

Modeling charged defects and defect levels in semiconductors and oxides with DFT: *An improved inside-out perspective*

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Unlimited Release

Why model defects in semiconductors and oxides?

Radiation effects in electronics

Process modeling for semiconductors

Radiation detectors

Defect chemistry in nuclear fuels and nuclear waste

Goals:

(1) Qualitative understanding

Augment experiments

- incomplete, inconclusive, unavailable, expensive

(2) Quantitative characterization

Predictive simulations, inform coarser models

- not just publishable, but defensible to engineers

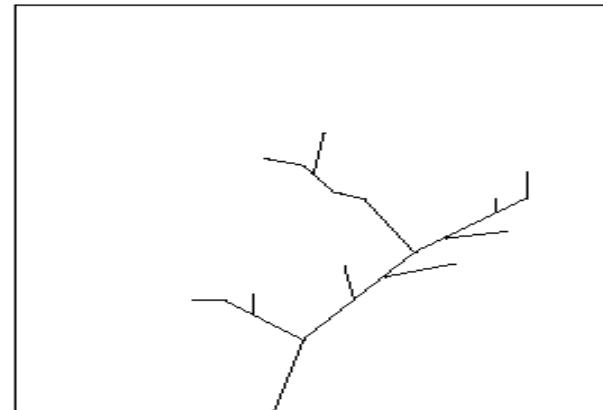
Defects: from atoms to devices

Initial defect distribution

Radiation creates displacement damage:

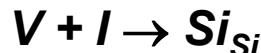


and charge carriers (electrons and holes)

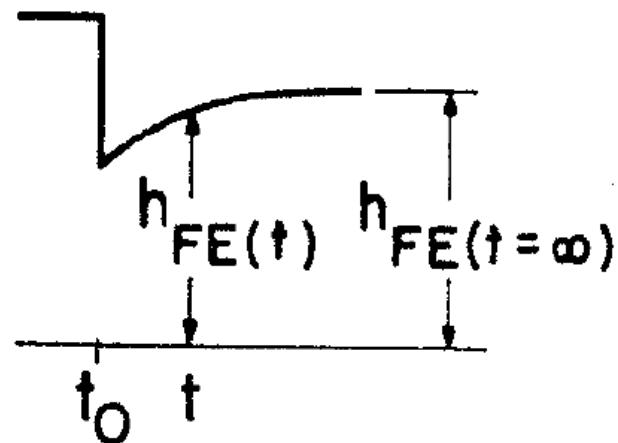


Defect evolution

Defects react with each other, and with other dopants and impurities:

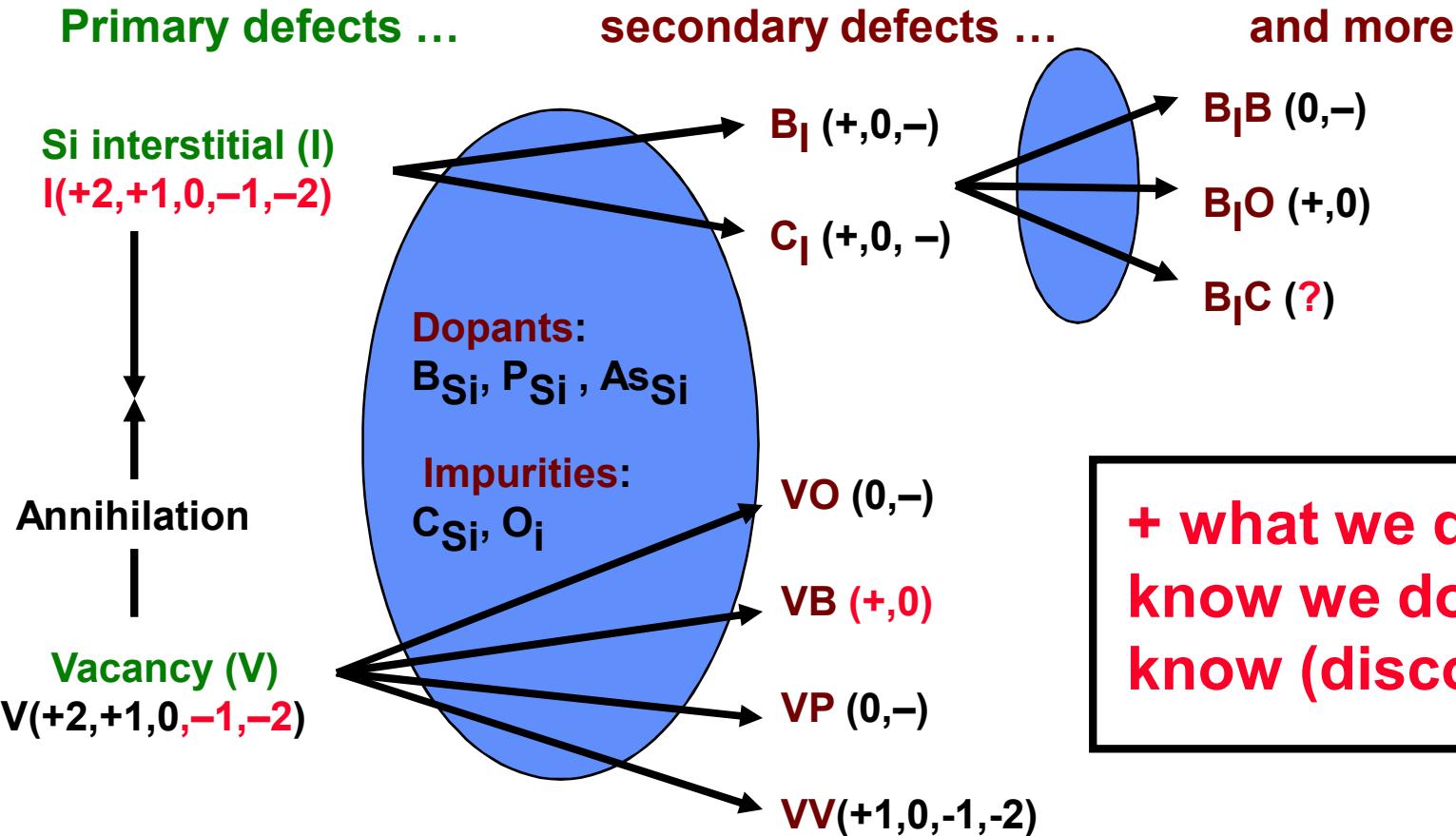


Defects recombine electrons and holes, modifying currents:



Radiation/implant/processing creates evolving chemistry of defects. Those defects govern the performance of electronic devices.

