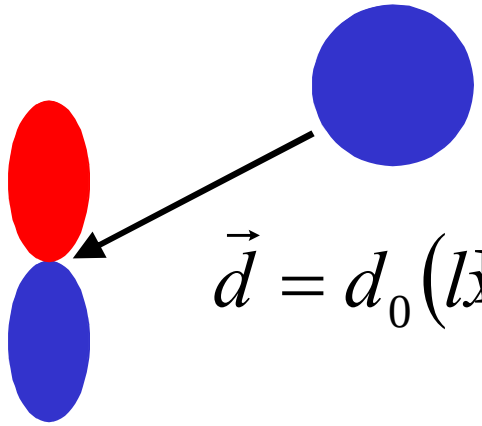


$$V_{sp\pi} = 0$$

ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING MATRIX ELEMENTS

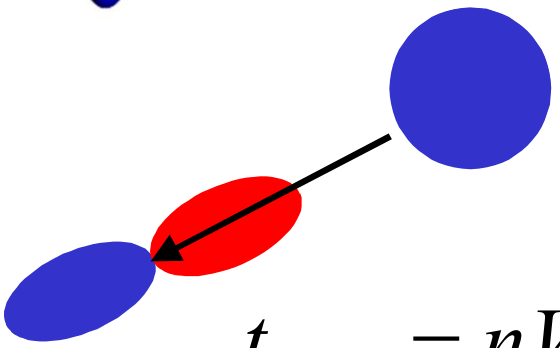
ZINCBLENDE LATTICE: TETRAHEDRAL COORDINATION



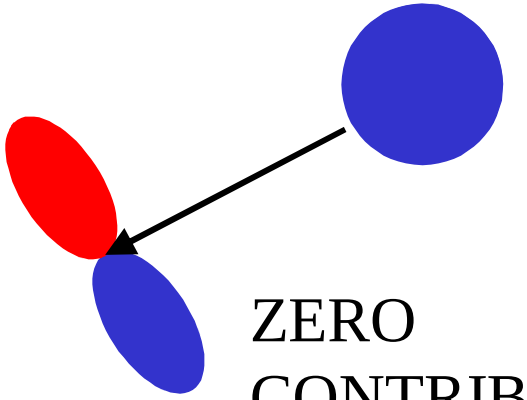


$$\vec{d} = d_0\left(l\check{E} + m\check{E} + n\check{E}\right)$$

DECOMPOSE ORBITALS:



$$t_{sa,zc} = nV_{sa,pc\sigma}$$



ZERO CONTRIBUTION

ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING MATRIX ELEMENTS

TABLE I. Energy integrals for crystal in terms of two-center integrals.

$E_{s,s}$	$(ss\sigma)$
$E_{s,x}$	$l(sp\sigma)$
$E_{x,x}$	$l^2(pp\sigma)+(1-l^2)(pp\pi)$
$E_{x,y}$	$lm(pp\sigma)-lm(pp\pi)$
$E_{x,z}$	$ln(pp\sigma)-ln(pp\pi)$
$E_{s,xy}$	$\sqrt{3}lm(sd\sigma)$
E_{s,x^2-y^2}	$\frac{1}{2}\sqrt{3}(l^2-m^2)(sd\sigma)$
$E_{s,3z^2-r^2}$	$[n^2-\frac{1}{2}(l^2+m^2)](sd\sigma)$
$E_{x,xy}$	$\sqrt{3}l^2m(pd\sigma)+m(1-2l^2)(pd\pi)$
$E_{x,yz}$	$\sqrt{3}lmn(pd\sigma)-2lmn(pd\pi)$
$E_{x,zx}$	$\sqrt{3}l^2n(pd\sigma)+n(1-2l^2)(pd\pi)$
E_{x,x^2-y^2}	$\frac{1}{2}\sqrt{3}l(l^2-m^2)(pd\sigma)+l(1-l^2+m^2)(pd\pi)$
E_{y,x^2-y^2}	$\frac{1}{2}\sqrt{3}m(l^2-m^2)(pd\sigma)-m(1+l^2-m^2)(pd\pi)$
E_{z,x^2-y^2}	$\frac{1}{2}\sqrt{3}n(l^2-m^2)(pd\sigma)-n(l^2-m^2)(pd\pi)$
$E_{x,3z^2-r^2}$	$l[n^2-\frac{1}{2}(l^2+m^2)](pd\sigma)-\sqrt{3}ln^2(pd\pi)$
$E_{y,3z^2-r^2}$	$m[n^2-\frac{1}{2}(l^2+m^2)](pd\sigma)-\sqrt{3}mn^2(pd\pi)$
$E_{z,3z^2-r^2}$	$n[n^2-\frac{1}{2}(l^2+m^2)](pd\sigma)+\sqrt{3}n(l^2+m^2)(pd\pi)$
$E_{xy,xy}$	$3l^2m^2(dd\sigma)+(l^2+m^2-4l^2m^2)(dd\pi)+(n^2+l^2m^2)(dd\delta)$
$E_{xy,yz}$	$3lm^2n(dd\sigma)+ln(1-4m^2)(dd\pi)+ln(m^2-1)(dd\delta)$
$E_{xy,zx}$	$3l^2mn(dd\sigma)+mn(1-4l^2)(dd\pi)+mn(l^2-1)(dd\delta)$
E_{xy,x^2-y^2}	$\frac{3}{2}lm(l^2-m^2)(dd\sigma)+2lm(m^2-l^2)(dd\pi)+\frac{1}{2}lm(l^2-m^2)(dd\delta)$
E_{yz,x^2-y^2}	$\frac{3}{2}mn(l^2-m^2)(dd\sigma)-mn[1+2(l^2-m^2)](dd\pi)+mn[1+\frac{1}{2}(l^2-m^2)](dd\delta)$
E_{zx,x^2-y^2}	$\frac{3}{2}nl(l^2-m^2)(dd\sigma)+nl[1-2(l^2-m^2)](dd\pi)-nl[1-\frac{1}{2}(l^2-m^2)](dd\delta)$
$E_{xy,3z^2-r^2}$	$\sqrt{3}lm[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)-2\sqrt{3}lmn^2(dd\pi)+\frac{1}{2}\sqrt{3}lm(1+n^2)(dd\delta)$
$E_{yz,3z^2-r^2}$	$\sqrt{3}mn[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}mn(l^2+m^2-n^2)(dd\pi)-\frac{1}{2}\sqrt{3}mn(l^2+m^2)(dd\delta)$
$E_{zx,3z^2-r^2}$	$\sqrt{3}ln[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}ln(l^2+m^2-n^2)(dd\pi)-\frac{1}{2}\sqrt{3}ln(l^2+m^2)(dd\delta)$
$E_{x^2-y^2,x^2-y^2}$	$\frac{3}{4}(l^2-m^2)^2(dd\sigma)+[l^2+m^2-(l^2-m^2)^2](dd\pi)+[n^2+\frac{1}{4}(l^2-m^2)^2](dd\delta)$
$E_{x^2-y^2,3z^2-r^2}$	$\frac{1}{2}\sqrt{3}(l^2-m^2)[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}n^2(m^2-l^2)(dd\pi)+\frac{1}{4}\sqrt{3}(1+n^2)(l^2-m^2)(dd\delta)$
$E_{3z^2-r^2,3z^2-r^2}$	$[n^2-\frac{1}{2}(l^2+m^2)]^2(dd\sigma)+3n^2(l^2+m^2)(dd\pi)+\frac{3}{4}(l^2+m^2)^2(dd\delta)$

$$l^2(pp\sigma)+(1-l^2)(pp\pi)$$

100 RULES
REDUCE 100 HOPPING TERMS
TO 21 NONTRIVIAL PARAMETERS

J. SLATER & G. KOSTER, PHYS. REV. **94,** 1498 (1954)

ELECTRONIC STRUCTURE CALCULATION
Sp3s* TIGHT BINDING HAMILTONIAN

$$
\mathbf{H}_{TB} = \begin{bmatrix}
\varepsilon^a_{S\downarrow} & 0 & 0 & 0 & 0 & & & & & \\
 & \varepsilon^a_{PX\downarrow} & i\Delta & 0 & 0 & & & & -\Delta & \\
 & & \varepsilon^a_{PY\downarrow} & 0 & 0 & & & & -i\Delta & \\
 & & & \varepsilon^a_{PZ\downarrow} & 0 & & \Delta & i\Delta & & \\
 & & & & \varepsilon^a_{S^*\downarrow} & & & & & \\
 & & & & & \varepsilon^a_{S\uparrow} & 0 & 0 & 0 & 0 \\
 & & & & & & \varepsilon^a_{PX\uparrow} & -i\Delta & 0 & 0 \\
 & & & & & & & \varepsilon^a_{PY\uparrow} & 0 & 0 \\
 & & & & & & & & \varepsilon^a_{PZ\uparrow} & 0 \\
 & & & & & & & & & \varepsilon^a_{S^*\uparrow}
\end{bmatrix}
$$

ANION

$$
\begin{bmatrix}
t_{SS} & t_{SPX} & t_{SPY} & t_{SPZ} & t_{SS^*} & & & & & \\
t_{PXS} & t_{PXPX} & t_{PXPY} & t_{PXPZ} & t_{PXS^*} & & & & & \\
t_{PYS} & t_{PYPX} & t_{PYPY} & t_{PYPZ} & t_{PYS^*} & & & & & \\
t_{PZS} & t_{PZPX} & t_{PZPY} & t_{PZPZ} & t_{PZS^*} & & & & & \\
t_{S^*S} & t_{S^*PX} & t_{S^*PY} & t_{S^*PZ} & t_{S^*S^*} & & & & & \\
 & & & & & t_{SS} & t_{SPX} & t_{SPY} & t_{SPZ} & t_{SS^*} \\
 & & & & & t_{PXS} & t_{PXPX} & t_{PXPY} & t_{PXPZ} & t_{PXS^*} \\
 & & & & & t_{PYS} & t_{PYPX} & t_{PYPY} & t_{PYPZ} & t_{PYS^*} \\
 & & & & & t_{PZS} & t_{PZPX} & t_{PZPY} & t_{PZPZ} & t_{PZS^*} \\
 & & & & & t_{S^*S} & t_{S^*PX} & t_{S^*PY} & t_{S^*PZ} & t_{S^*S^*}
\end{bmatrix}
$$

$$
\begin{bmatrix}
\varepsilon^c_{S\downarrow} & 0 & 0 & 0 & 0 & & & & & \\
 & \varepsilon^c_{PX\downarrow} & i\Delta & 0 & 0 & & & & -\Delta & \\
 & & \varepsilon^c_{PY\downarrow} & 0 & 0 & & & & -i\Delta & \\
 & & & \varepsilon^c_{PZ\downarrow} & 0 & & \Delta & i\Delta & & \\
 & & & & \varepsilon^c_{S^*\downarrow} & & & & & \\
 & & & & & \varepsilon^c_{S\uparrow} & 0 & 0 & 0 & 0 \\
 & & & & & & \varepsilon^c_{PX\uparrow} & -i\Delta & 0 & 0 \\
 & & & & & & & \varepsilon^c_{PY\uparrow} & 0 & 0 \\
 & & & & & & & & \varepsilon^c_{PZ\uparrow} & 0 \\
 & & & & & & & & & \varepsilon^c_{S^*\uparrow}
\end{bmatrix}
$$

CATION

$h.c.$

SPIN-ORBIT INTERACTION AFTER CHADI ET AL., PHYS. REV. B

TIGHT-BINDING PARAMETERS FROM BULK BAND STRUCTURE

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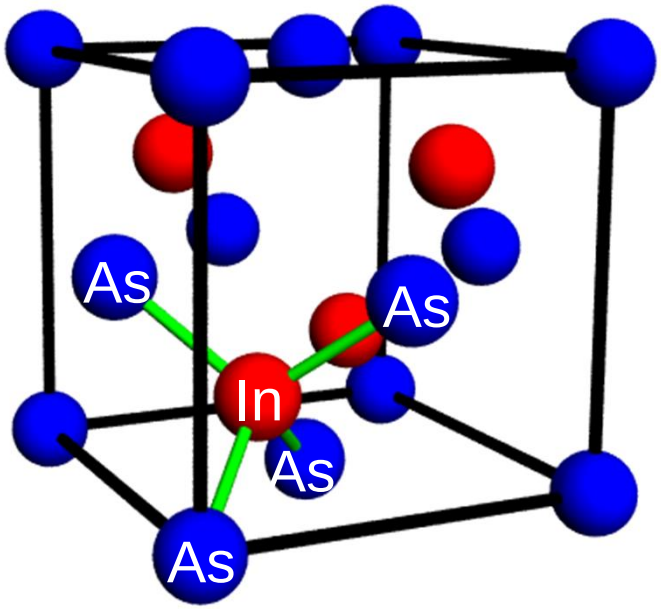
TIGHT-BINDING PARAMETERS FROM BULK BAND STRUCTURE

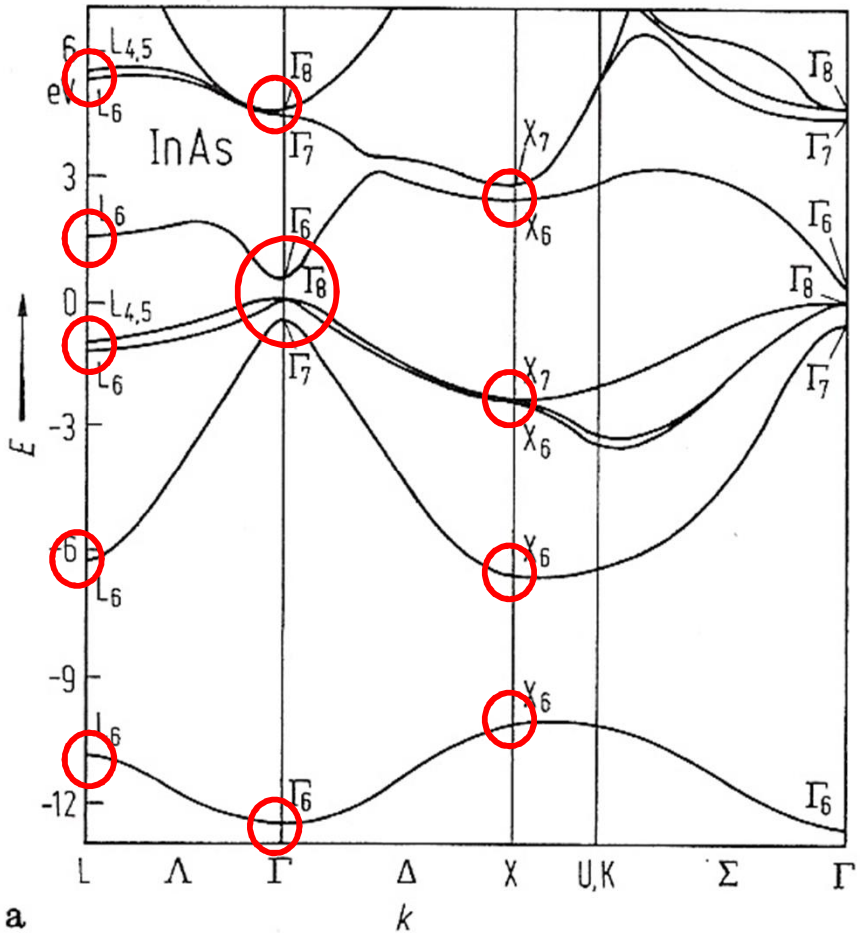


BLOCH STATES

$$\left|\Psi_{ANION}\right\rangle = \sum_{\alpha=1}^{20} A_{\alpha}^{ANION} \left(\frac{1}{\sqrt{N}} \sum_{i,BLUE} e^{ikR_i} u_{\alpha}\left(\vec{r} - \vec{R}_i\right) \right)$$

$$\left|\Psi_{CATION}\right\rangle = \sum_{\alpha=1}^{20} B_{\alpha}^{CATION} \left(\frac{1}{\sqrt{N}} \sum_{j,RED} e^{ikR_j} u_{\alpha}\left(\vec{r} - \vec{R}_j\right) \right)$$

ELECTRONIC STRUCTURE CALCULATION
FITTING BULK BANDSTRUCTURE

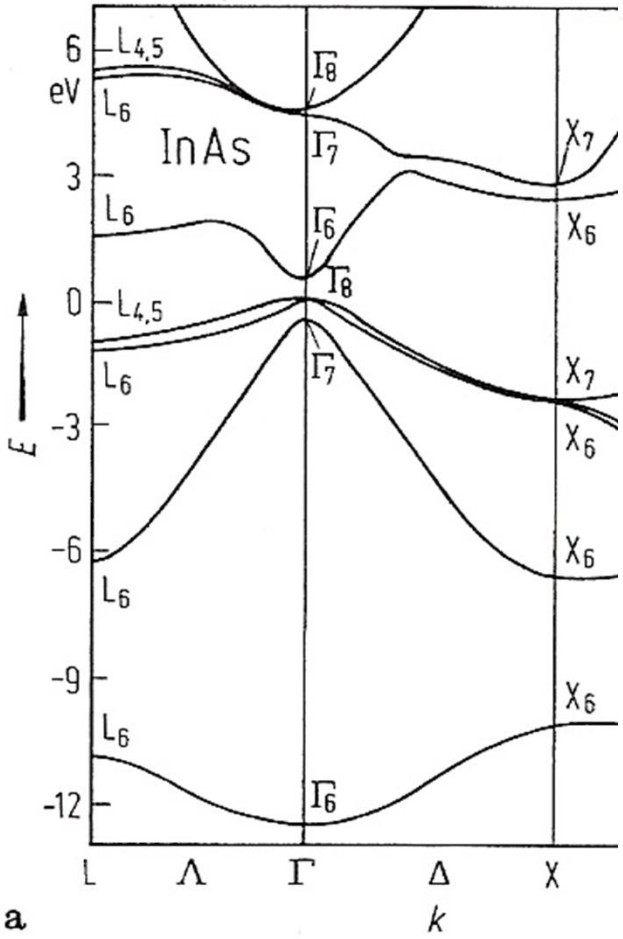


ENERGIES AND AVAILABLE EFFECTIVE MASSES FITTED USING GENETIC ALGORITHM

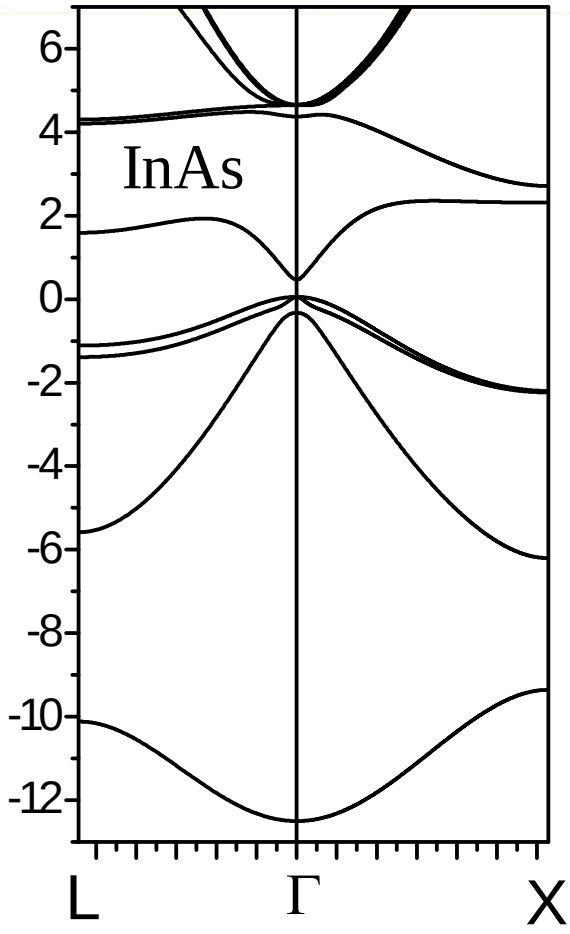
EXAMPLE: InAs

NONLOCAL PSEUDOPOTENTIAL, CHELIKOVSKY & COHEN, PRB

ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING BULK BANDSTRUCTURE



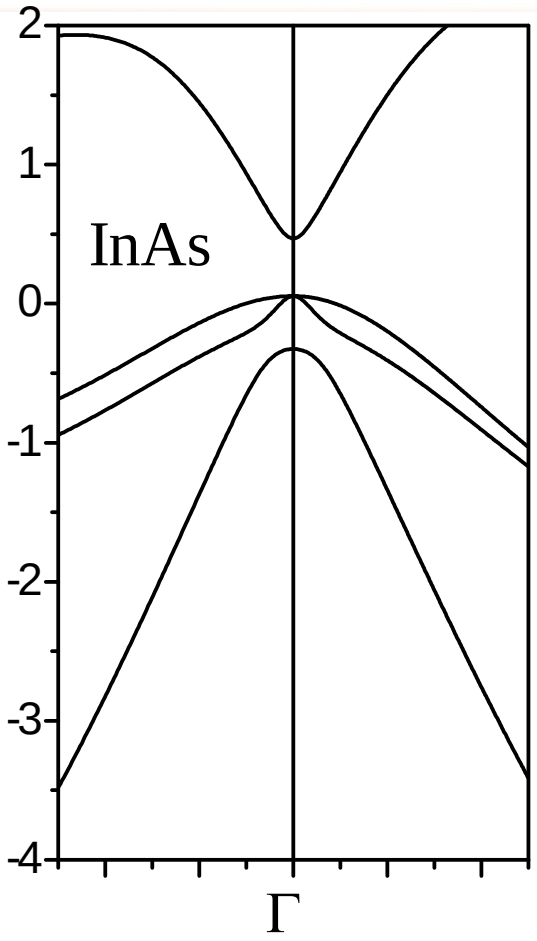
CHELIKOVSKY&COHEN



Tight binding

KORKUSINSKI, NRC1

ELECTRONIC STRUCTURE CALCULATION
TIGHT BINDING BULK BANDSTRUCTURE



OUR FIT

	TARGET	FITTED
E_g	0.418 eV	0.413 eV
Δ_{SO}	0.38 eV	0.381 eV
m_e	0.024 m_0	0.025 m_0
m_{lh}	0.026 m_0	0.029 m_0 [100] 0.029 m_0 [111]
$m_{hh\ [100]}$	0.35 m_0	0.369 m_0
$m_{hh\ [111]}$	0.43 m_0	0.471 m_0
m_{so}	0.14 m_0	0.098 m_0