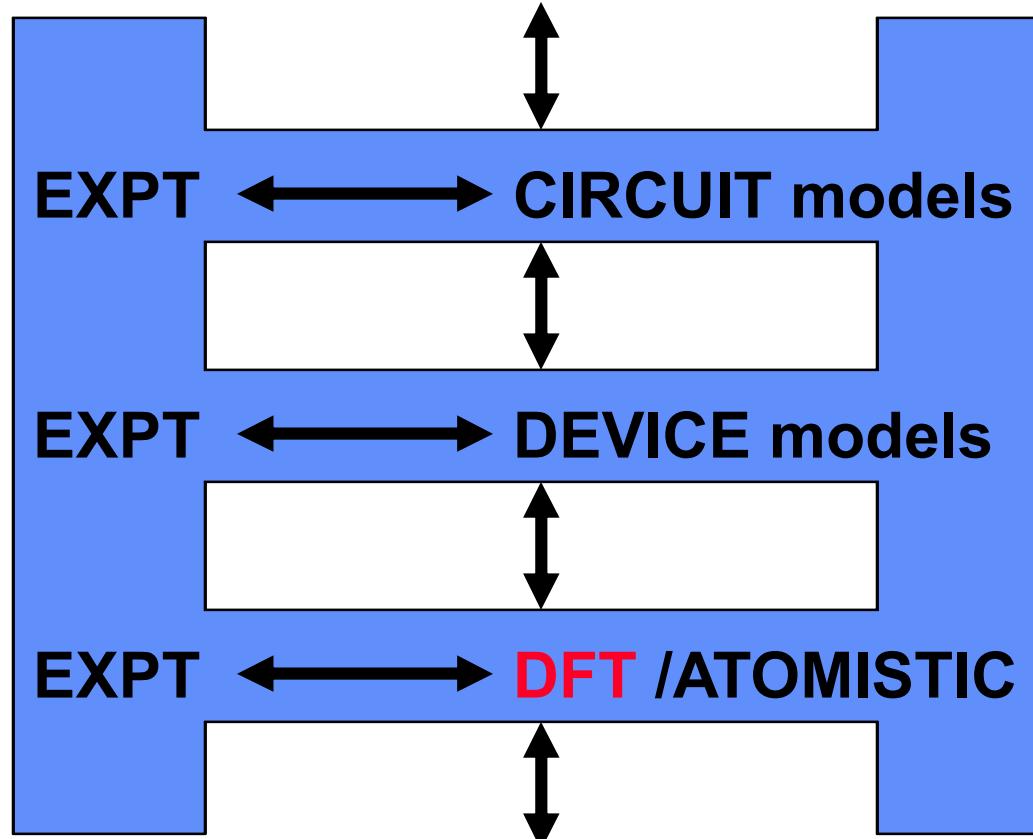
The radiation effect defect universe: Si



Need DFT - density functional theory - to fill gaps in defect physics: defect band gap energy levels, diffusion activation

Multiscale ladder for radiation damage

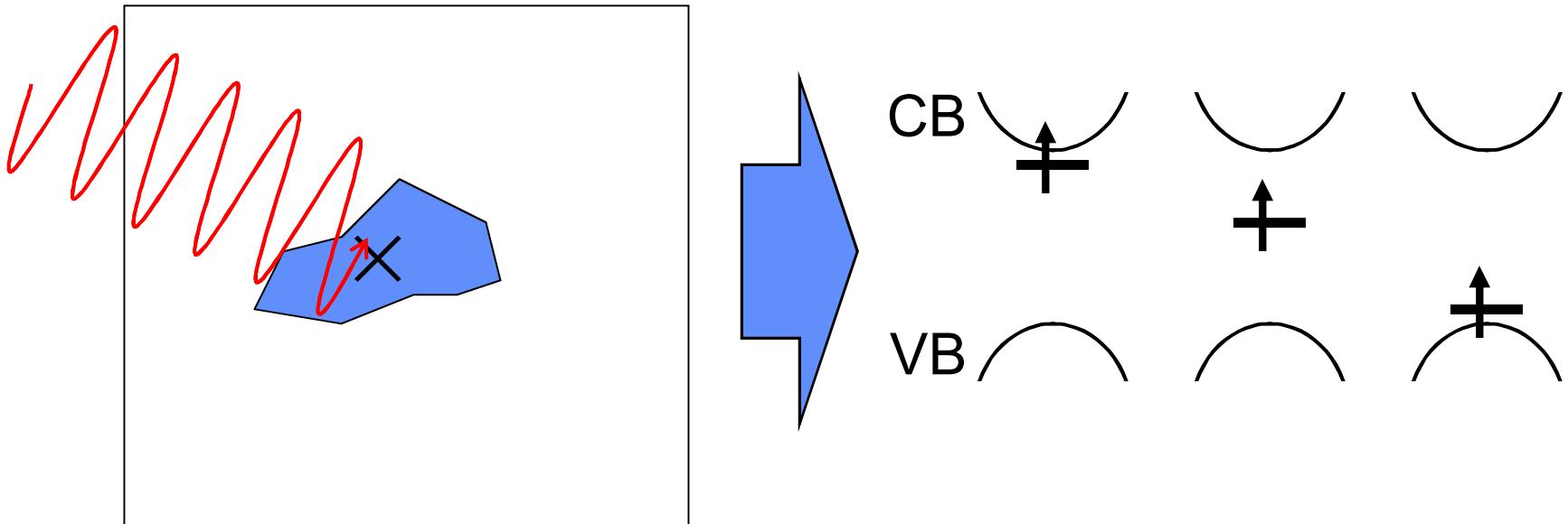
Electrical system response



Require: quantitative confidence
Verification, validation, uncertainty

Radiation damage and defects levels

Radiation damage ...

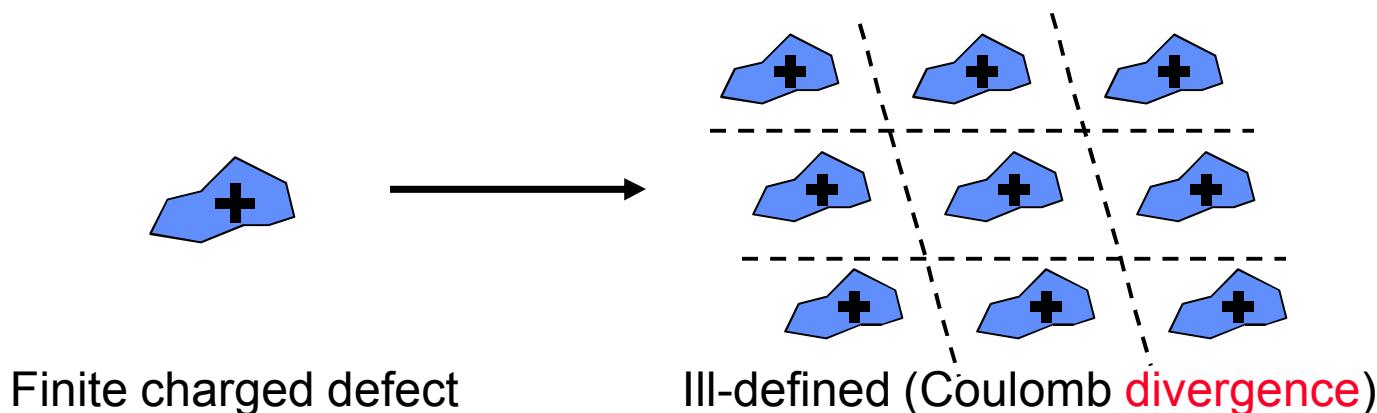


produces defects ... and introduces electronic transitions

... and we need to quantify these transitions; DFT

Challenges for density functional theory

- **Conventional DFT fails for defect levels in semiconductors**
 - (1) Physical accuracy: e.g., “band gap problem”
 - (2) Computational model size limitations
 - (3) Shortage of good data for validation
 - (4) Supercell problem for charged defects:



Lots of DFT calculations, no robust, predictive method

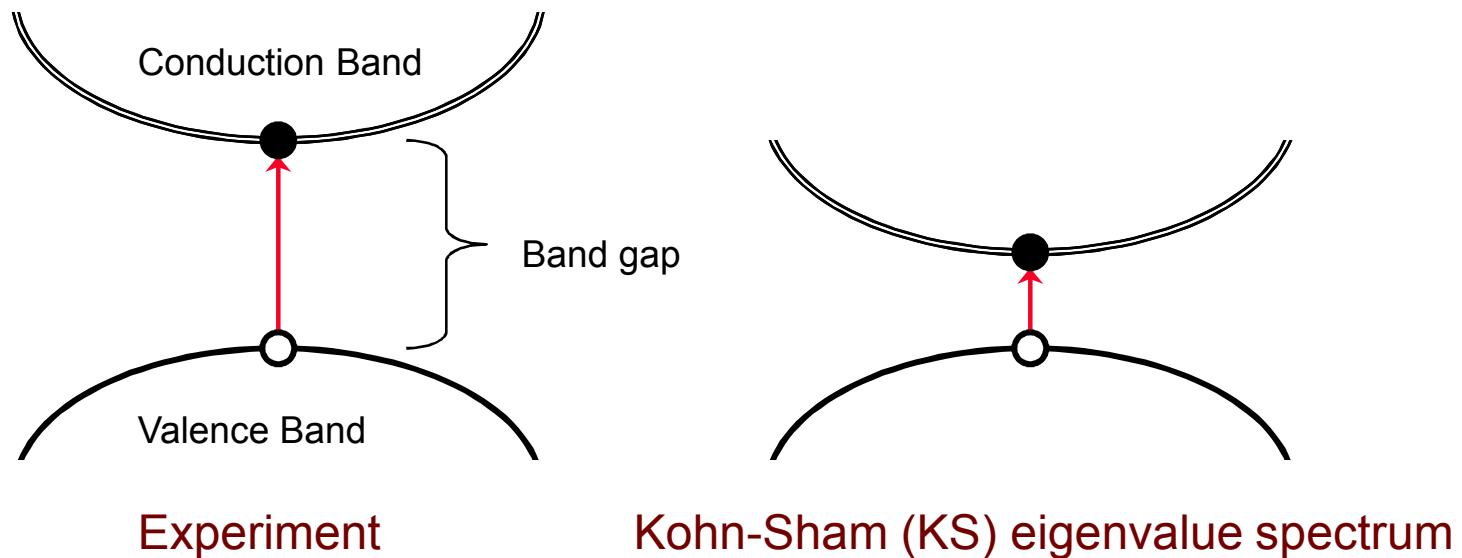
DFT “band gap problem”

DFT gap. i.e., in KS eigenvalues, significantly underestimates experiment

[L.J. Sham and M. Schlüter, PRL **51**, 1888 (1983); PRB **32**, 3883 (1985)]

Si: expt: 1.2 eV, DFT/LDA: 0.5 eV

GaAs: expt. 1.5 eV, DFT/LDA: 0.5 eV



The band gap defines the energy scale for defect levels

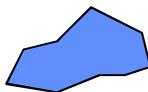
Fundamental impediment to quantitative predictions?

The Supercell Approximation

Fast Fourier Transforms are convenient means to solve 3D Poisson Equation.

DFT codes typically assume periodic boundary conditions.

However, our finite defect is not periodic ...