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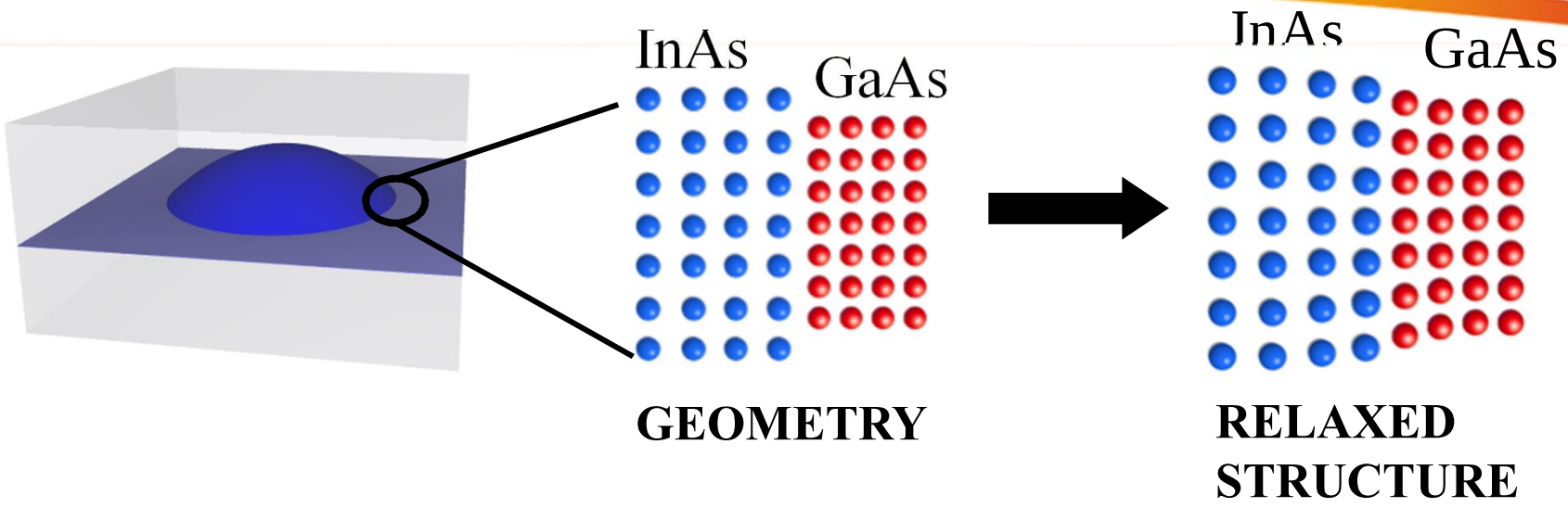
INTERFACES

ELECTRONIC STRUCTURE CALCULATION INTERFACES



- TB PARAMETERS ACROSS THE INTERFACE
  - -INTERFACE PARAMETERS – NOT A PROBLEM FOR GaAs/InAs
  - -**BAND OFFSETS** IN DIAGONAL MATRIX ELEMENTS

- MODIFIED ATOMIC POSITIONS

→ **STRAIN**

QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

OUTLINE:

INTRODUCTION
ATOMIC STRUCTURE DEFINITION
STRAIN
ELECTRONIC STRUCTURE CALCULATION
- **TIGHT BINDING METHOD**
- **EFFECT OF STRAIN**
- **SURFACE PASSIVATION**
- **EXTERNAL FIELDS**

MANY-BODY EFFECTS
- **MULTI-EXCITON COMPLEXES**
- **CHARGED EXCITONS**

EXAMPLES:
- **InAs/GaAs SELF-ASSEMBLED DOTS**
- **CdSe NANOCRYSTAL**

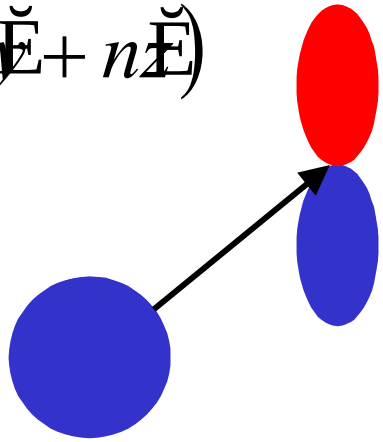
REFERENCES

TB HAMILTONIAN WITH STRAIN

RESCALE MATRIX ELEMENTS BY DIRECTIONAL COSINES AND BOND STRETCHING TERMS (HARRISON'S LAW)

NO STRAIN

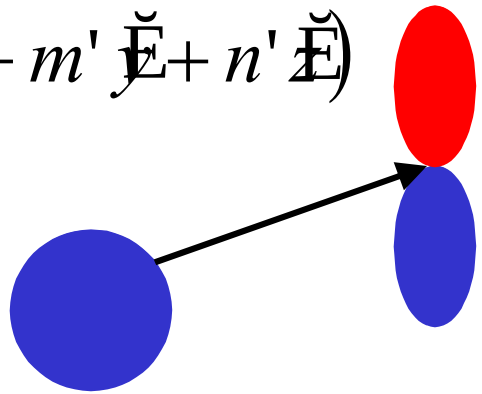
$$\vec{d} = d_0\left(l\check{\mathbf{E}}+ m\check{\mathbf{E}}+ n\check{\mathbf{E}}\right)$$



$$t_{sa,zc} = nV_{sa,pc\sigma}$$

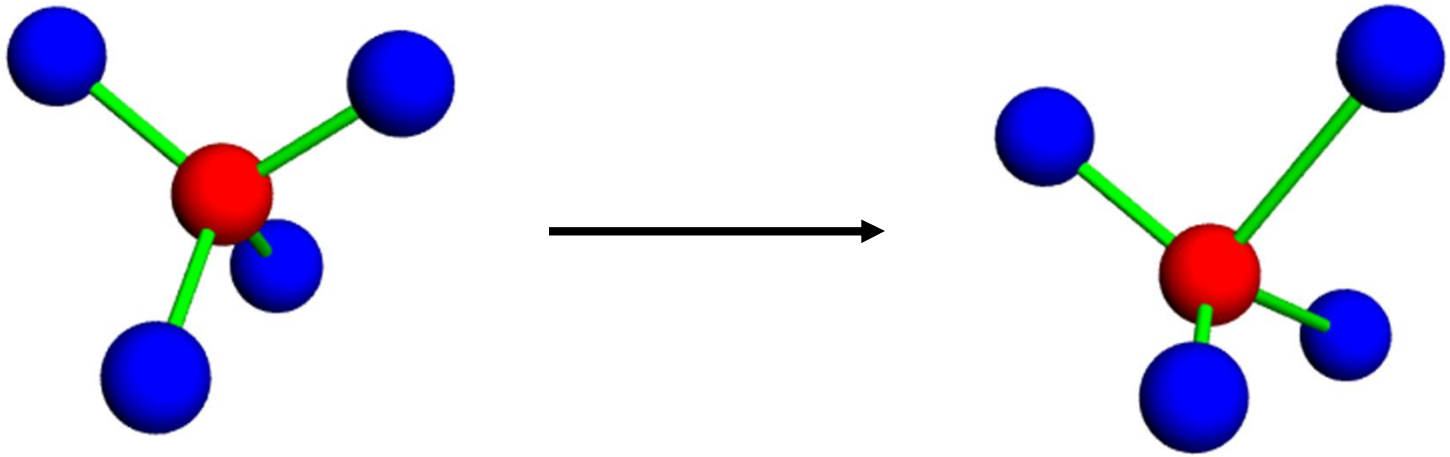
WITH STRAIN

$$\vec{d}' = d'\left(l'\check{\mathbf{E}}+ m'\check{\mathbf{E}}+ n'\check{\mathbf{E}}\right)$$



$$t'_{sa,zc} = n'V_{sa,pc\sigma}\left(\frac{d}{d_0}\right)^{\eta_{SPz}}$$

SHIFTS OF DIAGONAL TERMS



LOEWDIN-ORTHOGONALIZED BASIS:

$$\left|\Phi\right\rangle_i = \left|R,\alpha\right\rangle - \frac{1}{2}\sum_{R'\beta} S_{R\alpha,R'\beta}\left|R',\beta\right\rangle$$

S MATRIX CHANGES AS ATOMS ARE DISPLACED

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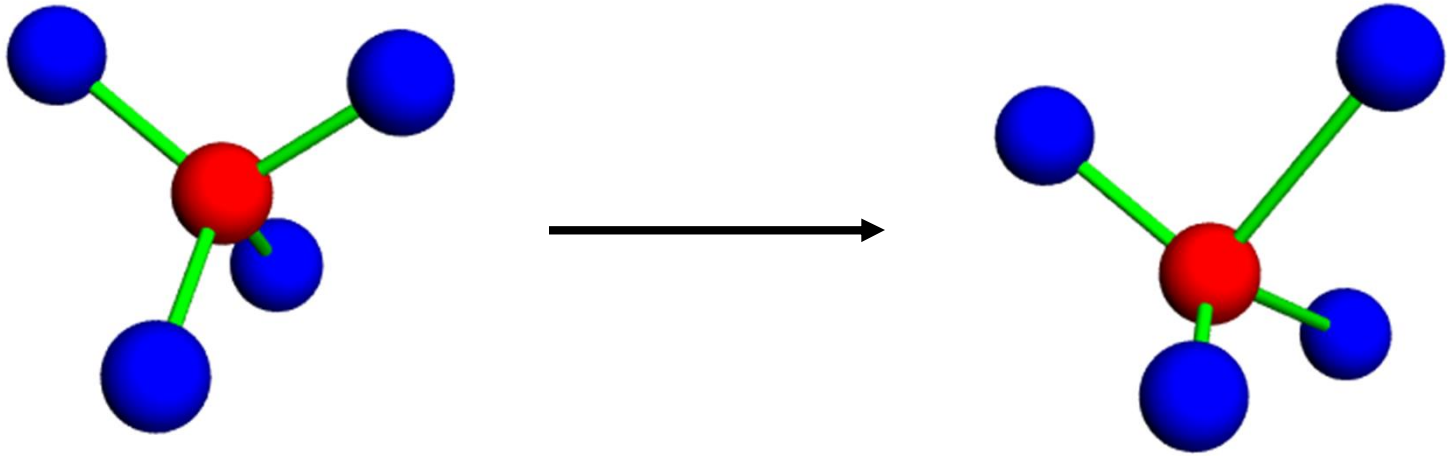
SHIFTS OF DIAGONAL TERMS



DIAGONAL HAMILTONIAN ELEMENTS

$$\varepsilon_{R\alpha} = {}_i\langle \Phi | H | \Phi \rangle_i \approx \langle R,\alpha | H | R,\alpha \rangle - \sum_{R'\beta} S_{R\alpha,R'\beta} \langle R,\alpha | H | R',\beta \rangle$$

SENSITIVE TO STRAIN!

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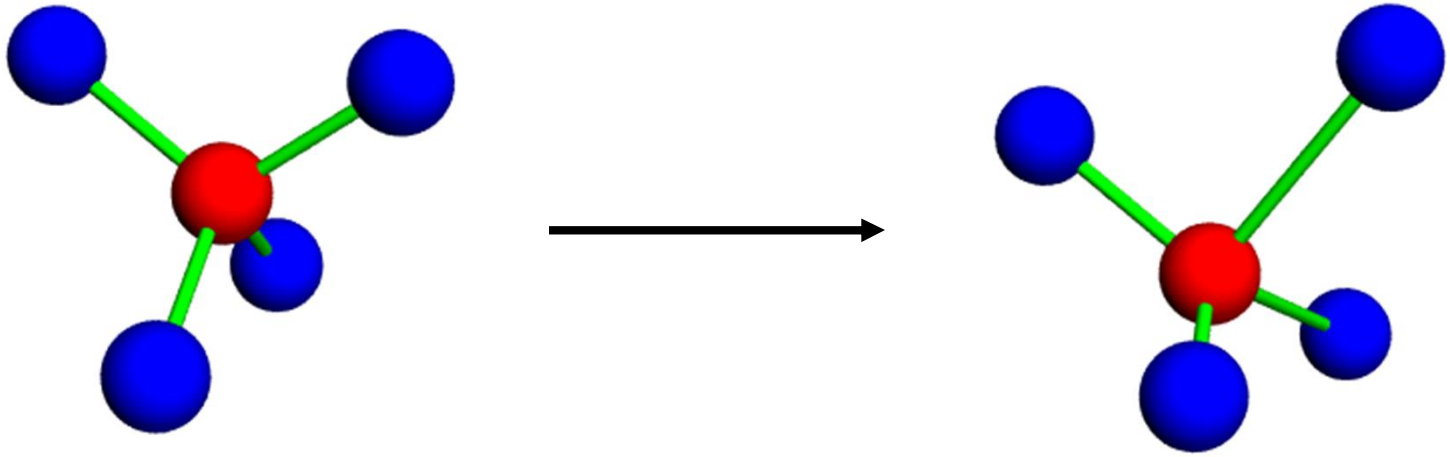
SHIFTS OF DIAGONAL TERMS



PROCEDURE: USE EXTENDED HUECKEL RULE:

$$S_{R\alpha,R'\beta} \approx A \frac{t_{R\alpha,R'\beta}}{\varepsilon_{R\alpha}^{ATOM} + \varepsilon_{R'\beta}^{ATOM}}$$

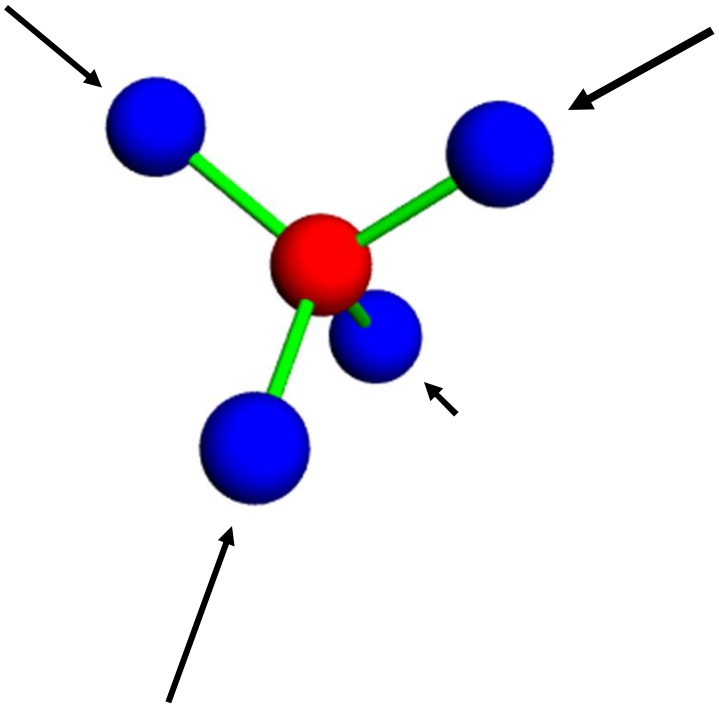
ñBAREò ATOMIC ENERGIES

$$\varepsilon_{\vec{R}\alpha} = \varepsilon_{\vec{R}\alpha}^{0} + \sum_{\vec{R}'\in nn} \sum_{\beta} C_{(\vec{R}\alpha,\vec{R}'\beta)} \frac{\left(t_{\vec{R}\alpha,\vec{R}'\beta}^{0}\right)^2 - \left(t_{\vec{R}\alpha,\vec{R}'\beta}^{'}\right)^2}{\varepsilon_{\vec{R}\alpha}^{0} + \varepsilon_{\vec{R}'\beta}^{0} - \Delta E_{ATOM}}$$

C ï PARAMETERS TO BE FITTED

FITTING OF STRAIN

HYDROSTATIC ï BIR-PIKUS MODEL



LINEAR SHIFTS OF BAND EDGES

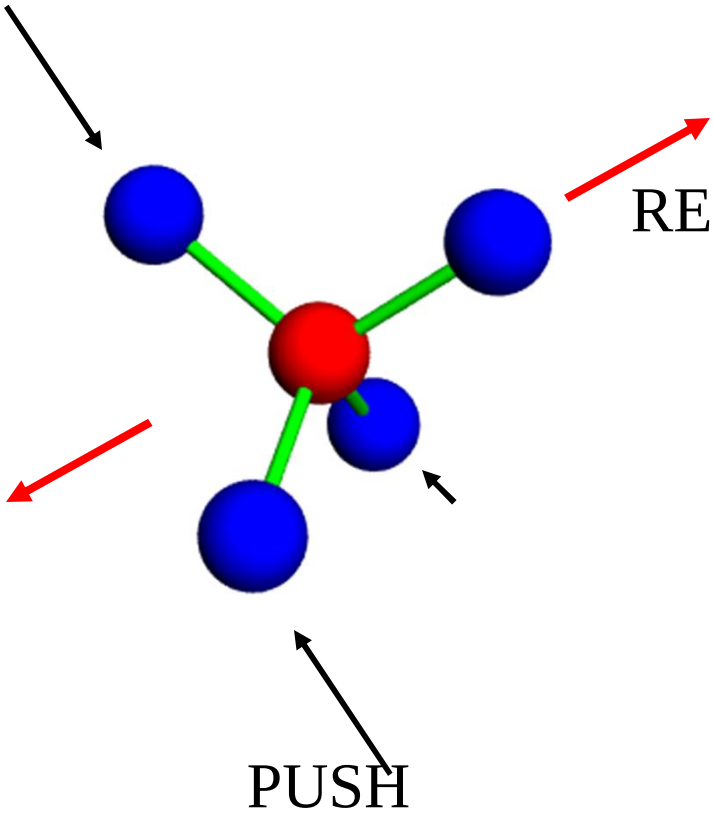
$$E_{CB} = E_{CB}^{0} + a_C\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right)$$

$$E_{VB,HH} = E_{VB,HH}^{0} + a_V\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right)$$

$$E_{SO} = E_{SO}^{0} + a_V\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right)$$

a_C, a_V - DEFORMATION POTENTIALS

FITTING OF STRAIN



BIAXIAL STRAIN

NONTRIVIAL BEHAVIOR-
FIT TO AB INITIO RESULTS

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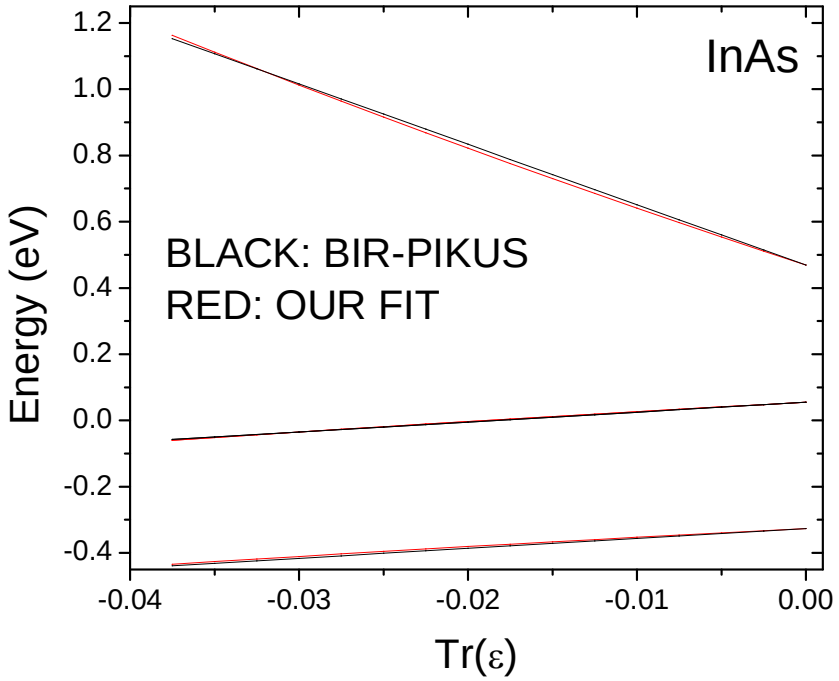
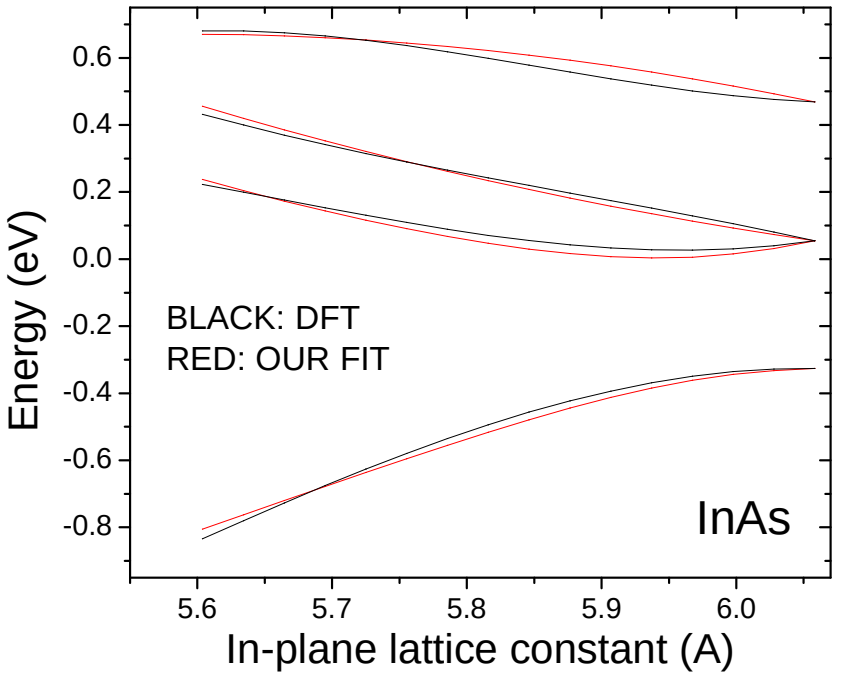
BAND EDGES AS A FUNCTION OF STRAIN

Hydrostatic strain fitted to Bir-Pikus model



Biaxial strain fit to DFT (LDA) model



Kadantsev et al. JAP2010

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STRAIN IN TIGHT BINDING MODEL

SUMMARY :

STRAIN EFFECTS CHANGE BONDS ANGLES AND LENGTHS.

Bonds angles: Slater-Koster formalism

Bonds lengths: a generalized version of Harrison law

$$V_{\alpha\beta\gamma} = V^{0}_{\alpha\beta\gamma}\left(d_{ij}^{\,0} / d_{ij}\right)^{\eta_{\alpha\beta\gamma}}$$

d_{ij} is bond length, 0 superscript = values without strain

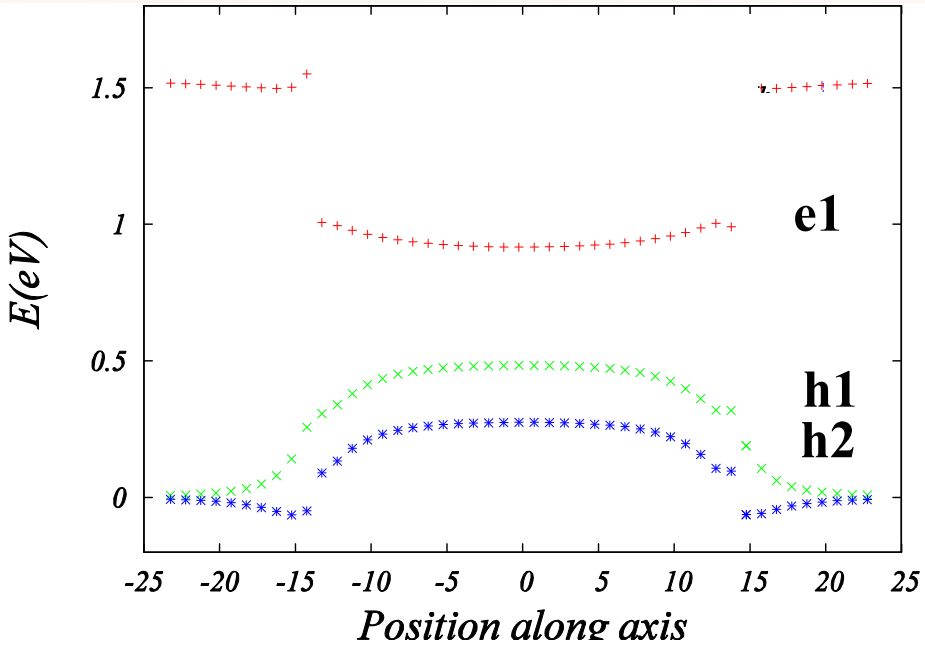
Diagonal elements vary in response to displacement of neighbours:

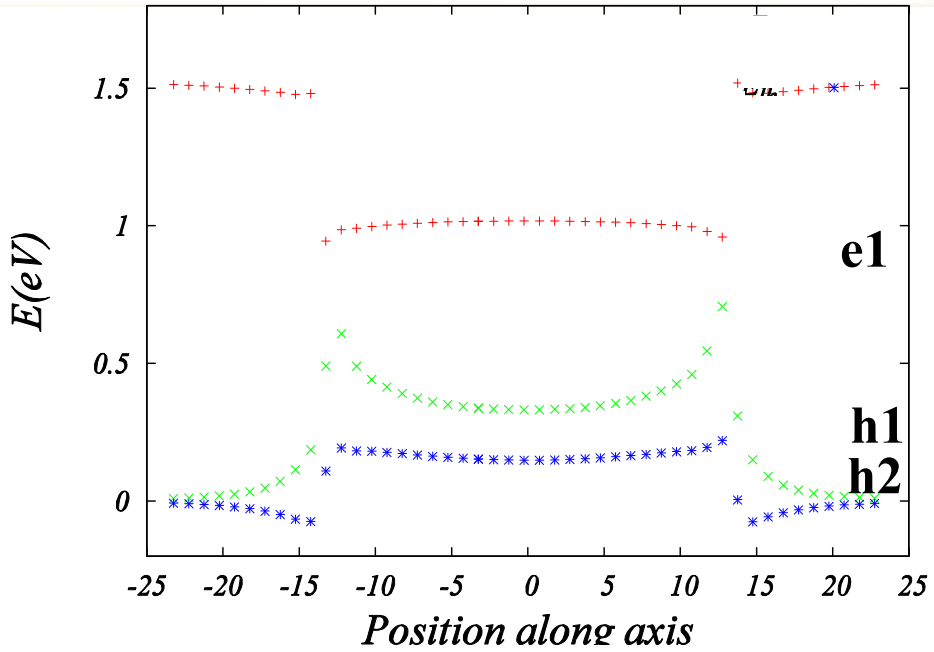
$$\varepsilon_{\vec{R}\alpha} = \varepsilon^{0}_{\vec{R}\alpha} + \sum_{\vec{R}'\in nn}\sum_{\beta} C_{(\vec{R}\alpha,\vec{R}'\beta)} \frac{\left(t^{0}_{\vec{R}\alpha,\vec{R}'\beta}\right)^2 - \left(t_{\vec{R}\alpha,\vec{R}'\beta}\right)^2}{\varepsilon^{0}_{\vec{R}\alpha} - \varepsilon^{0}_{\vec{R}'\beta}}$$

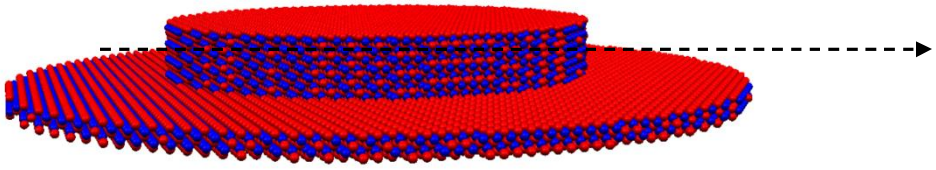
Ůdiagonal and t off-diagonal Hamiltonian matrix eler

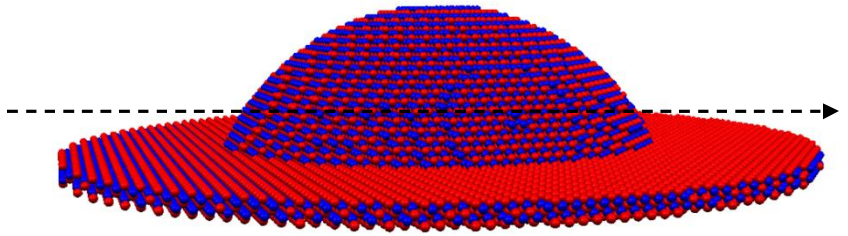
ɖ, C empirical parameters

TB CONFINING POTENTIAL PROFILES ALONG X-AXIS









Disc D=16 nm, h=2 nm

Lens D=16 nm, h=5 nm

QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

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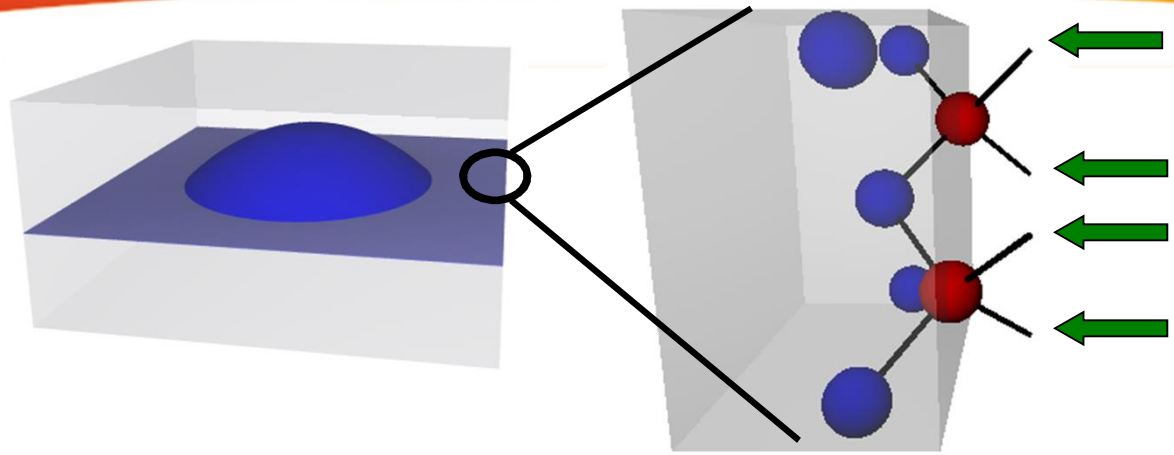
  - CdSe NANOCRYSTAL
- REFERENCES

SURFACE PASSIVATION-BOUNDARIES



ENERGIES OF DANGLING BONDS IN THE SAME RANGE AS ENERGIES OF QDOT STATES

1. ROTATE THE sp^3 BASIS INTO HYBRIDIZED ORBITALS

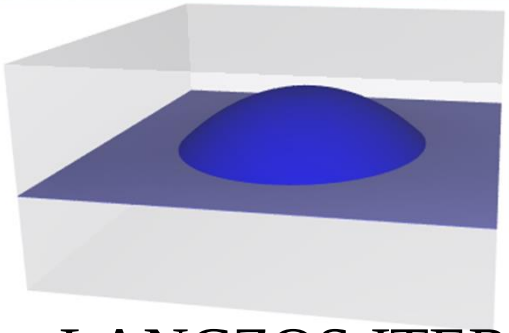
$$\left|sp_1^3\right\rangle = \frac{1}{2}\left(\left|s\right\rangle + \left|p_x\right\rangle + \left|p_y\right\rangle + \left|p_z\right\rangle\right) \qquad \left|sp_2^3\right\rangle = \frac{1}{2}\left(\left|s\right\rangle + \left|p_x\right\rangle - \left|p_y\right\rangle - \left|p_z\right\rangle\right)$$

$$\left|sp_3^3\right\rangle = \frac{1}{2}\left(\left|s\right\rangle - \left|p_x\right\rangle + \left|p_y\right\rangle - \left|p_z\right\rangle\right) \qquad \left|sp_4^3\right\rangle = \frac{1}{2}\left(\left|s\right\rangle - \left|p_x\right\rangle - \left|p_y\right\rangle + \left|p_z\right\rangle\right)$$

2. IDENTIFY DANGLING BONDS, SHIFT THEIR ENERGIES

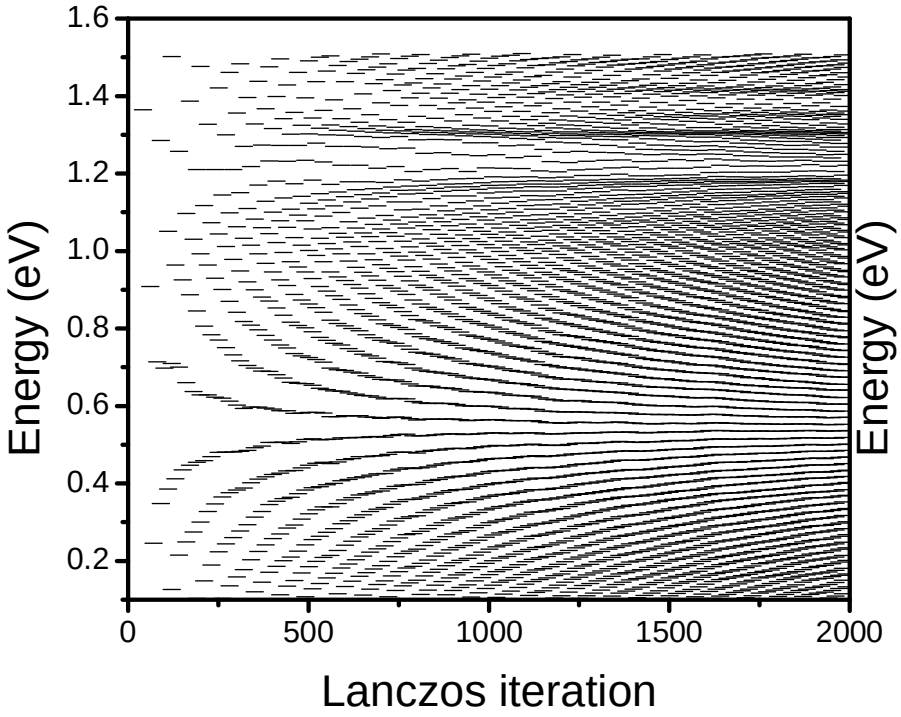
3. ROTATE HYBRIDIZED ORBITALS BACK TO sp^3 BASIS

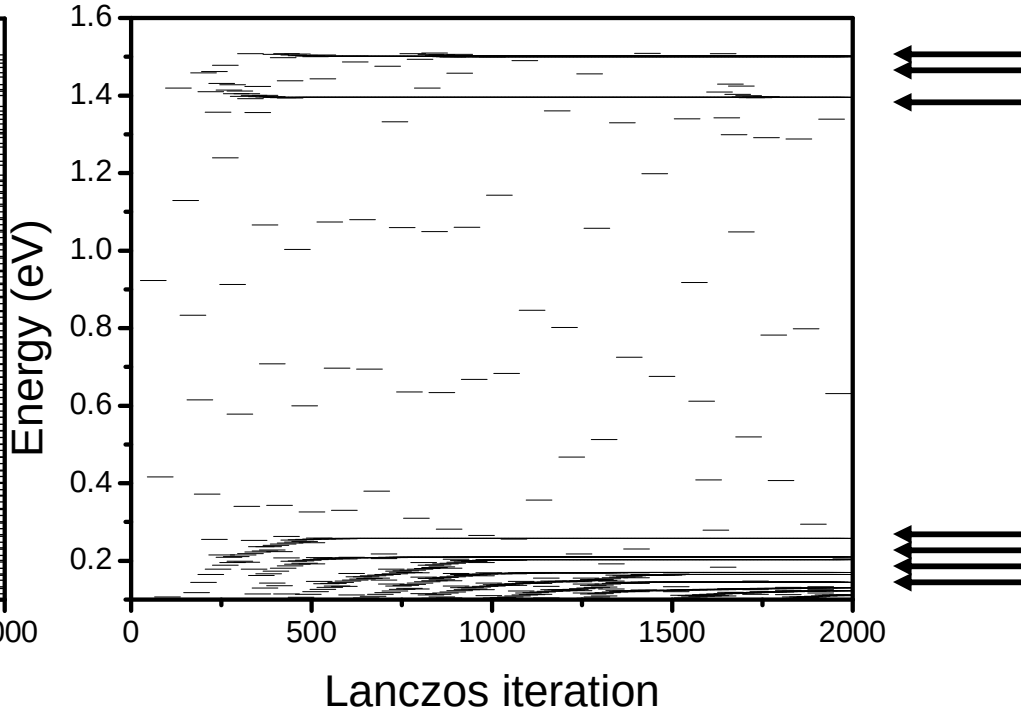
SURFACE PASSIVATION-BOUNDARIES



IS IT IMPORTANT?