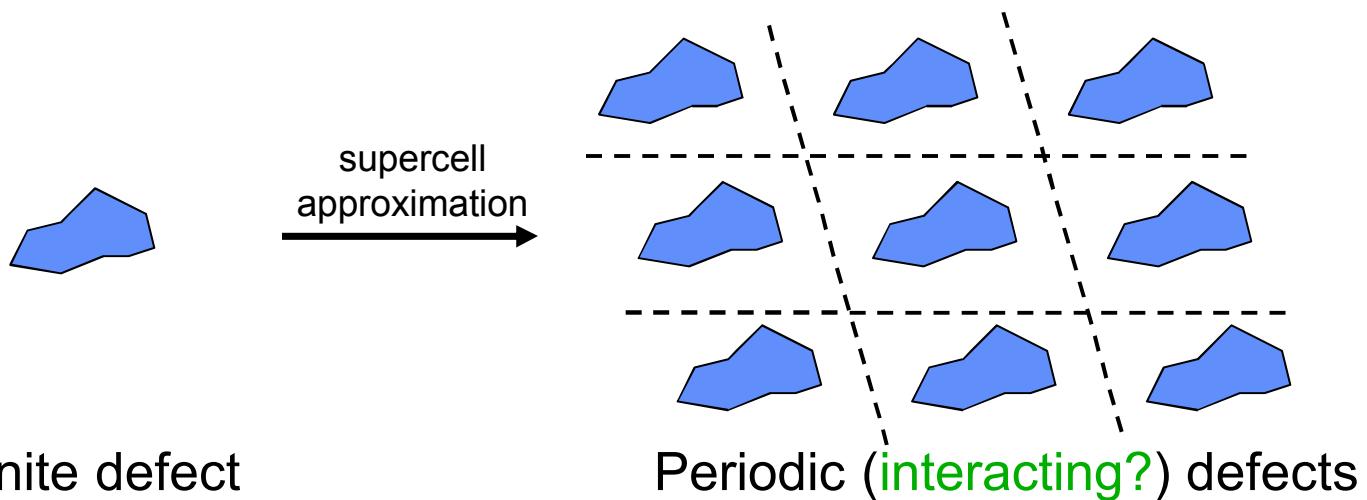
Finite defect

The Supercell Approximation

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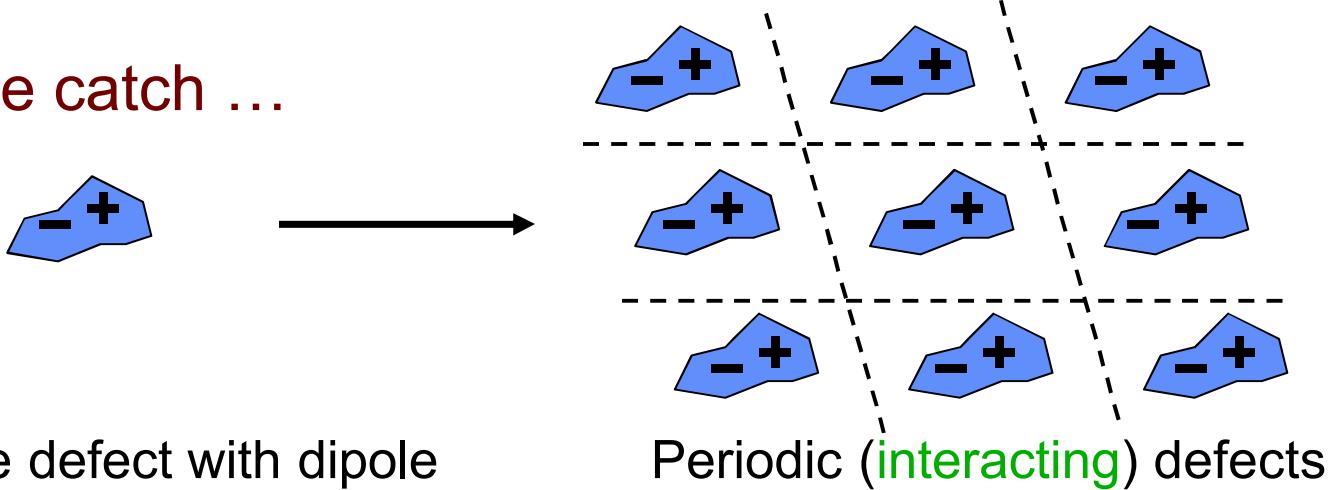


The supercell Idea:

Surround perturbed defect region with enough material to buffer defects.
In the limit of large enough supercells approach an isolated defect.

The Supercell Approximation

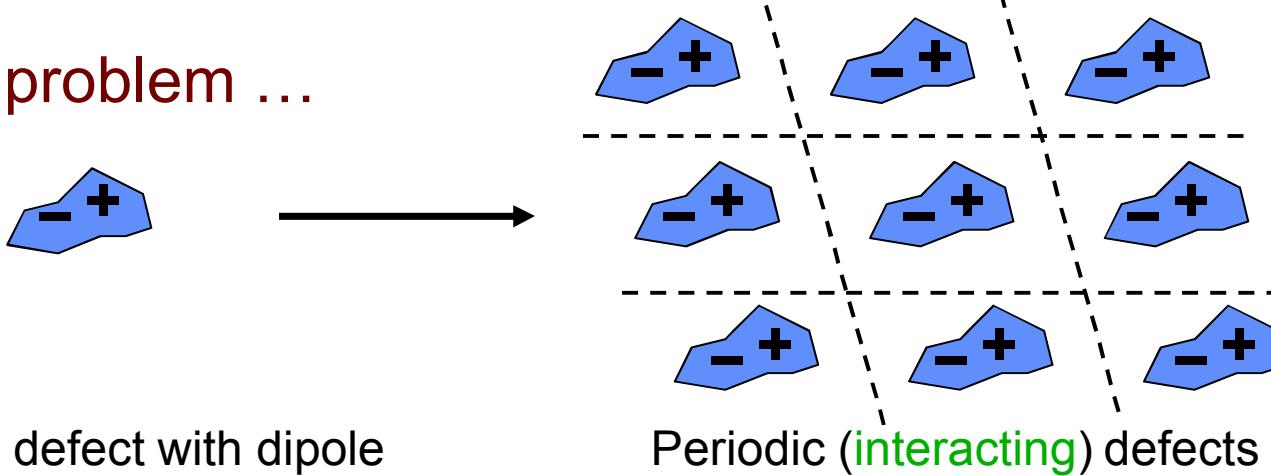
the catch ...



DFT expense limits size of supercell - defects interact

The supercell approximation

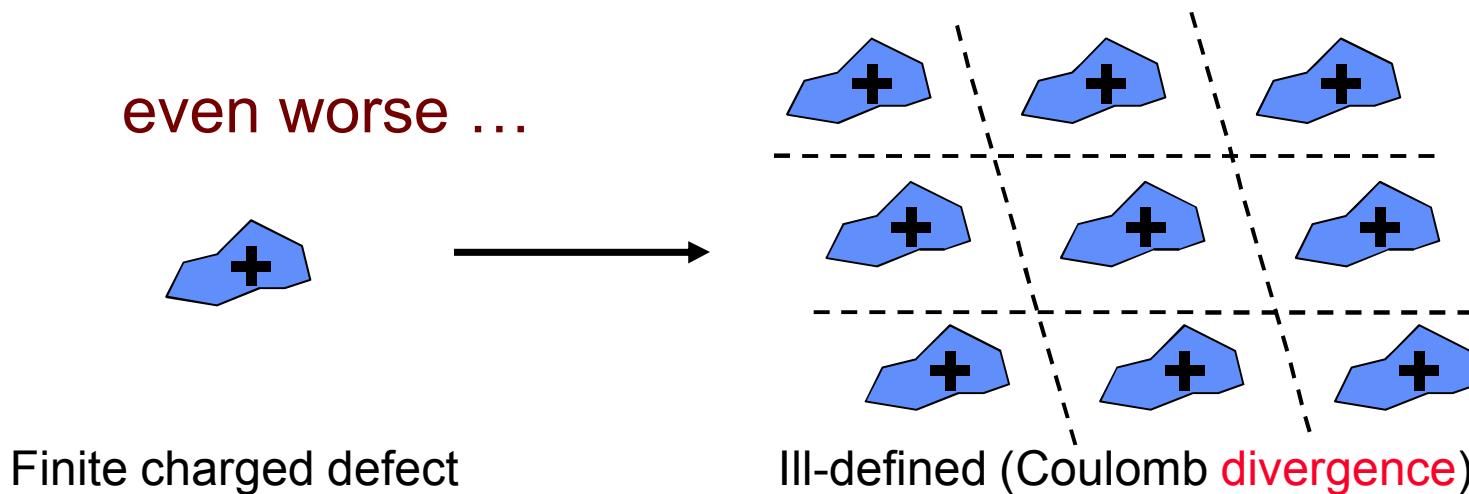
A problem ...



Finite defect with dipole

Periodic (interacting) defects

even worse ...



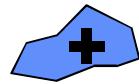
Finite charged defect

III-defined (Coulomb divergence)

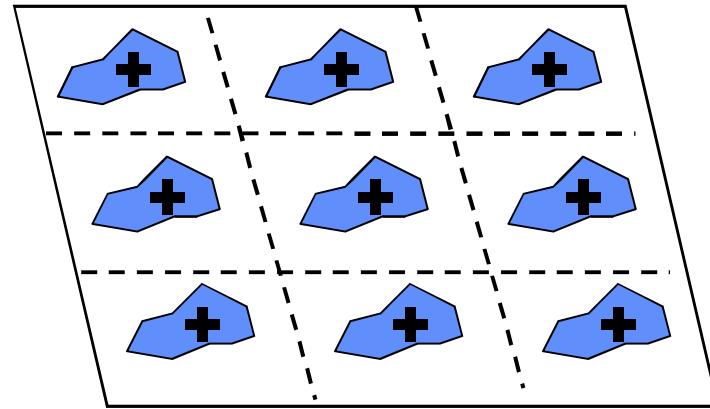
Interactions and divergence are key issues

Jellium to eliminate divergence?

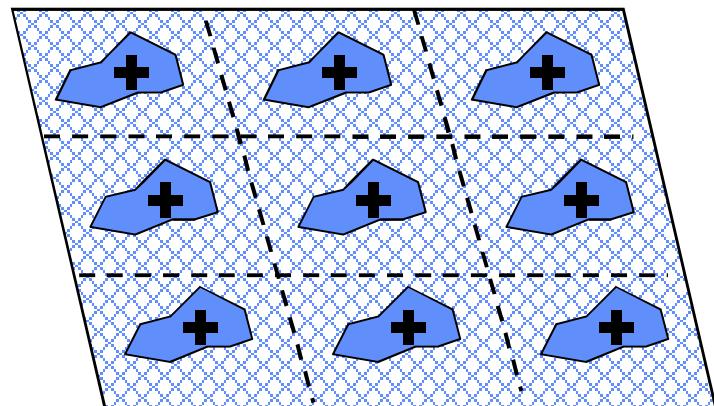
Isolated defect ...



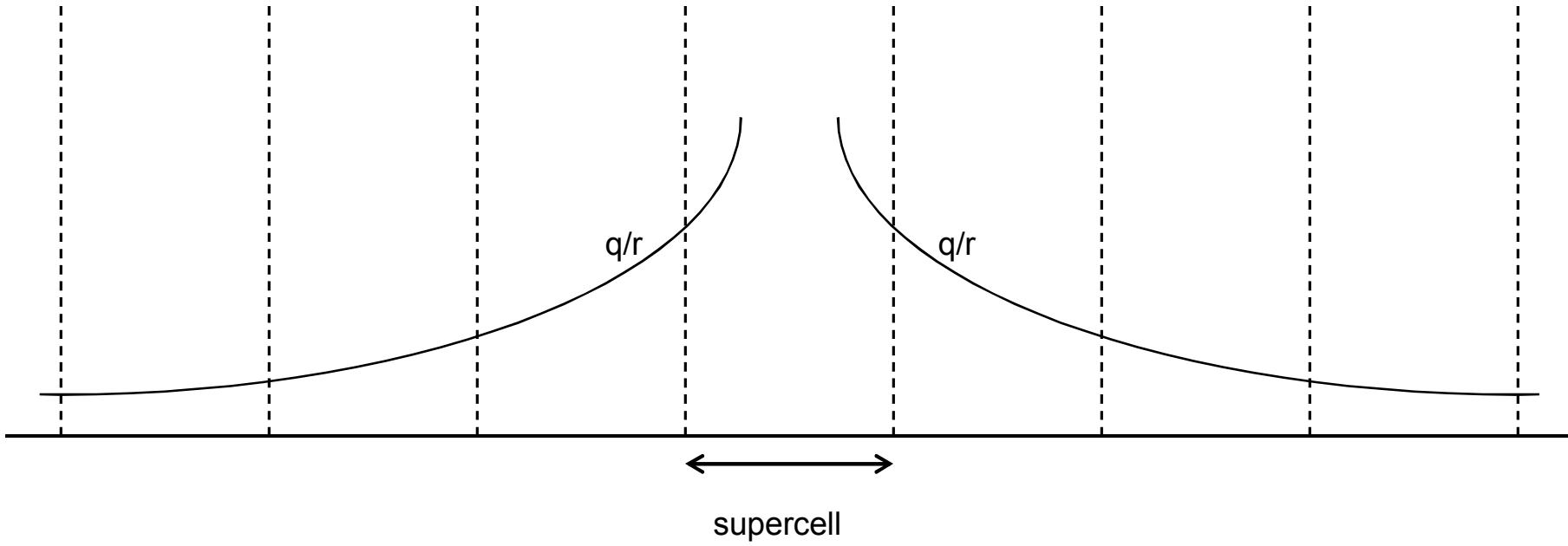
Apply supercell approximation ...



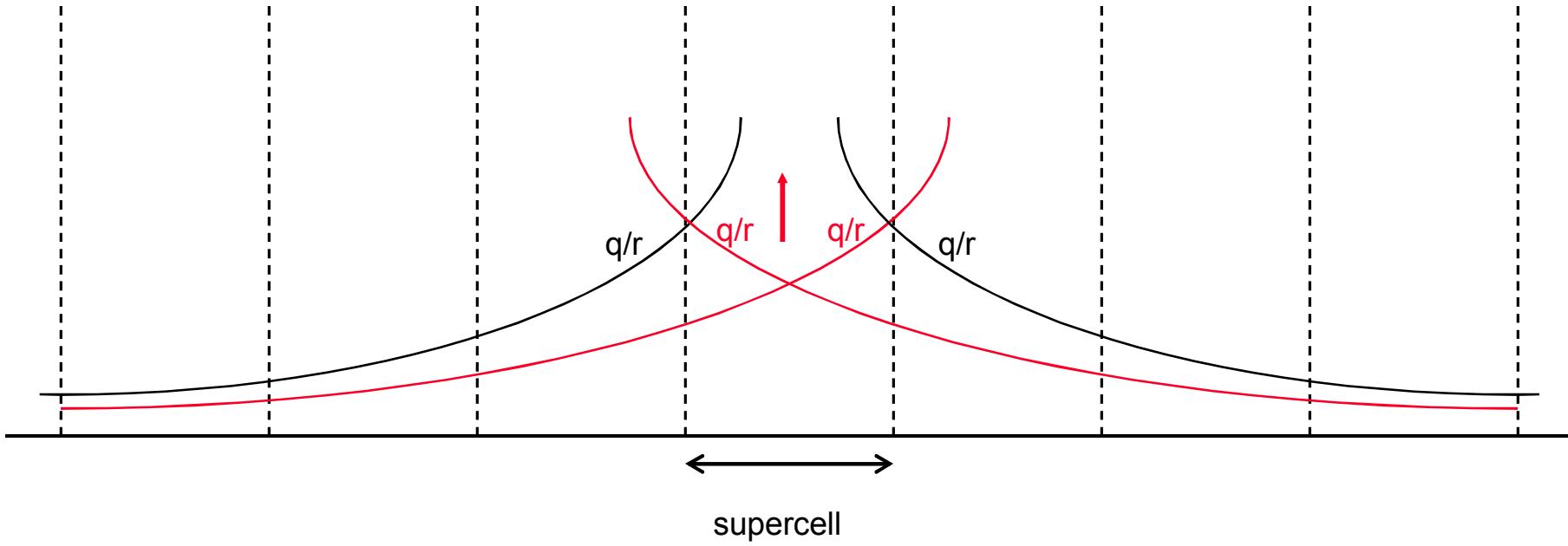
Neutralize with flat
background charge:
“jellium”