LANCZOS ITERATIVE DIAGONALIZATION





NO SURFACE PASSIVATION

SURFACE PASSIVATION

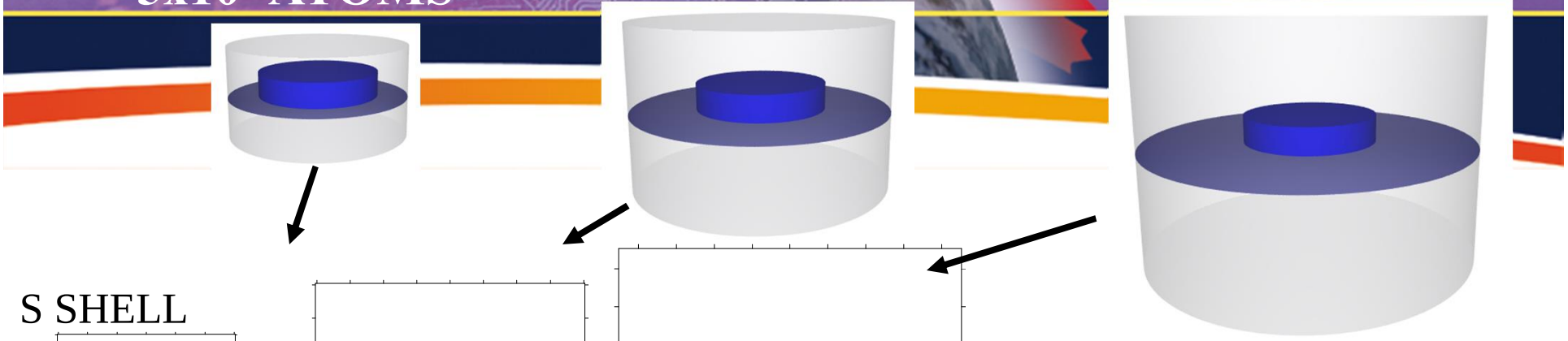
M.Korkusinski

TESTING THE ELECTRONIC SOLVER

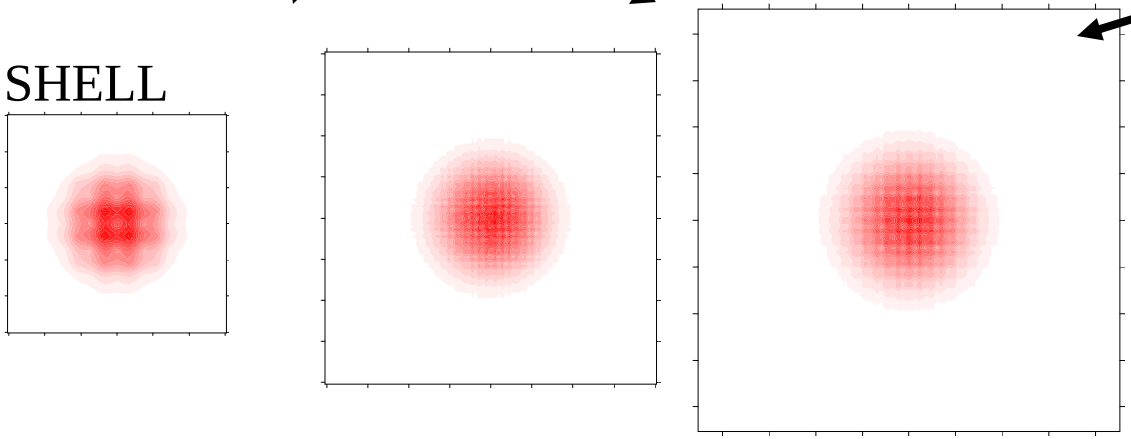
$5x10^5$ ATOMS

$1.2x10^6$ ATOMS

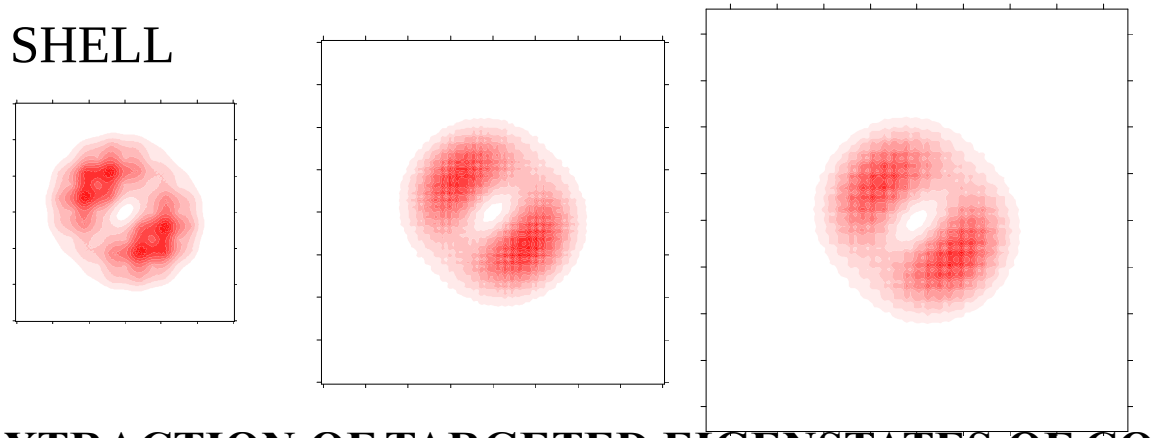
$1.8x10^6$ ATOMS

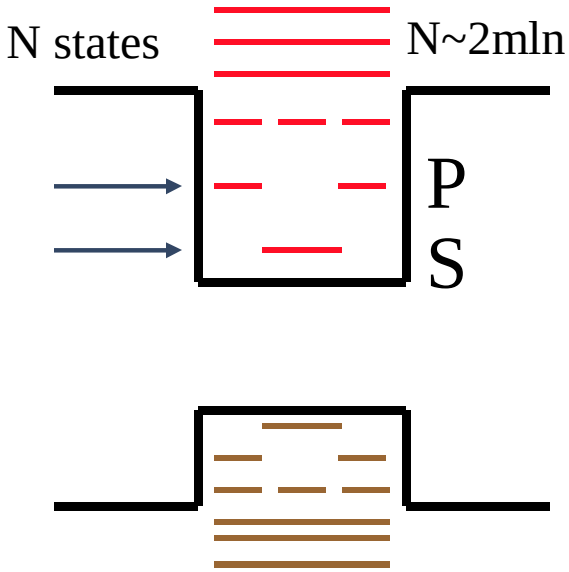


S SHELL



P SHELL





EXTRACTION OF TARGETED EIGENSTATES OF CORRECT SYMMETRY WITH LANCZOS ITERATIVE ALGORITHM

M.Korkusinski

EXTERNAL FIELDS

$$\varepsilon_{\alpha\vec{R}}{}^{0} = \left\langle \alpha\vec{R} \middle| \mathbf{H}^{0} \middle| \alpha\vec{R} \right\rangle$$

$$t_{\alpha\vec{R},\alpha'\vec{R}'}{}^{0} = \left\langle \alpha'\vec{R}' \middle| \mathbf{H}^{0} \middle| \alpha\vec{R} \right\rangle$$

$$\varepsilon_{\alpha\vec{R}} = \varepsilon_{\alpha\vec{R}}{}^{0} - e\Phi\left(\vec{R}\right) + \frac{1}{2} g_0 \mu_B \vec{\sigma} \cdot \vec{B}$$

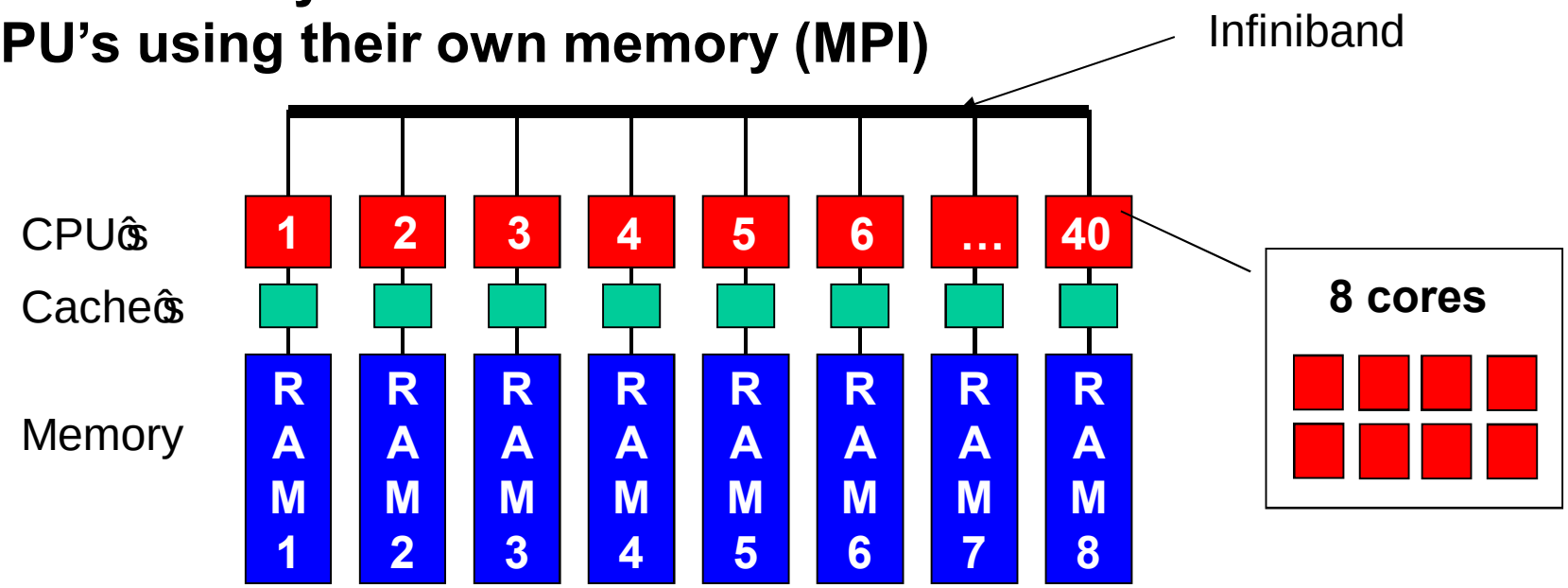
$$t_{\alpha\vec{R},\alpha'\vec{R}'} = t_{\alpha\vec{R},\alpha'\vec{R}'}{}^{0} \exp\left\{ -\frac{ie}{2\hbar} \vec{B} \cdot \left(\vec{R} \times \vec{R}'\right) \right\}$$

Under symmetric gauge

P.Vogl, C. Strahberger
phys. stat. sol. (b) 234, No. 1, 472ï 477 (2002)

PARALLELIZATION – DISTRIBUTION-SATURN

Distributed memory =
many CPU's using their own memory (MPI)

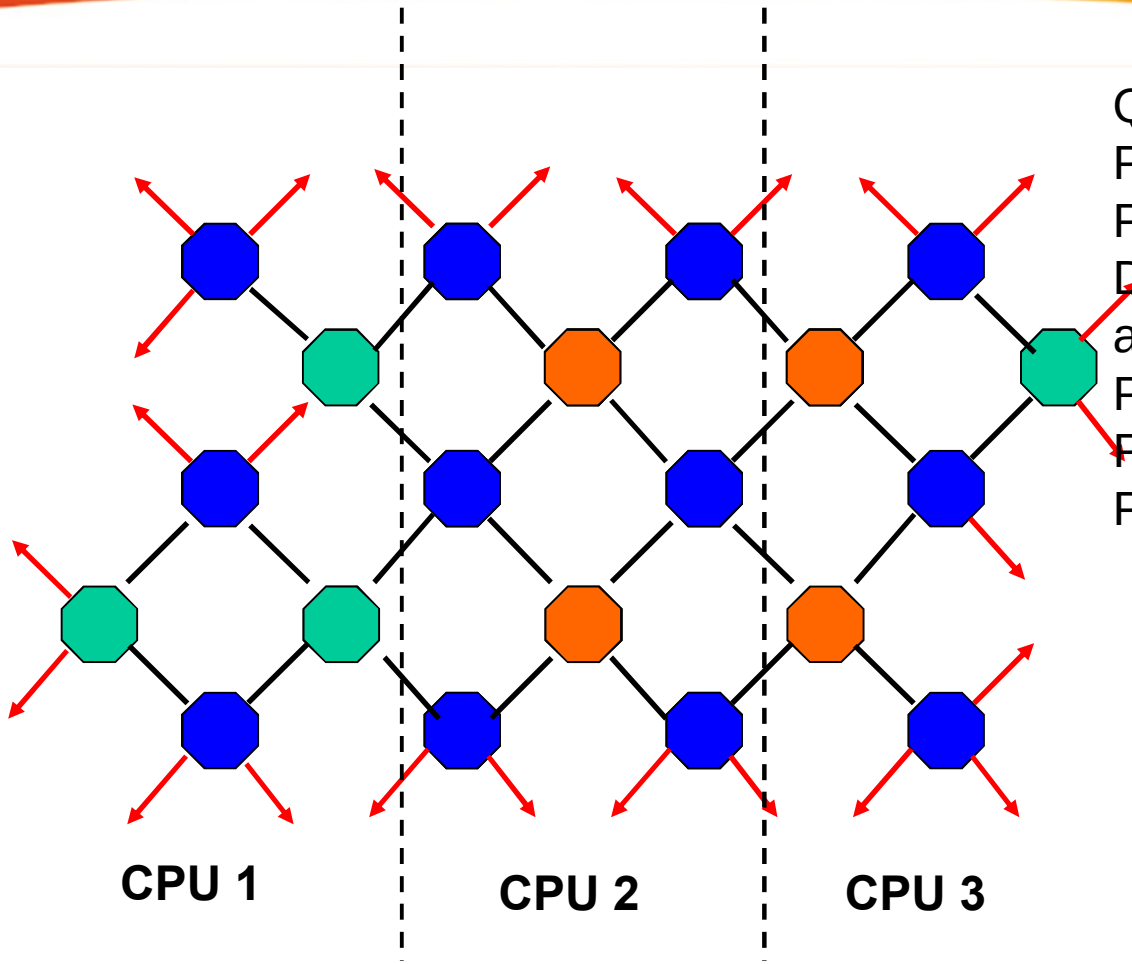


Distribution both of computational effort and memory resources.

ñinexpensiveò cluster of ñdesktopò computers

Hard to code (320 cores!)

CRYSTAL LATTICE DISTRIBUTION



QNANO:
Parallel conjugate-gradient (VFF)
Parallel Lanczos (TB)
Distribution of TB matrix
and TB matrix-vector product
Parallel Coulomb ME
Parallel fits (genetic alg.)
Parallel LCAO

Including

1. Equal distribution
   (load balancing)
2. Proper (no deadlocks)
   and minimal (speed!)
   communication

QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

OUTLINE:

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STRAIN
ELECTRONIC STRUCTURE CALCULATION
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- **EXTERNAL FIELDS**

MANY-BODY EFFECTS
- **MULTI-EXCITON COMPLEXES**
- **CHARGED EXCITONS**

EXAMPLES:
- **InAs/GaAs SELF-ASSEMBLED DOTS (Zielinski et al PRB2010)**
- **CdSe NANOCRYSTAL**

REFERENCES

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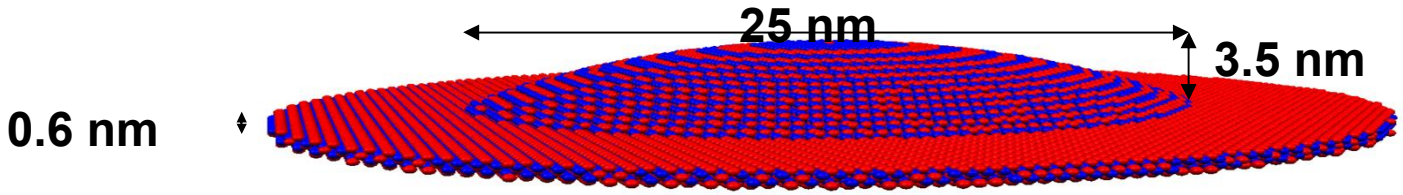
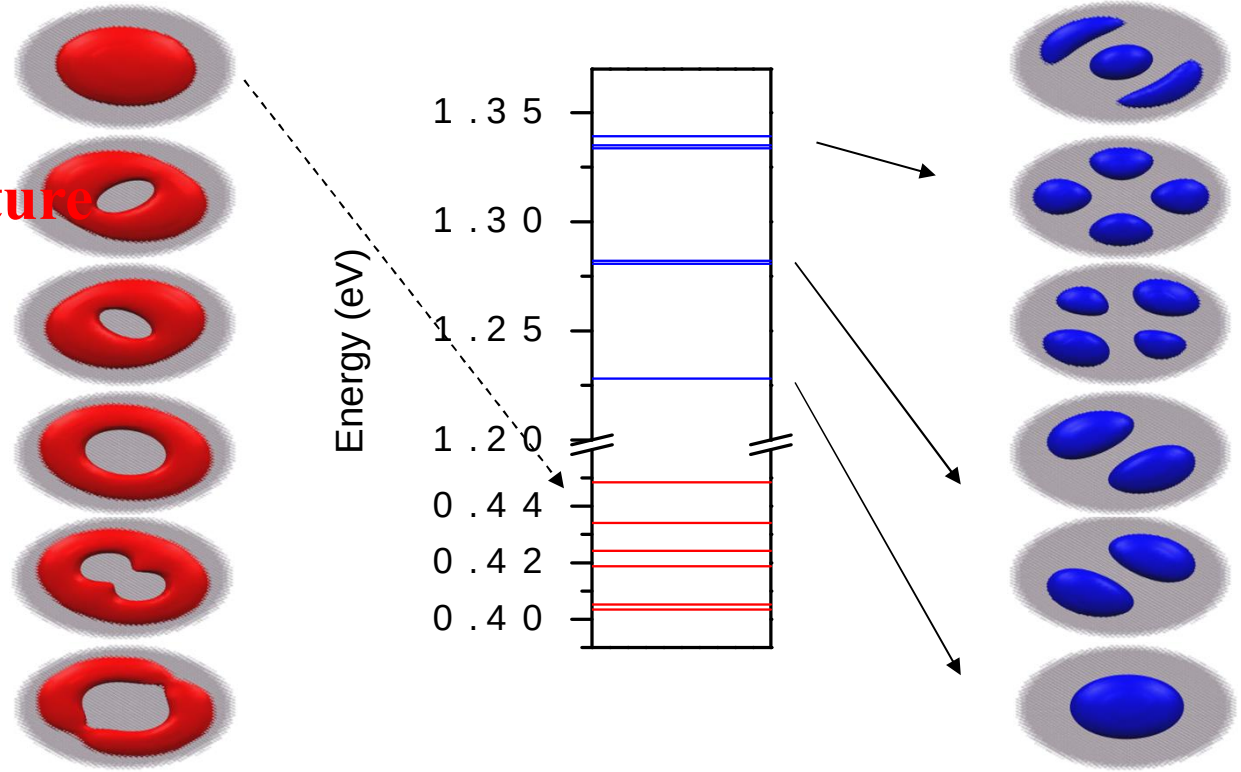
EFFECT OF STRAIN AND VALENCE BAND OFFSETS ON ELECTRONS AND HOLES: DIFFERENT MODELS



No Shell Structure For holes



Shell Structure For electrons

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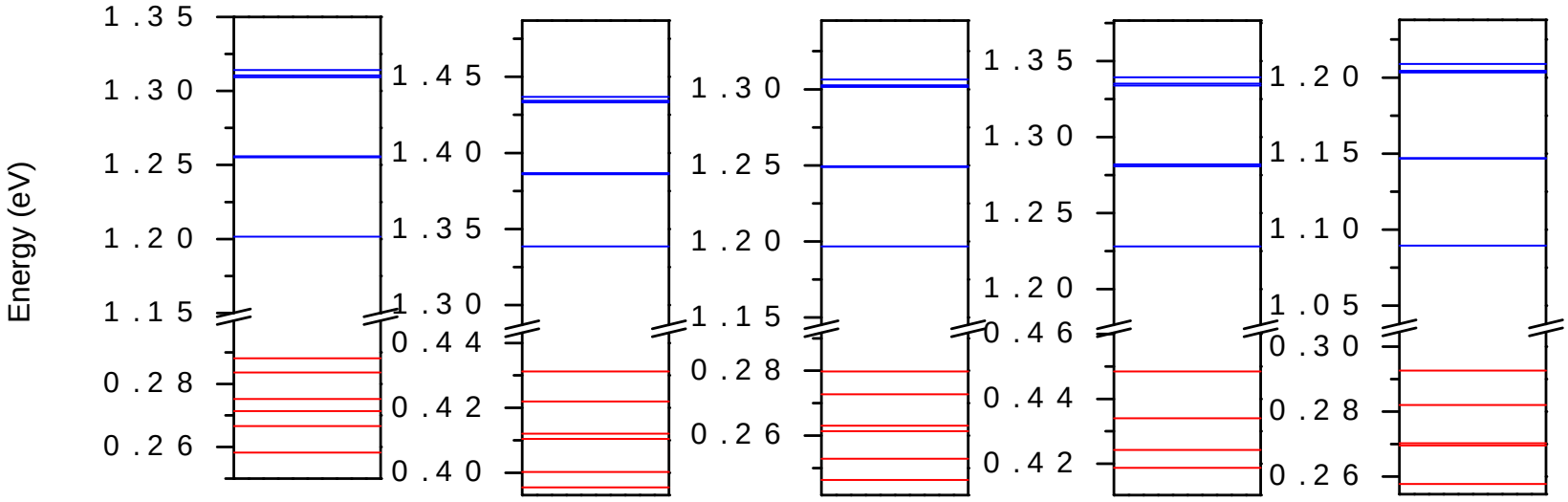
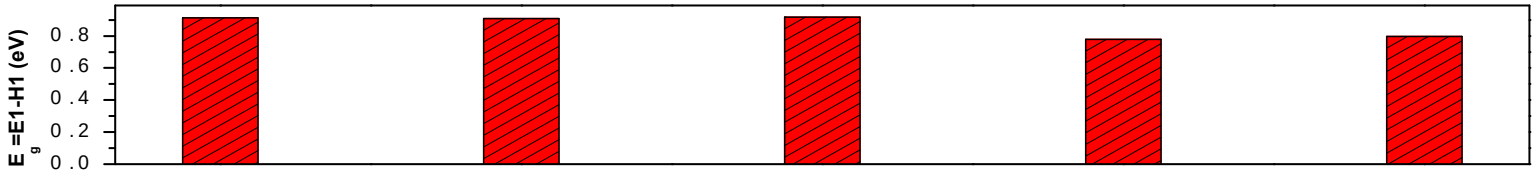
SAME QDOT, DIFFERENT STRAIN AND VALENCE BAND OFFSETS : DIFFERENT MODELS

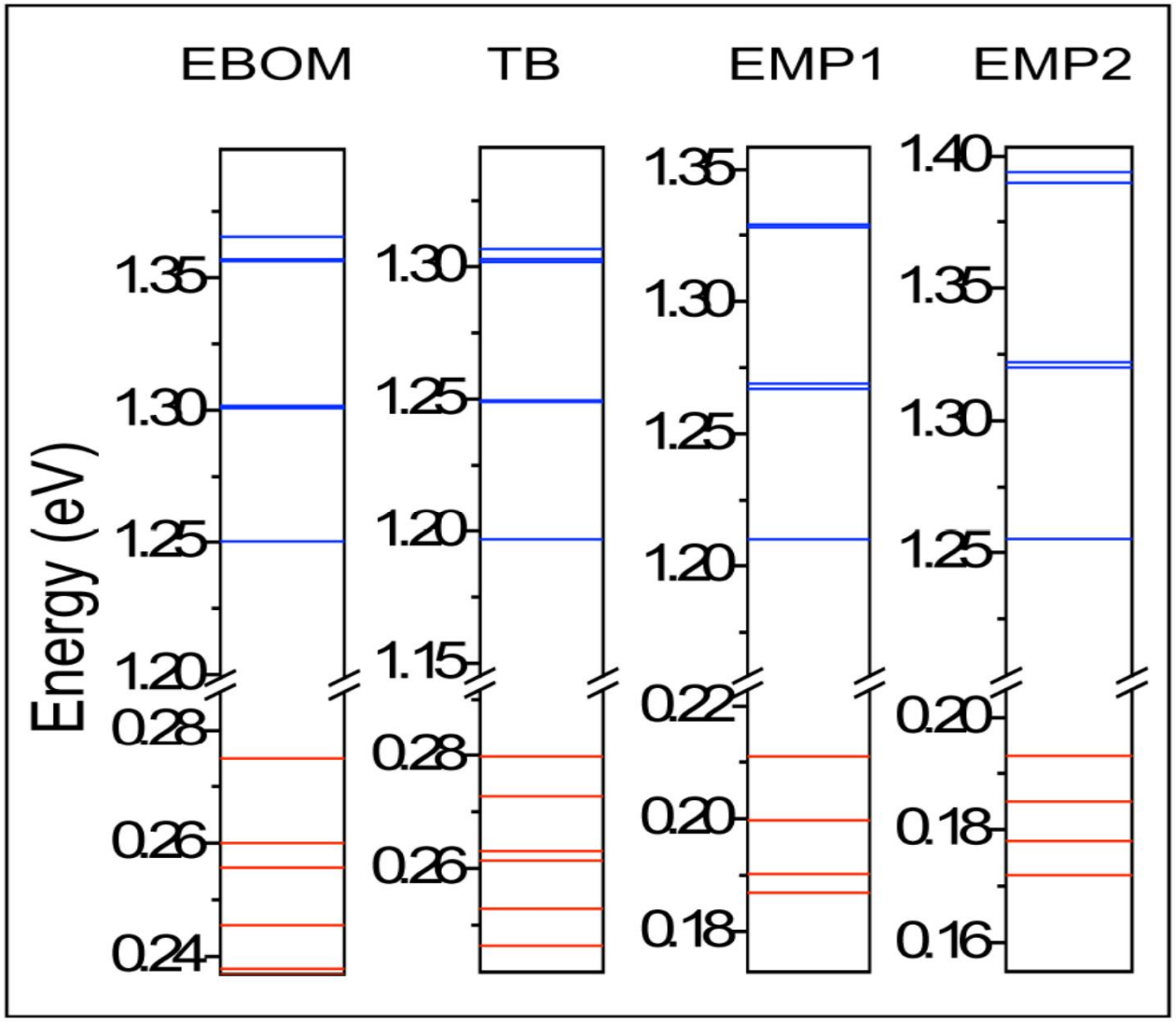
Strain Fit	BP	BP	BP	DFT	DFT
a_v (eV)	+1.0	-1.0	-1.0	-0.88	-0.88
VBO (meV)	**210**	**210**	**60**	**210**	**60**



E_1-H_1 (eV)	0.9136	0.9073	0.9169	0.7797	0.7969



SAME QDOT DIFFERENT METHODOLOGY



EBOM-effective bond orbital model,W.Sheng et al, PRB2005.

TB – Zielinski et al, PRB2010

EMP1(2) ï empirical pseudopotential results , He et al Phys. Rev. B 73, 115324 (2006)

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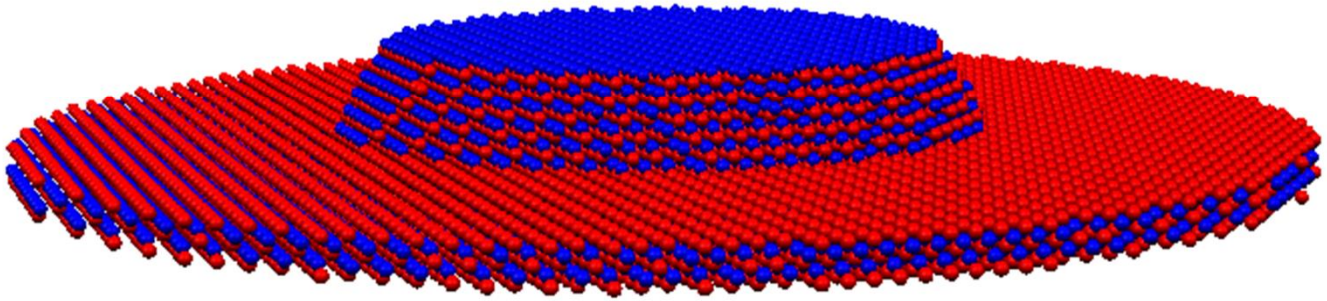
InAs/GaAs In-FLUSH GROWN DOT

IMS In-flush growth technique ï Wasilewski et al J.Cryst.Growth,1999



QD diameter 12.5 nm, height 2.0 nm
VFF domain: 32.2 mln atoms
TB domain : 0.298 mln atoms

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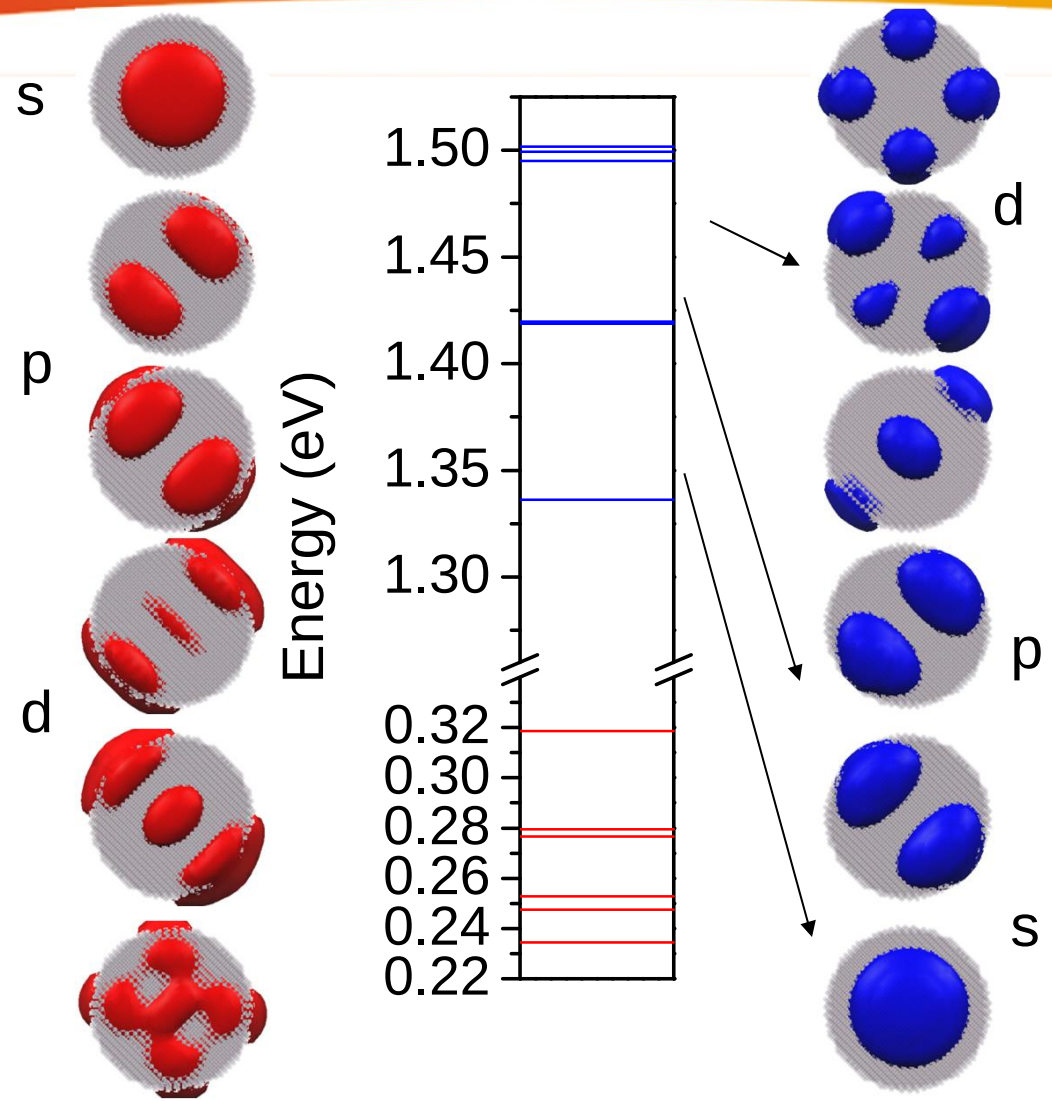
InAs/GaAs In-FLUSH GROWN DOT



SHELL STRUCTURE OF HOLES!

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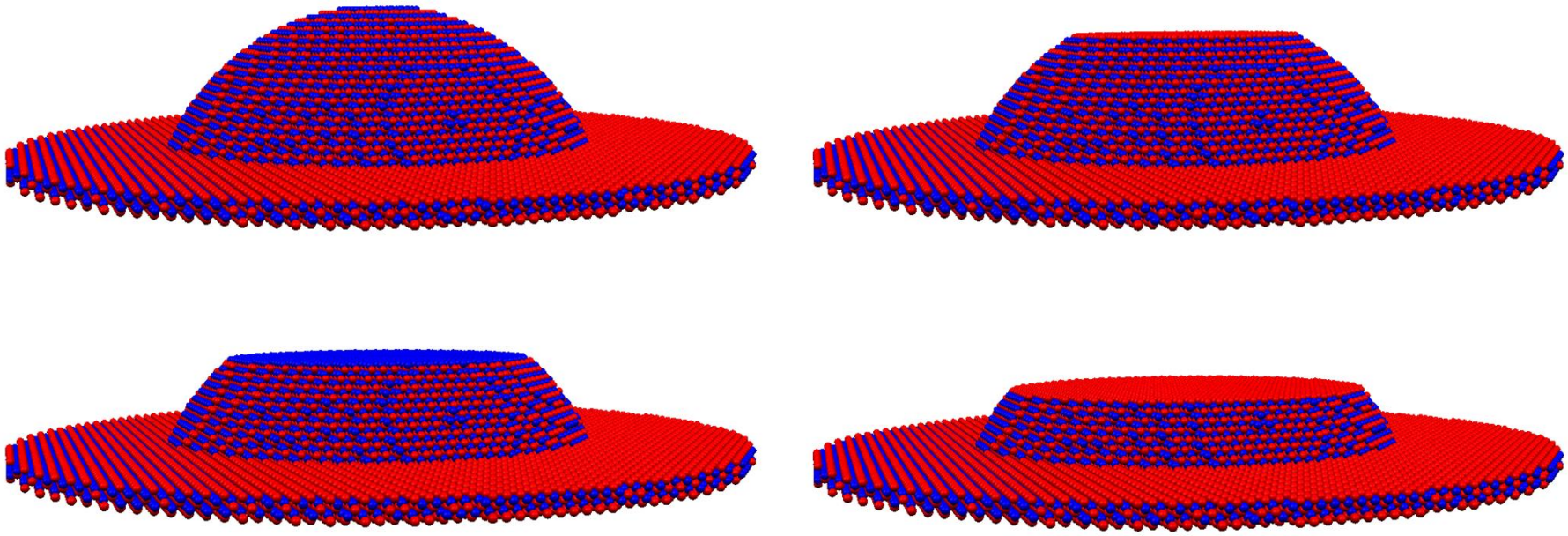
InAs/GaAs LENS TO DISC QD



QD diameter 16.0 nm, height from 5.0 nm to 2.0 nm
VFF domain: 32.2 mln atoms
TB domain : 0.44 mln atoms

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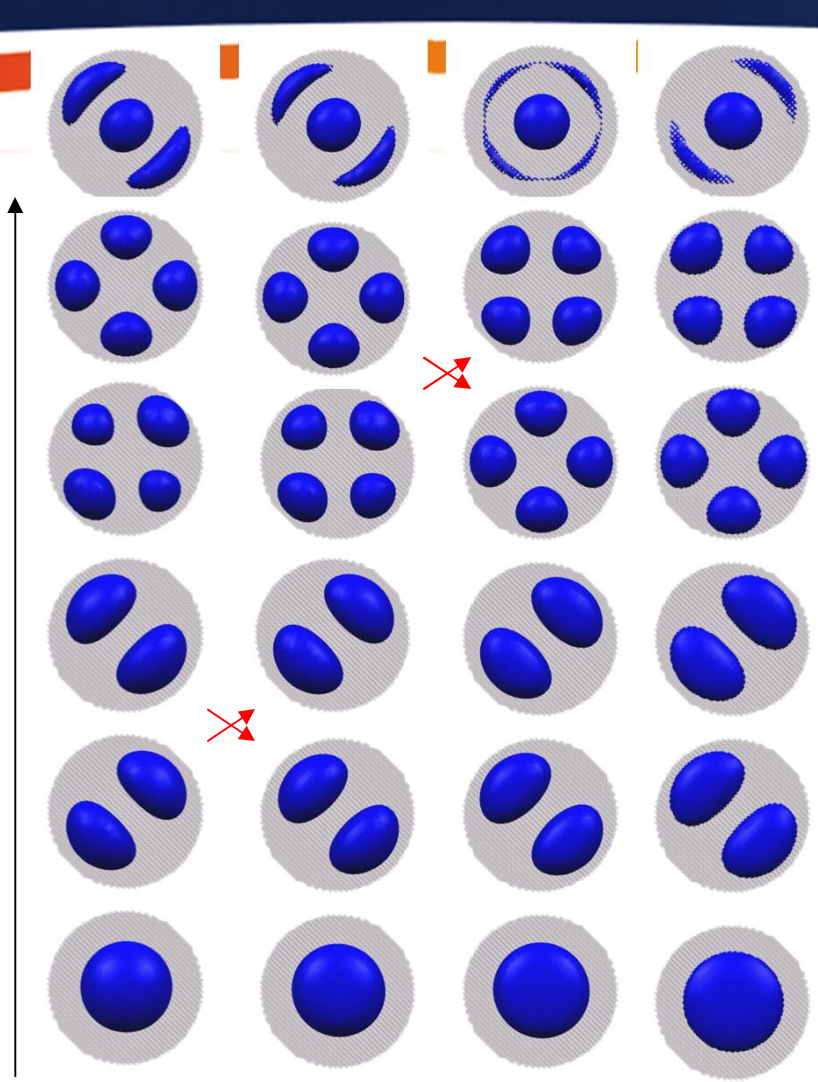
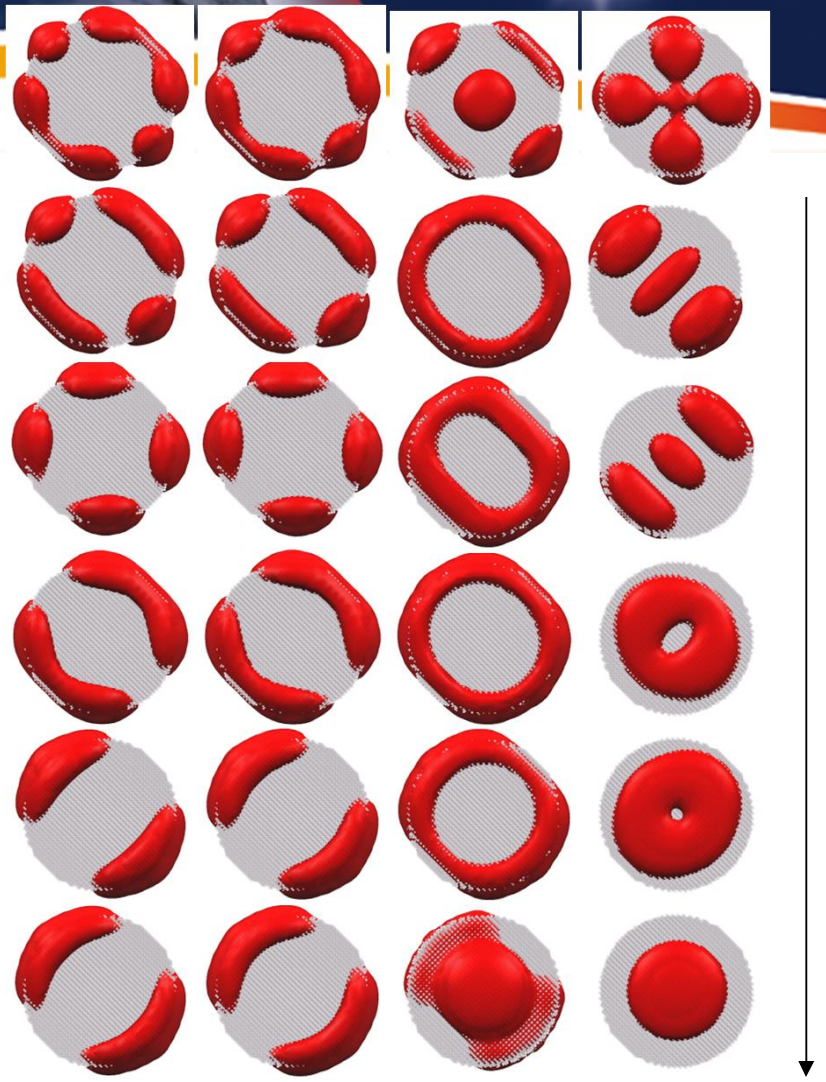
QD STATES VS CUT-OFF HEIGHT