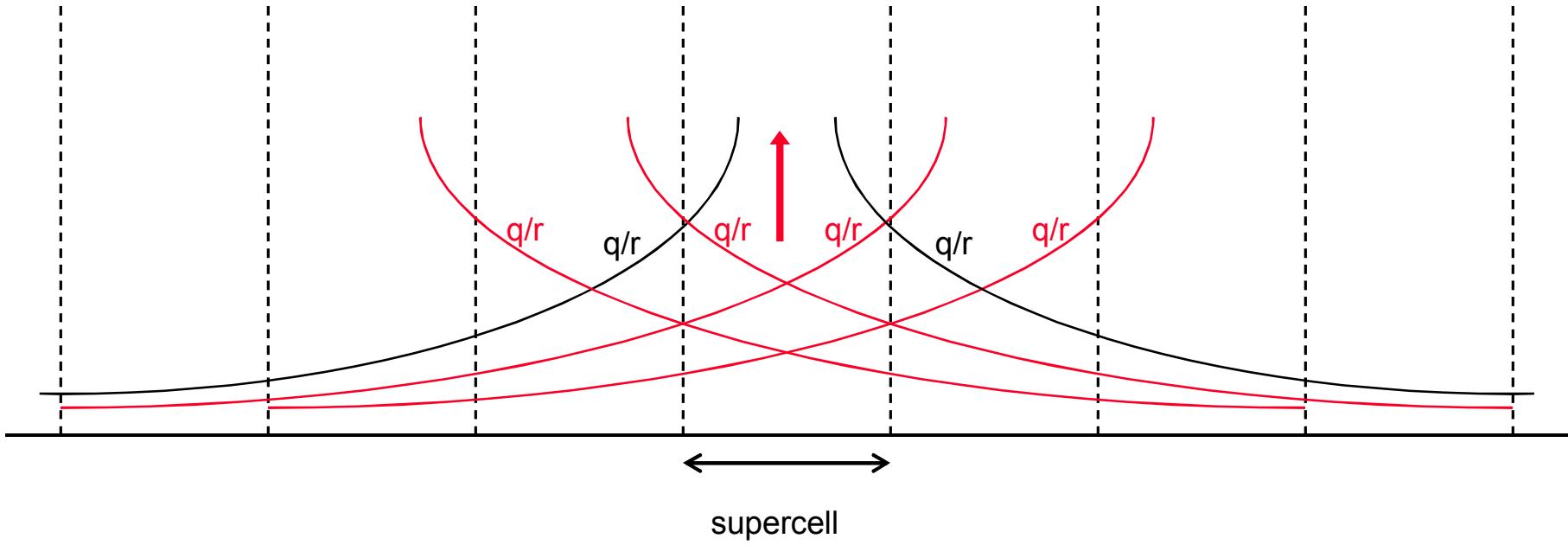
Whence the divergence?



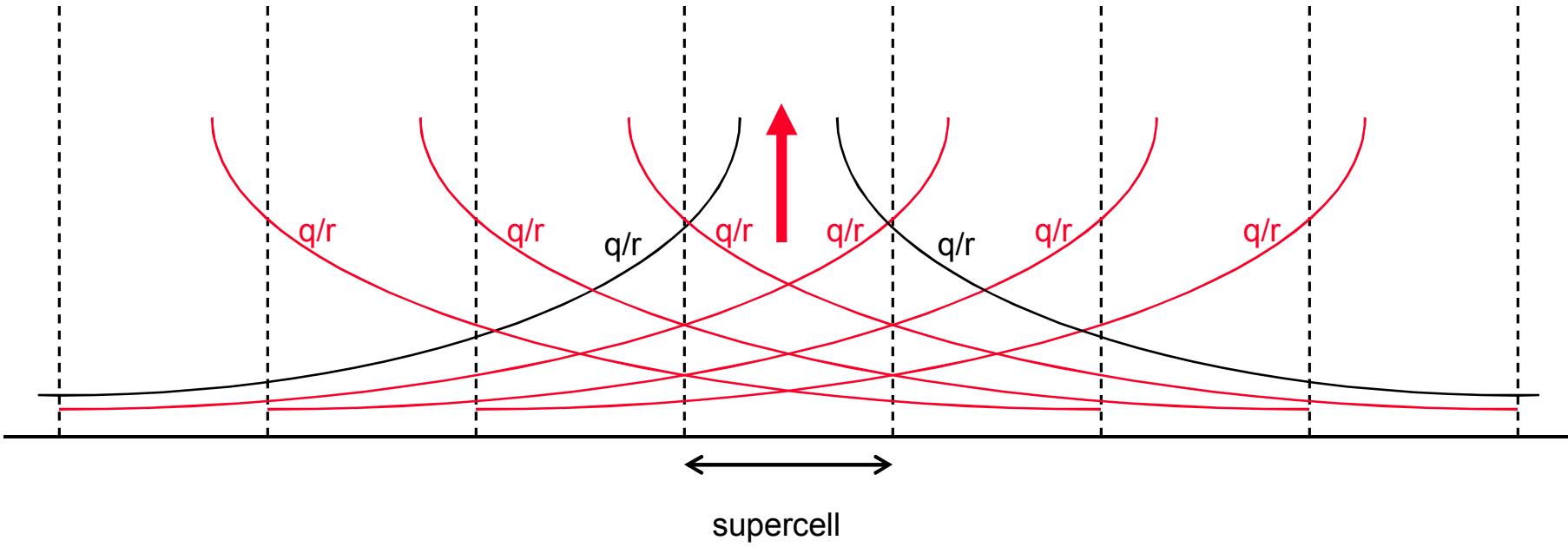
Whence the divergence?