5 nm 4 nm 3 nm 2 nm

Electrons



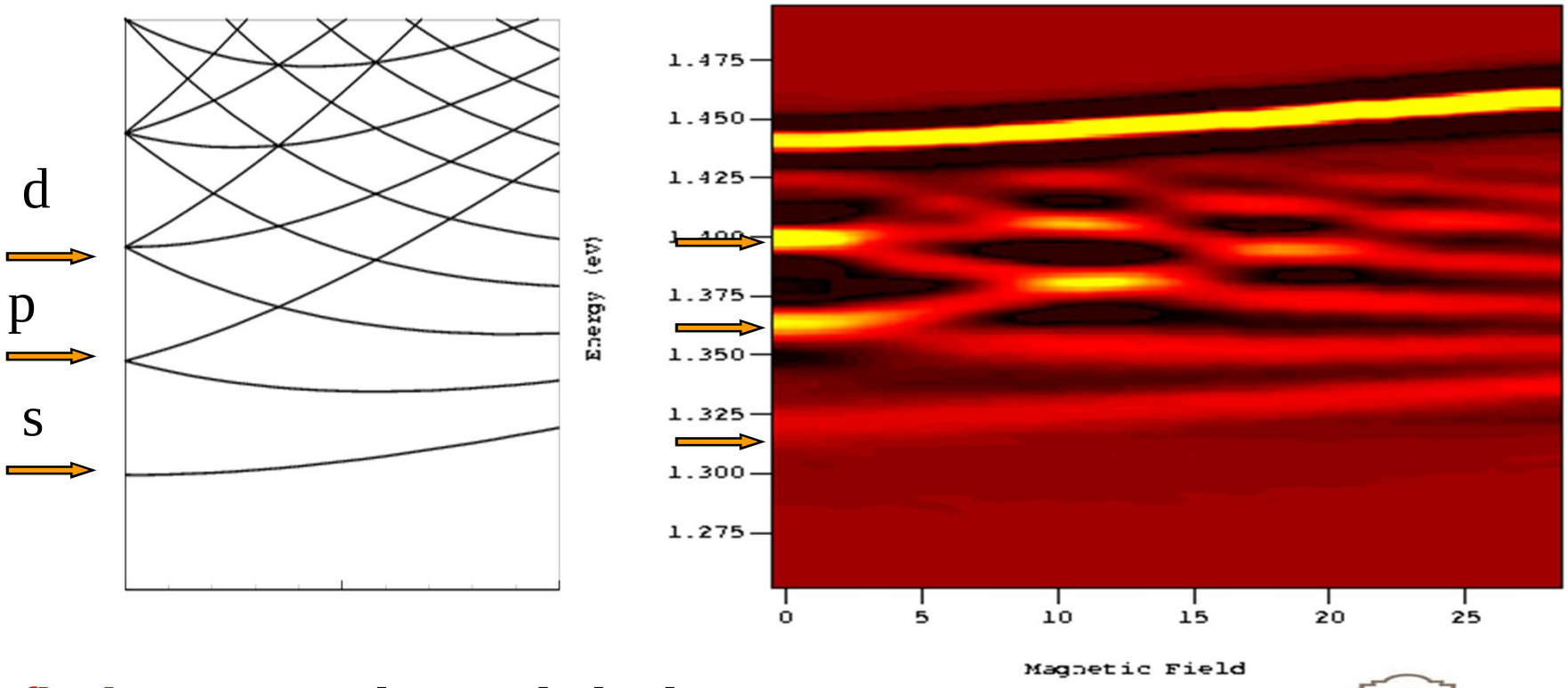
5 nm 4 nm 3 nm 2 nm

Holes

FOCK-DARWIN SPECTRUM OF In FLUSH QDOTS

SINGLE PARTICLE SPECTRUM

$$E(m,n) = \Omega_{-}(m+1/2) + \Omega_{+}(n+1/2)$$



In-flush grown and annealed qdots

Raymond et al, PRL 2004, IMS/Grenoble/Dortmund

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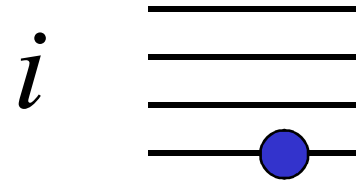
MULTI-EXCITON COMPLEXES

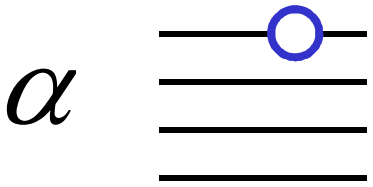
INTERACTING ELECTRONS AND HOLES

QUASIPARTICLES



QUASIELECTRON

$$\left|\alpha_1, i_1\right\rangle = c_{i1}^{+} h_{\alpha 1}^{+} \left| GS \right\rangle$$



QUASIHOLE

ENERGY OF QUASI_ELECTRON_QUASI_HOLE PAIR

$$E(\alpha_1, i_1) = (\varepsilon_{i1} + \Sigma(i_1)) - (\varepsilon_{\alpha 1} + \Sigma(\alpha_1)) - V(\alpha_1, i_1) + V_X(\alpha_1, i_1)$$

$$E(\alpha_1, i_1) = \varepsilon_{i1}^{TB} - \varepsilon_{\alpha 1}^{TB} - V(\alpha_1, i_1) + V_X(\alpha_1, i_1)$$

INTERACTING ELECTRONS AND HOLES

HAMILTONIAN OF QUASI-ELECTRONS QUASI-HOLES:

$$\check{H}=\sum_i E_i^{(e)} c_i^+ c_i + \frac{1}{2}\sum_{ijkl}\langle i,j|V_{ee}|k,l\rangle c_i^+ c_j^+ c_k c_l$$

ELECTRON SP STATES, E-E INTERACTION

$$+\sum_j E_j^{(h)} h_j^+ h_j + \frac{1}{2}\sum_{ijkl}\langle i,j|V_{hh}|k,l\rangle h_i^+ h_j^+ h_k h_l$$

HOLE SP STATES, H-H INTERACTION

$$-\sum_{ijkl\sigma\sigma'}\left(\langle i_e,j_h|V_{eh,dir}|k_h,l_e\rangle - \langle i_e,j_h|V_{eh,xchg}|l_h,k_e\rangle\right) c_i^+ h_j^+ h_k c_l$$

ELECTRON-HOLE DIRECT AND EXCHANGE INTERACTION

1. Build configurations $|p\rangle = c_i^+ c_j^+ h_k^+ h_l^+ ..|0\rangle$

2.Build $\langle s|H|p\rangle$ 3.Diagonalize H, obtain eigenstates and eigenvalues

OPTICAL SPECTRA

EMISSION SPECTRA – FERMI'S GOLDEN RULE

$$I(\omega) = \sum_f \left| \langle f, N-1 | P^- | i, N \rangle \right|^2 \delta\left(E_i - E_f - \hbar\omega\right) \qquad P^- = \sum_{lm} \langle l_e | \vec{\varepsilon} \cdot \vec{r} | m_h \rangle c_l h_m$$

$$\langle l_e | x | m_h \rangle = \sum_{R,\alpha} R a^{(e)*}_{R,\alpha} a^{(h)}_{R,\alpha} + \sum_{R,\alpha} \sum_{\beta \neq \alpha} a^{(e)*}_{R,\alpha} a^{(h)}_{R,\beta} \langle \alpha | x | \beta \rangle + \sum_{R,\alpha} \sum_{R',\beta} a^{(e)*}_{R,\alpha} a^{(h)}_{R',\beta} \langle R, \alpha | x | R', \beta \rangle$$

ONSITE DIAGONAL

ONSITE OFFDIAGONAL

NEAREST NEIGHBORS

INTERACTIONS

IN PRNCIPLE, WE SHOULD SOLVE FOR SCREENED COULOMB INTERACTIONS

$$\check{W}(r_1, r_2, \omega) = \check{V}(r_1, r_2) + \check{V}(r_1, r') \Pi(r', r'', \omega) \check{W}(r'', r_2, \omega)$$

POLARIZATION OPERATOR

BUT WE TAKE STATICALLY SCREENED INTERACTIONS

$$\check{W}(r_1, r_2) = \frac{e^2}{\varepsilon(r_1, r_2)|r_1 - r_2|}$$

COULOMB MATRIX ELEMENTS

$$\left|\Psi_{TB}^{e,h}\right\rangle = \sum_{atoms\,\vec{R}} \sum_{orbitals\,\alpha} c_{\vec{R}\alpha}^{e.h} \left|\vec{R}\alpha\right\rangle$$

$$\left\langle \Psi_i \Psi_j \left| V \right| \Psi_k \Psi_l \right\rangle = \sum_{R_1\alpha_1} \sum_{R_2\alpha_2} \sum_{R_3\alpha_3} \sum_{R_4\alpha_4} a_{R_1\alpha_1}^{(i)*} a_{R_2\alpha_2}^{(j)*} a_{R_3\alpha_3}^{(k)} a_{R_4\alpha_4}^{(l)} \left\langle R_1\alpha_1, R_2\alpha_2 \left| \frac{e^2}{\varepsilon \left|\vec{r}_1 - \vec{r}_2\right|} \right| R_3\alpha_3, R_4\alpha_4 \right\rangle$$

COMPUTATIONAL EFFORT NONTRIVIAL!

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COULOMB MATRIX ELEMENTS

$$\left\langle \Psi_i \Psi_j \left| V \right| \Psi_k \Psi_l \right\rangle = \sum_{R_1\alpha_1} \sum_{R_2\alpha_2} \sum_{R_3\alpha_3} \sum_{R_4\alpha_4} a^{(i)*}_{R_1\alpha_1} a^{(j)*}_{R_2\alpha_2} a^{(k)}_{R_3\alpha_3} a^{(l)}_{R_4\alpha_4} \left\langle R_1\alpha_1, R_2\alpha_2 \left| \frac{e^2}{\varepsilon \left| \vec{r}_1 - \vec{r}_2 \right|} \right| R_3\alpha_3, R_4\alpha_4 \right\rangle$$

$$\left\langle \Psi_i \Psi_j \left| V \right| \Psi_k \Psi_l \right\rangle = \sum_{R_1} \sum_{\alpha_1\alpha_2\alpha_3\alpha_4} a^{(i)*}_{R_1\alpha_1} a^{(j)*}_{R_1\alpha_2} a^{(k)}_{R_1\alpha_3} a^{(l)}_{R_1\alpha_4} \left\langle R_1\alpha_1, R_1\alpha_2 \left| \frac{e^2}{\left| \vec{r}_1 - \vec{r}_2 \right|} \right| R_1\alpha_3, R_1\alpha_4 \right\rangle + \quad \text{ON-SITE}$$

$$\sum_{R_1, R_{NN}} \sum_{\alpha_1\alpha_2\alpha_3\alpha_4} a^{(i)*}_{R_1\alpha_1} a^{(j)*}_{R_{1NN}\alpha_2} a^{(k)}_{R_{1NN}\alpha_3} a^{(l)}_{R_1\alpha_4} \left\langle R_1\alpha_1, R_{NN}\alpha_2 \left| \frac{e^2}{\varepsilon_{NN} \left| \vec{r}_1 - \vec{r}_2 \right|} \right| R_{NN}\alpha_3, R_1\alpha_4 \right\rangle + \quad \text{NN}$$

$$+ \sum_{R_1} \sum_{R_2 \neq R_1} \left[\sum_{\alpha_1} a^{(i)*}_{R_1\alpha_1} a^{(l)}_{R_1\alpha_1} \right] \left[\sum_{\alpha_2} a^{(j)*}_{R_2\alpha_2} a^{(k)}_{R_2\alpha_2} \right] \frac{e^2}{\varepsilon \left| \vec{R}_1 - \vec{R}_2 \right|} \quad \text{LONG-RANGE}$$

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COULOMB MATRIX ELEMENTS

ELECTRON HOLE EXCHANGE
MONOPOLE-MONOPOLE, MONOPOLE-DIPOLE, DIPOLE-DIPOLE

$$\langle v'c'|V^X|vc\rangle = \sum_{R_1\neq R_2}\sum_{a_1b_1}\sum_{a_2b_2}(a^{(v')}_{R_1b_1})(a^{(c')}_{R_1a_1})^*(a^{(v)}_{R_2b_2})^*(a^{(c)}_{R_2\alpha_2})\langle R_1a_1, R_2b_2|\frac{1}{|\vec{r}_1-\vec{r}_2|}|R_2a_2, R_1b_1\rangle$$

$$\langle R_1a_1, R_2b_2|\frac{1}{|\vec{r}_1-\vec{r}_2|}|R_2a_2, R_1b_1\rangle = \iint dr_1dr_2\,\varphi^*_{b1}(r_1-R_1)\varphi_{a1}(r_1-R_1)\frac{1}{|r_1-r_2|}\varphi_{b2}(r_2-R_2)\varphi^*_{a2}(r_2-R_2)$$

El-hole complex
On atom at R1

El-hole complex
On atom at R2

COULOMB MATRIX ELEMENTS

ELECTRON HOLE EXCHANGE
MONOPOLE-MONOPOLE,MONOPOLE-DIPOLE,DIPOLE-DIPOLE

$$\langle v'c'|V^X|vc\rangle = \sum_{R_1\neq R_2}\sum_{a_1b_1}\sum_{a_2b_2}(a^{(v')}_{R_1b_1})(a^{(c')}_{R_1a_1})^*(a^{(v)}_{R_2b_2})^*(a^{(c)}_{R_2\alpha_2})\left\langle R_1a_1, R_2b_2\left|\frac{1}{|\vec{r}_1-\vec{r}_2|}\right|R_2a_2, R_1b_1\right\rangle$$

$$\left\langle R_1a_1, R_2b_2\left|\frac{1}{|\vec{r}_1-\vec{r}_2|}\right|R_2a_2, R_1b_1\right\rangle = \iint dr_1dr_2\,\varphi^*_{b1}(r_1-R_1)\varphi_{a1}(r_1-R_1)\frac{1}{|r_1-r_2|}\varphi_{b2}(r_2-R_2)\varphi^*_{a2}(r_2-R_2)$$

$$\frac{1}{|\vec{r}_1-\vec{r}_2|} = \frac{1}{|\vec{R}_1-\vec{R}_2|} - [(\vec{r}_1-\vec{R}_1)-(\vec{r}_2-\vec{R}_2)]\frac{(\vec{R}_1-\vec{R}_2)}{|\vec{R}_1-\vec{R}_2|^3}$$

$$+\sum_{i,j}(\vec{r}_1-\vec{R}_1)_i(\vec{r}_1-\vec{R}_1)_j\left(\frac{|\vec{R}_1-\vec{R}_2|^2\delta_{ij}-3(\vec{R}_1-\vec{R}_2)_i(\vec{R}_1-\vec{R}_2)_j}{|\vec{R}_1-\vec{R}_2|^5}\right)+$$

COULOMB MATRIX ELEMENTS

ELECTRON HOLE EXCHANGE
MONOPOLE-MONOPOLE,é

$$\iint dr_1 dr_2 \, \varphi^*_{b1}(r_1 - R_1)\varphi_{a1}(r_1 - R_1)\frac{1}{|r_1 - r_2|}\varphi_{b2}(r_2 - R_2)\varphi^*_{a2}(r_2 - R_2)$$

Monopole-monopole contribution

$$\frac{1}{|\vec{r}_1 - \vec{r}_2|} = \frac{1}{|\vec{R}_1 - \vec{R}_2|} +$$

This term is related to
ñsò state content in the hole state
and
ñpò state content in the electron state

$$\frac{\delta_{a1b1}\delta_{a2b2}}{|\vec{R}_1 - \vec{R}_2|} +$$

Other terms: dipole-monopole and dipole-dipole

MULTI-EXCITON COMPLEXES

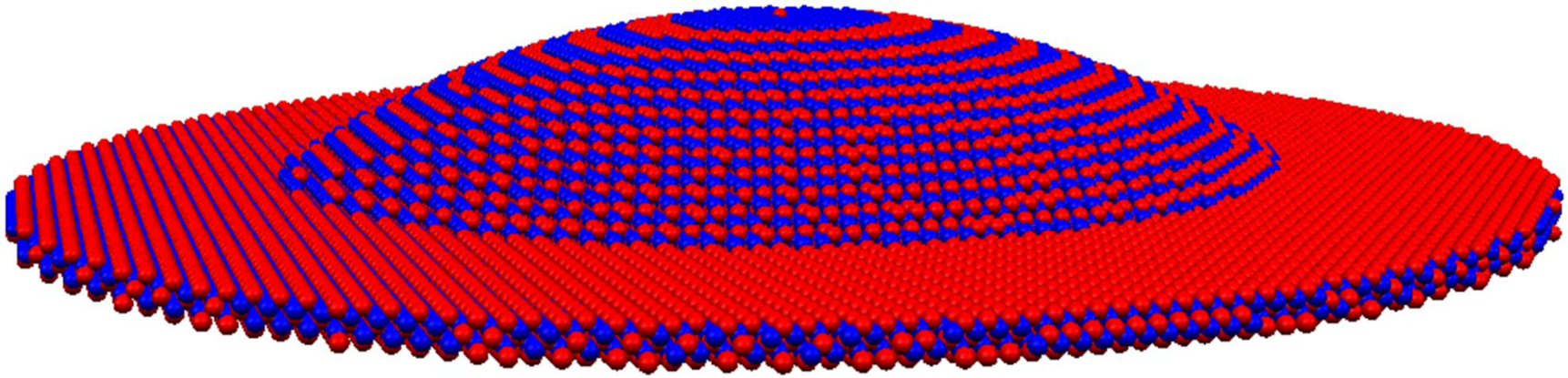
INTERACTING ELECTRONS AND HOLES

EXAMPLE

MULTI-EXCITON COMPLEXES

MULTI_EXCITON COMPLEXES IN A BENCHMARK QD

For pseudopotential calculations see
L. He and A. Zunger Phys. Rev. B 73, 115324 (2006)



QD diameter 25nm, height 3.5 nm
VFF domain: 50.3 mln atoms
TB domain : 0.561 mln atoms

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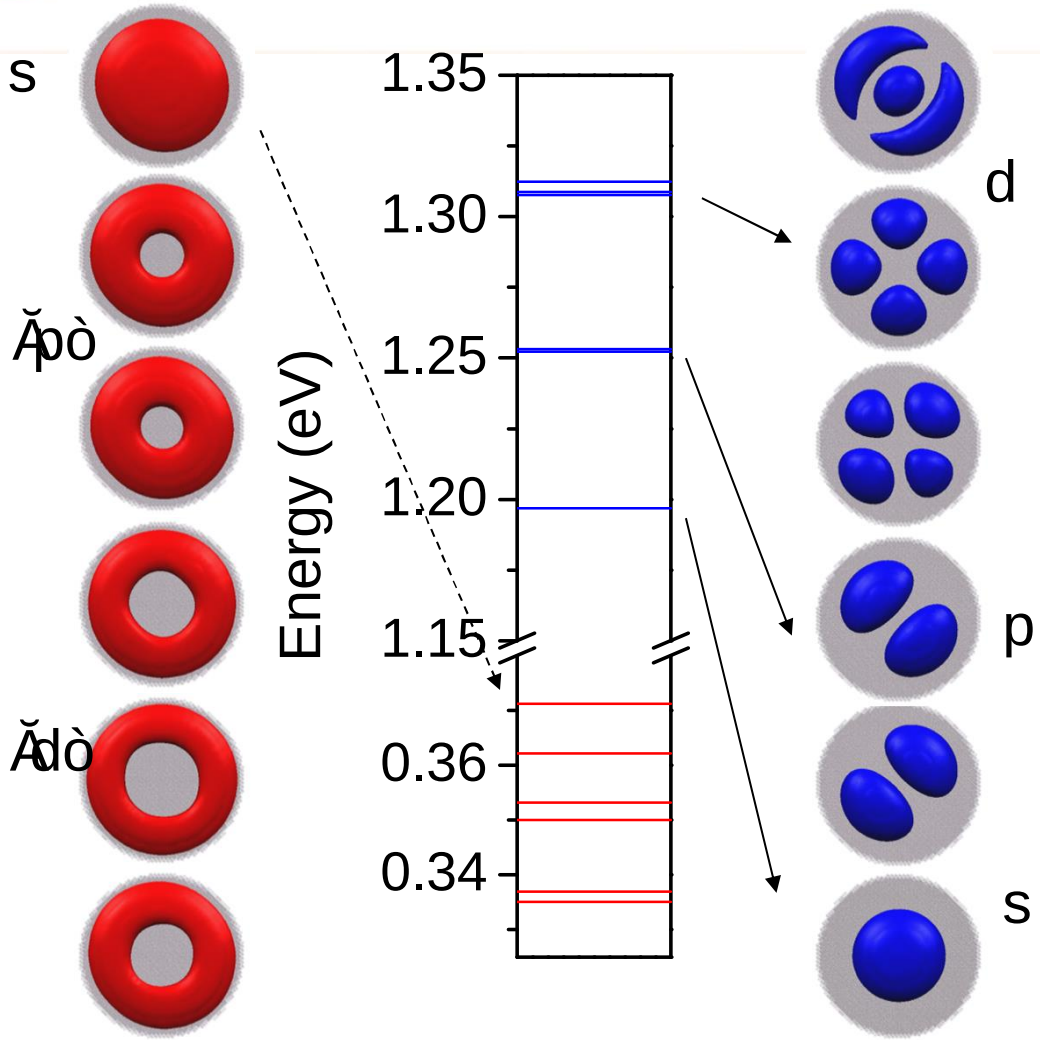
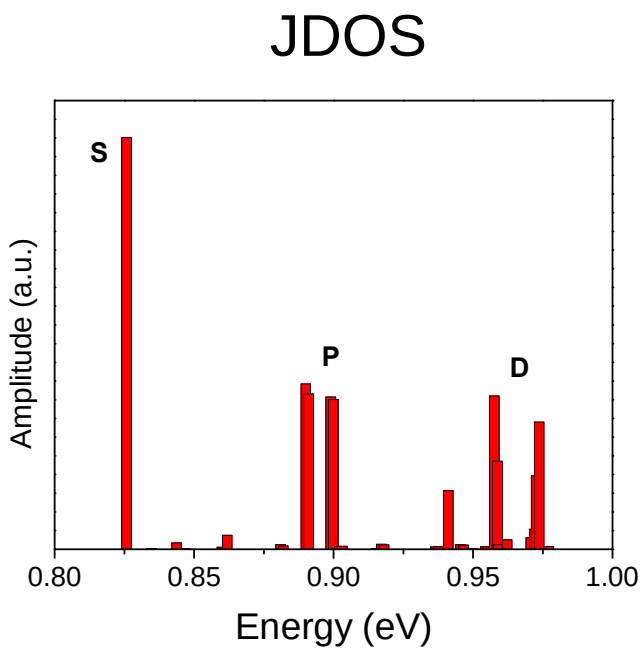
SINGLE PARTICLE STATES AND OPTICAL DENSITY OF STATES





InAs/GaAs lens type QD: D=25nm, h=3.5nm

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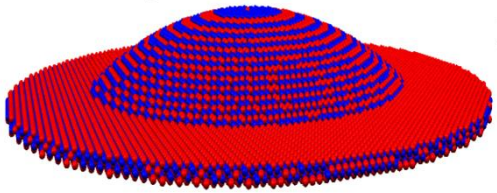
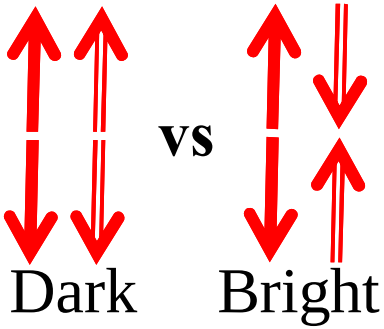
EXCITON FINE STRUCTURE



Electron-hole exchange splitting



Anisotropic EH exchange splitting.

But QD is cylindricalé

Cylindrical symmetry reduced by crystal lattice!

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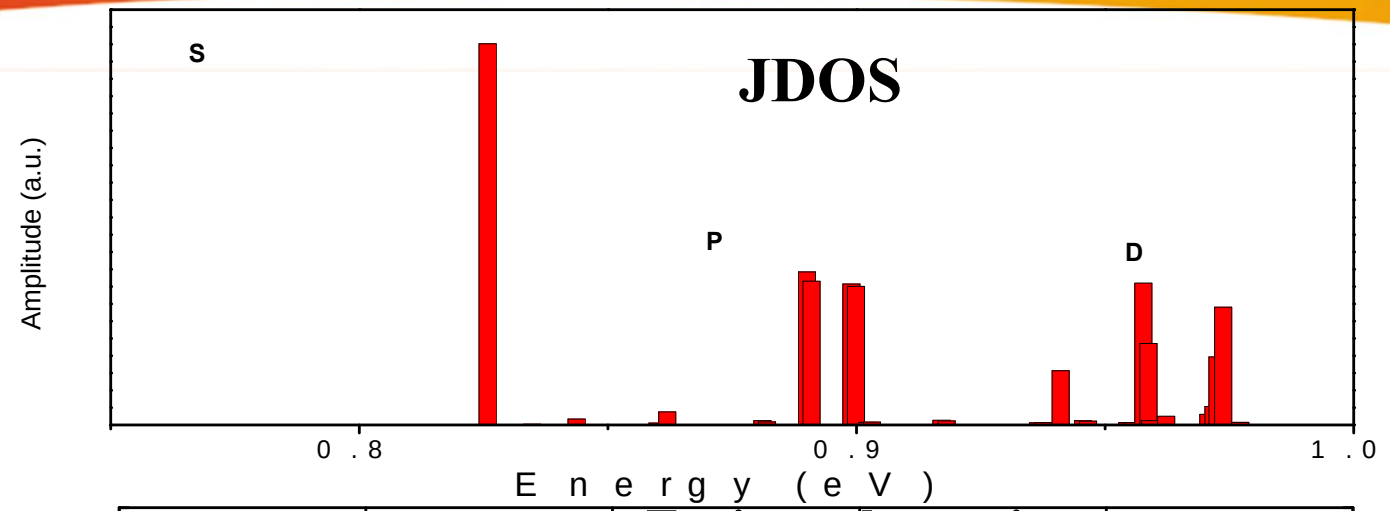
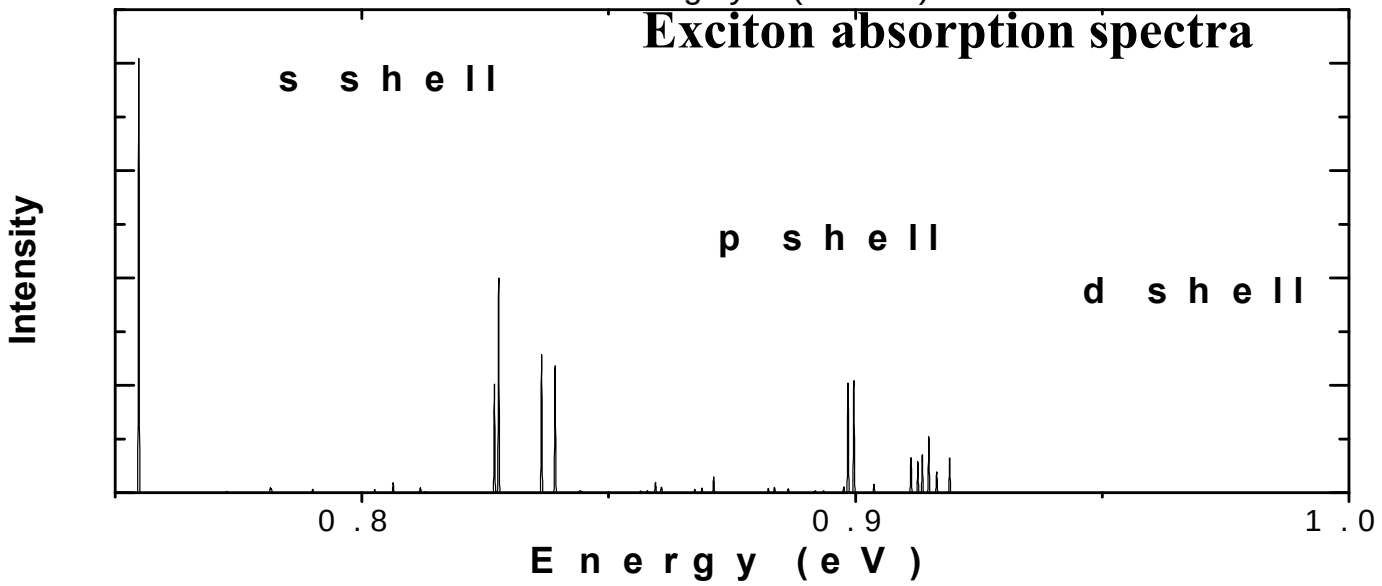
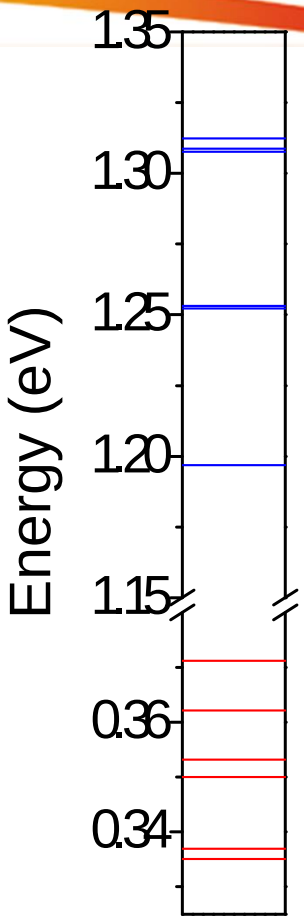
EXCITONIC ABSORPTION SPECTRUM







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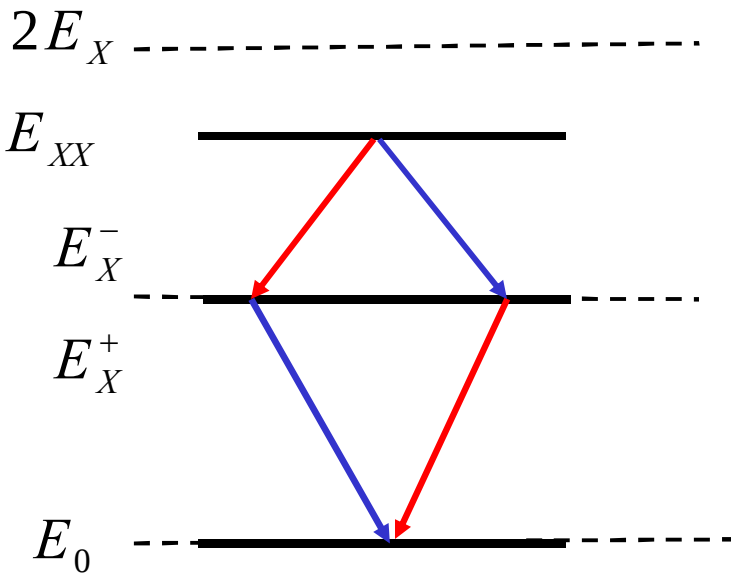
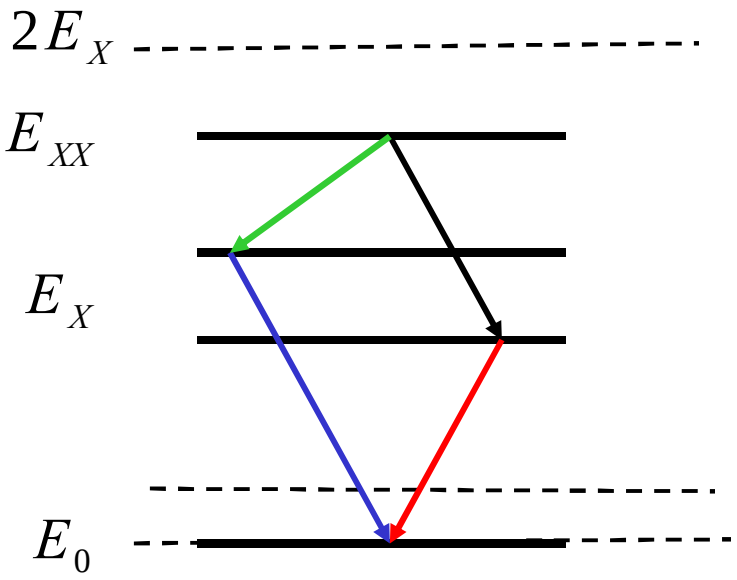
ENTANGLED PHOTON PAIR FROM EXCITON-BIEXCITON CASCADE



Benson et al

A



Real life

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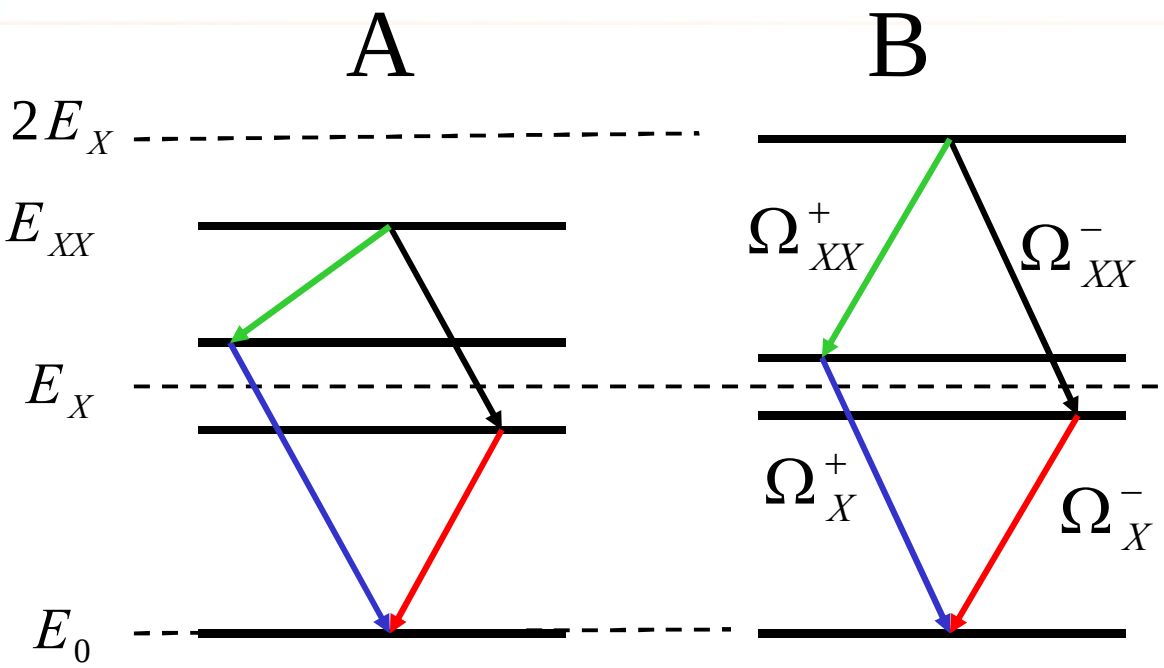
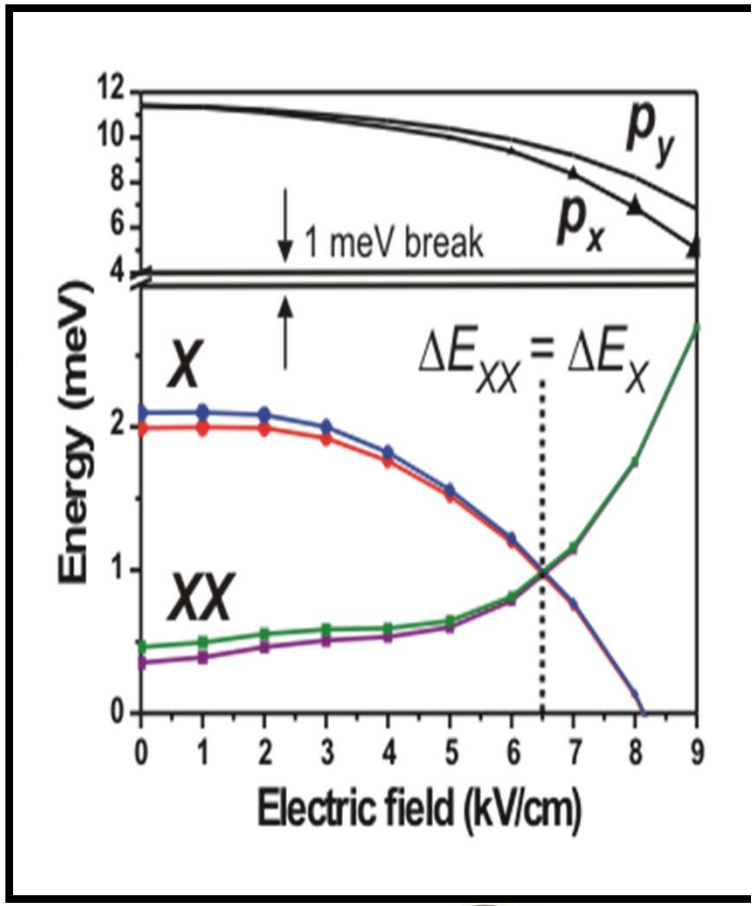
ENTANGLED PHOTON PAIR FROM EXCITON-BIEXCITON CASCADE IN LATERAL FIELD



On X-XX resonance B



$$\Psi = \frac{1}{\sqrt{2}}\left(V_{xx}V_x + H_{xx}H_x\right)$$

Even if two X are different

Reimer,Williams, Korkusinski,PH PRB2008,PRB2009

Theory

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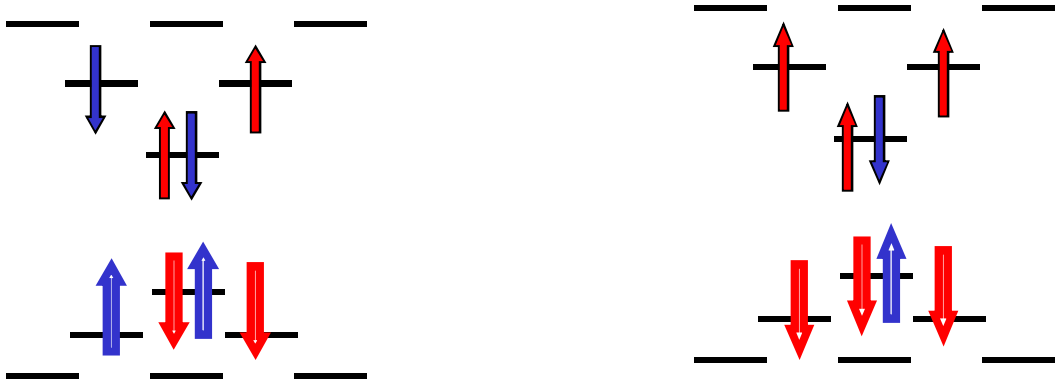
MULTIEXCITON COMPLEXES

HIDDEN SYMMETRIES
IN MULTI-EXCITON COMPLEXES



A.Wojs,PH, Solid State Comm. 100, 487 (1996).,P. H, Phys. Rev. B60, 5597 (1999); M.Bayer,I

HIDDEN SYMMETRIES ON DEGENERATE SHELLS

Interband polarisation operator $P^{+} = \sum_i c_i^{+} h_i^{+}$

On shell $[\, H \;,\; P^{+} \,] = E_X P^{+}$

$| N >= (P^{+})^{N} | 0 > .$ **E(N)= N Ex**

multiplicative states=exciton condensate

Pairing (XX) operator

$$Q^{+} = \frac{1}{2} \sum_{i,j} (c^{+}_{i\downarrow} c^{+}_{j\uparrow} + c^{+}_{j\downarrow} c^{+}_{i\uparrow})(h^{+}_{i\uparrow} h^{+}_{j\downarrow} + h^{+}_{j\uparrow} h^{+}_{i\downarrow})$$

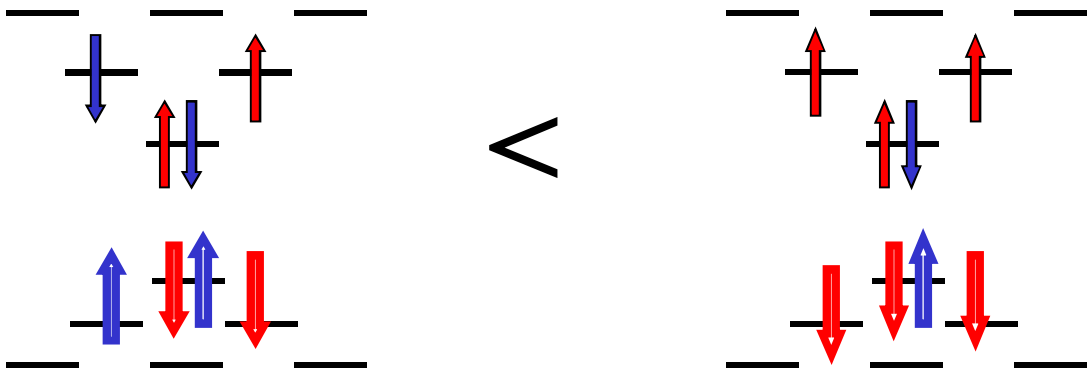
$$[\, H \;, Q^{+} \,] = E_{XX} Q^{+}$$

$$E\,(Q^{+} \,|\, 0 >) = E\,((\, P^{+})^{2} \,|\, 0 >)$$

A.Wojs,PH, Solid State Comm. 100, 487 (1996).,P. H, Phys. Rev. B60, 5597 (1999); M.Bayer,P. H, Nature 2000.