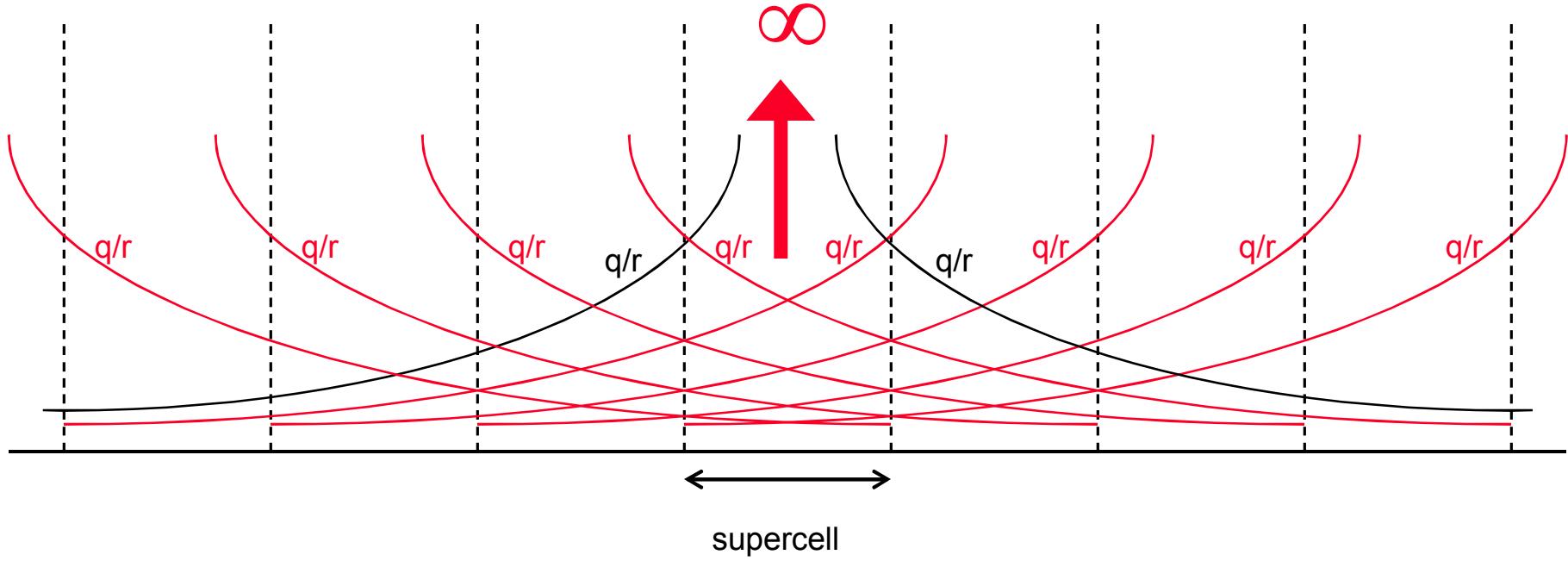
Whence the divergence?



Whence the divergence?



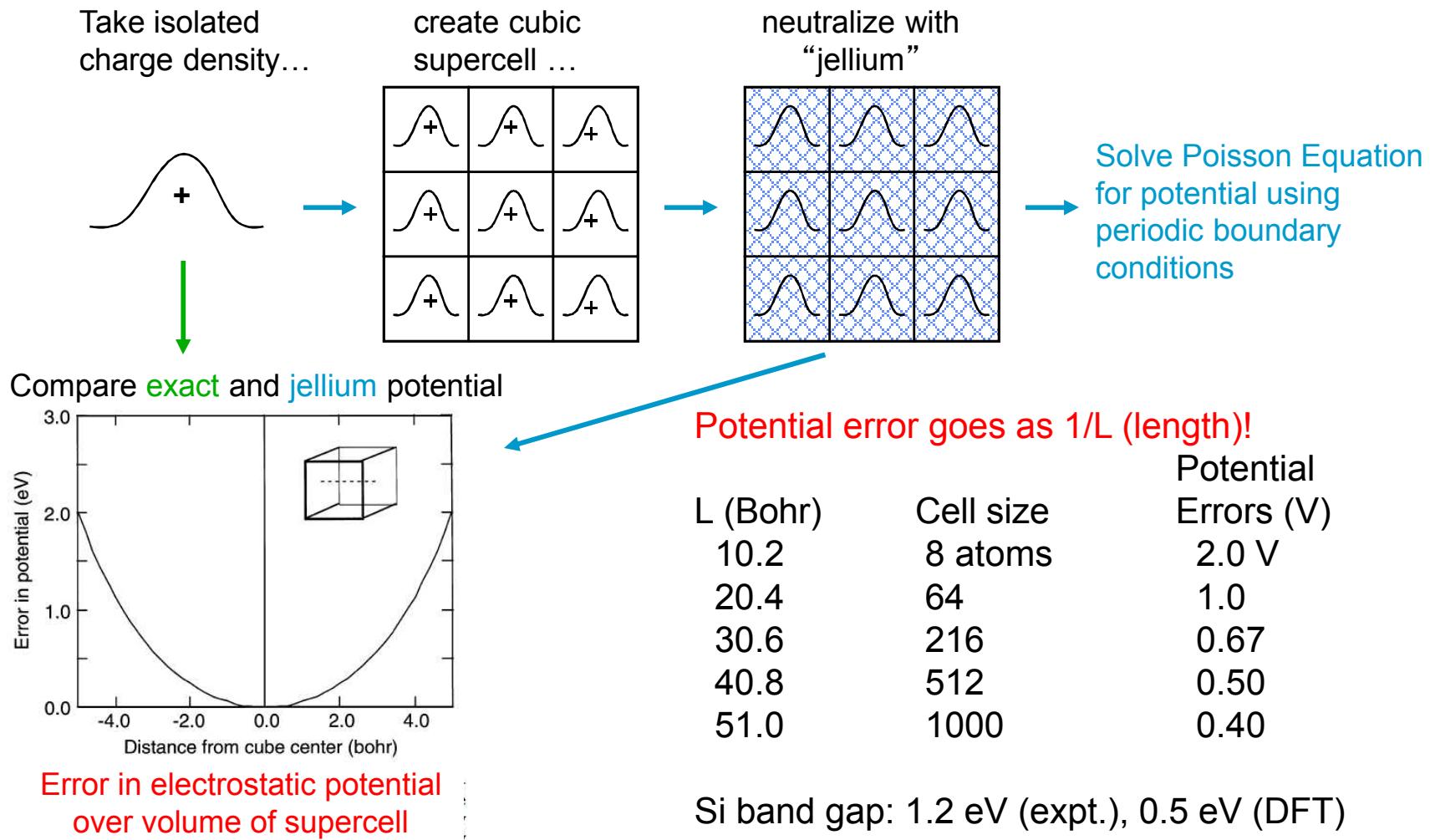
Whence the divergence?