EMERGENCE OF RULES IN MX COMPLEXES

$$E\,(Q^{+}\mid 0>)\;=\;E\,((P^{+})^{2}\mid 0>)$$

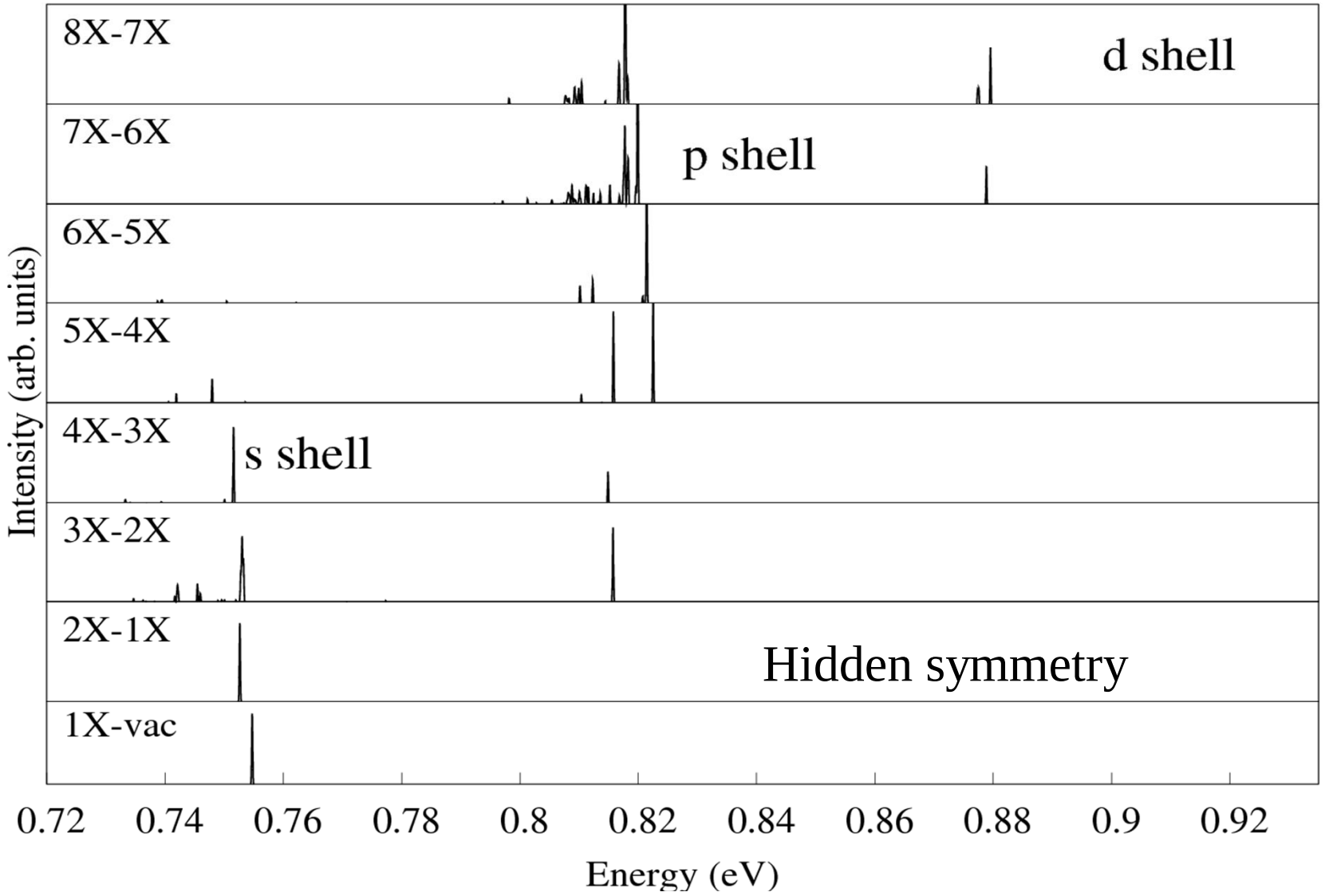


singlet triplet

HIDDEN SYMMETRIES
REPLACE HUNDS RULES IN
EXCITONIC ARTIFICIAL ATOMS

A.Wojs,PH, Solid State Comm. 100, 487 (1996).,P. H, Phys. Rev. B60, 5597 (1999); M.Bayer,P. H, Nature 2000.

MULTIEXCITON EMISSION SPECTRA



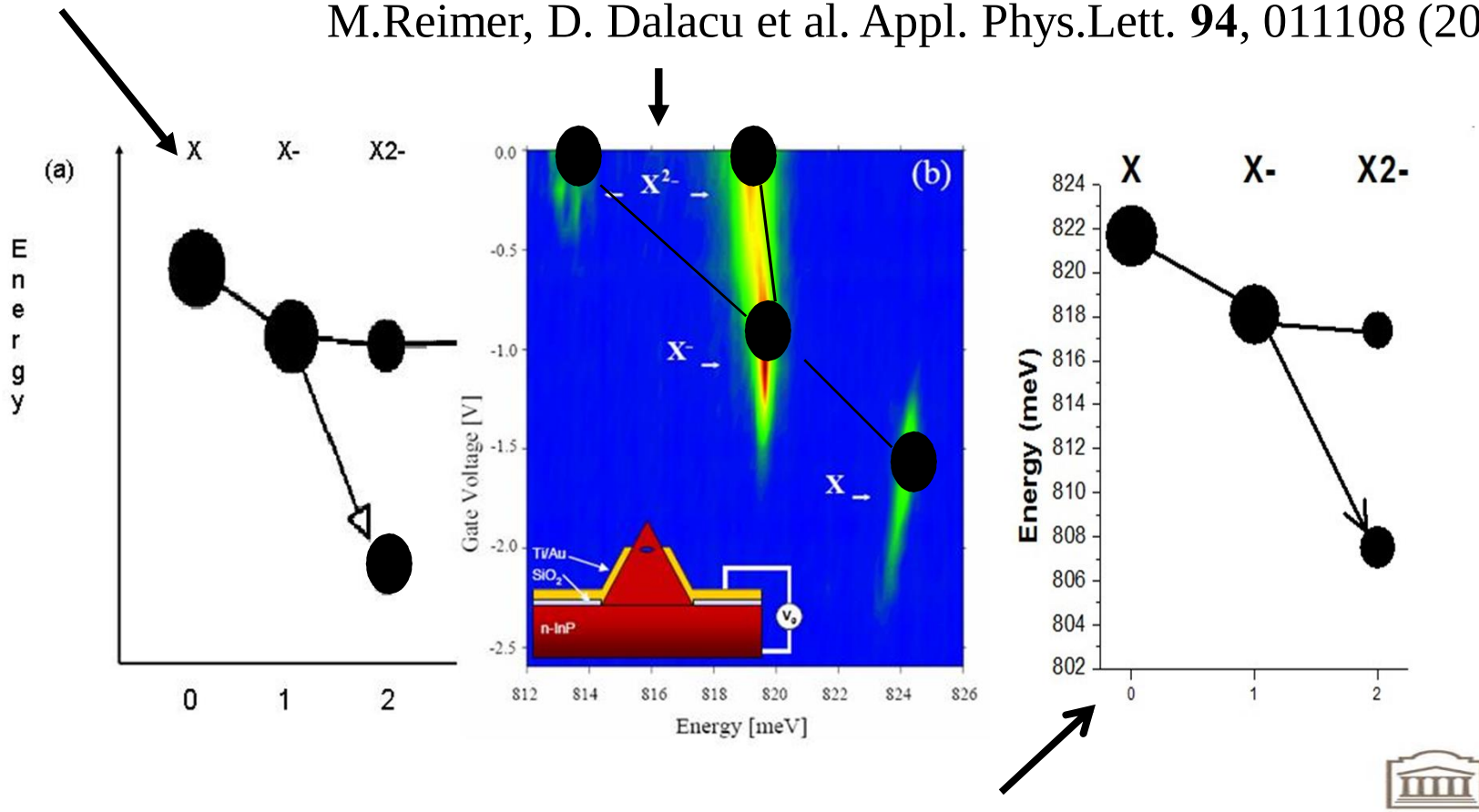
QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

SUMMARY:

CHARGED EXCITONS- SEMI-ANALITICAL THEORY, ATOMISTIC CI CALCULATION AND EXPERIMENT

A. Wojs and P. Hawrylak Phys. Rev. B 55, 13066 (1997), theory

M.Reimer, D. Dalacu et al. Appl. Phys.Lett. **94**, 011108 (2009).



Atomistic CI calculation (Zielinski et al)

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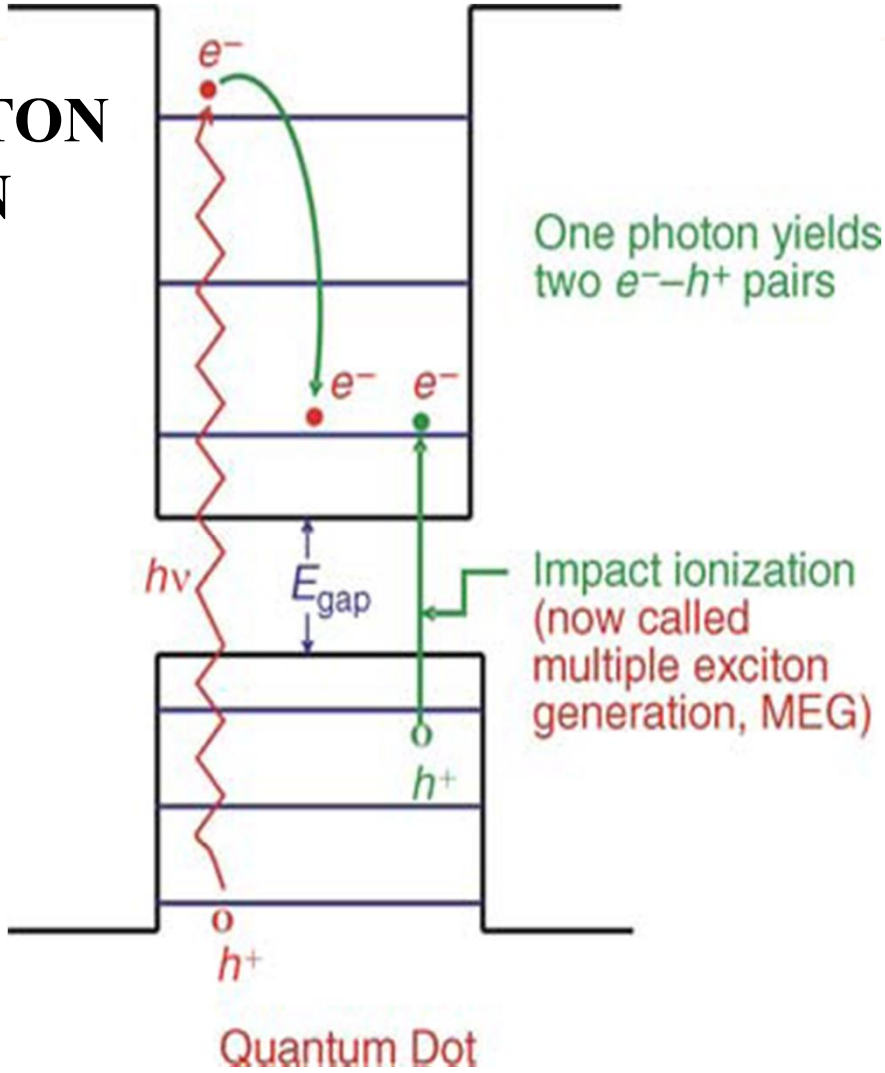
QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

SUMMARY:

MEG IN ABSORPTION IN NANOCRYSTALS

MULTI-EXCITON GENERATION IN QUANTUM DOT



Nozik,..
Klimov,é
Efros,é .
Zunger,é
é é
é é

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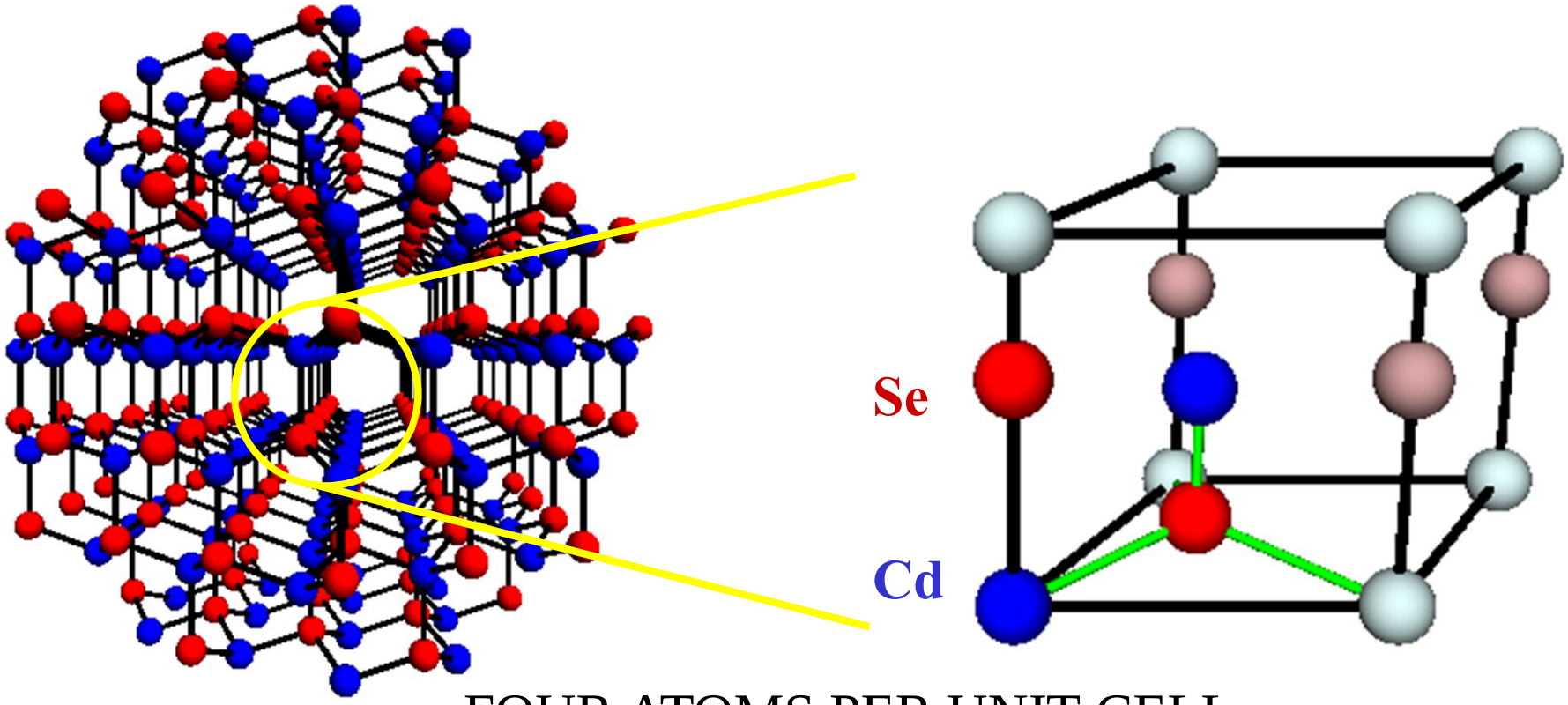
CADMIUM SELENIDE

WURTZITE CRYSTAL STRUCTURE



FOUR ATOMS PER UNIT CELL:
TWO CADMIUM ATOMS
TWO SELENIUM ATOMS

KORKUSINSKI
VOZNYY

INTERACTING ELECTRONS AND HOLES

ELECTRON-HOLE HAMILTONIAN

$$\hat{H} = \sum_{i\sigma} E^{(e)}_{i\sigma} c^{+}_{i\sigma} c_{i\sigma} + \frac{1}{2} \sum_{ijkl\sigma\sigma'} \langle i\sigma, j\sigma' | V_{ee} | k\sigma', l\sigma \rangle c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{k\sigma'} c_{l\sigma}$$

$$+ \sum_{j\sigma} E^{(h)}_{j\sigma} h^{+}_{j\sigma} h_{j\sigma} + \frac{1}{2} \sum_{ijkl\sigma\sigma'} \langle i\sigma, j\sigma' | V_{hh} | k\sigma', l\sigma \rangle h^{+}_{i\sigma} h^{+}_{j\sigma'} h_{k\sigma'} h_{l\sigma}$$

$$- \sum_{ijkl\sigma\sigma'} (\langle i\sigma, j\sigma' | V_{eh} | k\sigma', l\sigma \rangle - \langle i\sigma, j\sigma' | V_{eh} | l\sigma, k\sigma' \rangle) c^{+}_{i\sigma} h^{+}_{j\sigma'} h_{k\sigma'} c_{l\sigma}$$

ELECTRON SP STATES, E-E INTERACTION

HOLE SP STATES, H-H INTERACTION

ELECTRON-HOLE INTERACTION
DIRECT + EHXC

$$+ \sum_{ijkl\sigma\sigma'} \langle i\sigma, j\sigma' | V | k\sigma', l\sigma \rangle c^{+}_{i\sigma} c_{j\sigma'} c_{k\sigma'} h_{l\sigma}$$

$$+ \sum_{ijkl\sigma\sigma'} \langle i\sigma, j\sigma' | V | k\sigma', l\sigma \rangle h^{+}_{i\sigma} h_{j\sigma'} c_{k\sigma'} h_{l\sigma} + \ldots..$$

E-H NONCONSERVING TERMS

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QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

SUMMARY:

INTRODUCTION
ATOMIC STRUCTURE DEFINITION
STRAIN
ELECTRONIC STRUCTURE CALCULATION
- **TIGHT BINDING METHOD**
- **EFFECT OF STRAIN**
- **SURFACE PASSIVATION**
- **EXTERNAL FIELDS**

MANY-BODY EFFECTS
- **MULTI-EXCITON COMPLEXES**
- **CHARGED EXCITONS**

EXAMPLES:
- **InAs/GaAs SELF-ASSEMBLED DOTS**
- **CdSe NANOCRYSTAL,GRAPHENE**

REFERENCES:

QNANO:COMPUTATIONAL PLATFORM FOR ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

CONTRIBUTIONS:

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O. VOZNYY (IMS) – AB-INTIO, NCs,PV

I.OZFIDAN,P.POTASZ.D.GUCLU - GRAPHENE

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S.J.SHENG (IMS/NCTU) – EFF.MASS, B, CI