Divergence arises from infinite-ranged q/r potentials from periodic images

Divergence is not flat

Net charge boundary conditions - jellium

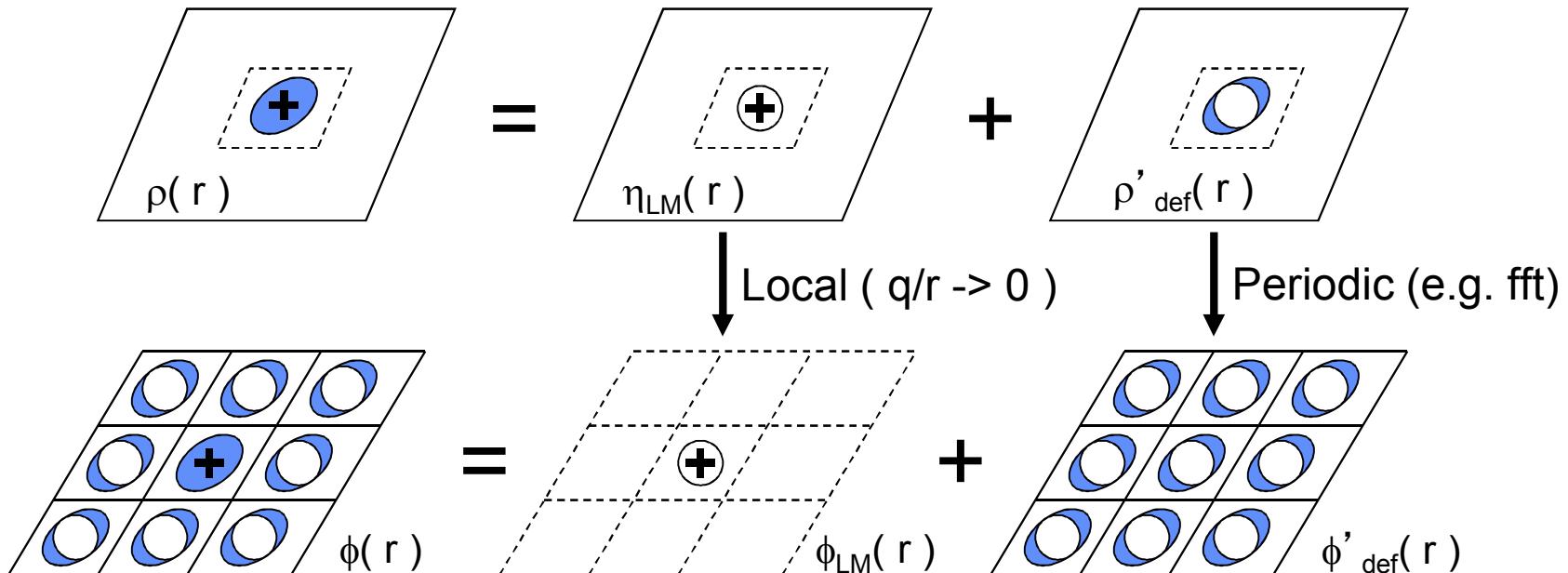


Standard jellium method has large $O(1/L)$ error in potential
Error propagated into density distribution and into energy

Local Moment CounterCharge (LMCC)

P.A. Schultz, PRB **60**, 1551 (1999)

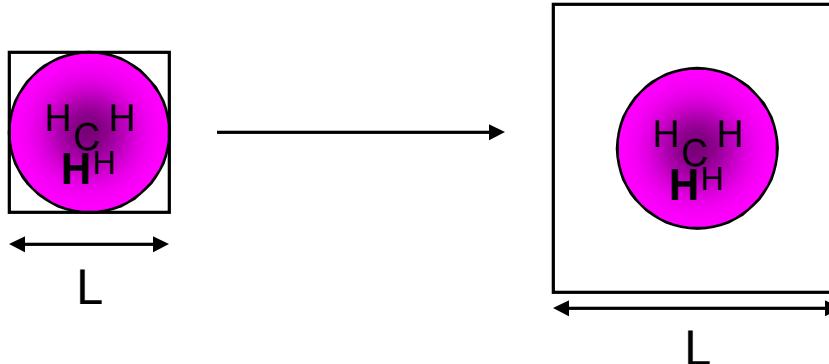
- Solution of Poisson Equation is linear in the density
- LMCC: split total density $\rho(r)$ into two pieces ...
 - (1) model local density $\eta_{LM}(r)$ matching multipole (charge) of $\rho(r)$
 - (2) remainder (momentless) density $\rho'_{def}(r) = \rho(r) - \eta_{LM}(r)$



Gives proper $r \rightarrow \infty$ asymptotic boundary condition
 Avoid (not ignore!) Coulomb divergence

Charged cell convergence - LMCC

P.A. Schultz, PRB **60**, 1551 (1999)



Charged, no dipole: $\text{CH}_4 \rightarrow \text{CH}_4[+]$... Ionization Potential

$L = 18.0 - 30.0$ bohr (9.5-15.9 Å) IP varies $< 10^{-5}$ eV

Dipole, no charge: $\text{Na}-\text{Cl}$ diatomic molecule ... Total Energy

$L = 16.8 - 30.0$ bohr (8.9-15.9 Å) TE varies $< 10^{-5}$ eV

Dipole, charge: $\text{OH} \rightarrow \text{OH}[-]$... Electron Affinity

$L = 18.0 - 30.0$ bohr (9.5-15.9 Å) EA varies $< 10^{-3}$ eV

Total energy, levels, i.e. full Hamiltonian are all immediately converged.
-> electrostatic *potential* correctly represented by LMCC, not just energy

A supercell theory of defect energies

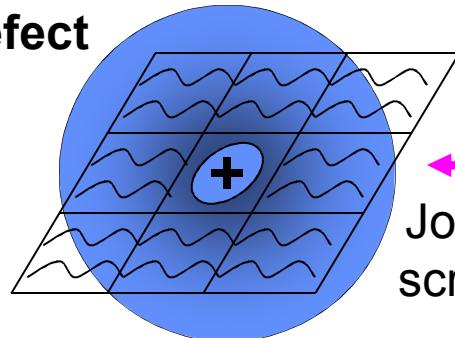
Peter A. Schultz, Phys. Rev. Lett. **96**, 246401 (2006).

Target system:
isolated defect

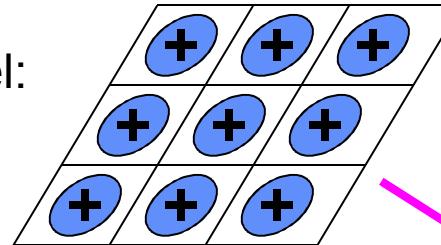
=

Computational
model for
isolated defect

(+ DDO
for defect
banding)



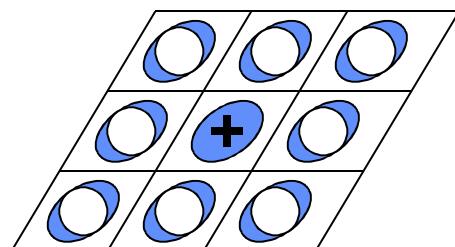
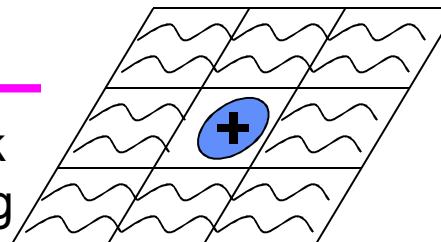
Standard
DFT model:
Supercell



LMCC to fix
boundary
conditions

Finite Defect Supercell Model

Jost Bulk
screening



Crystal embedding
to fix μ_e

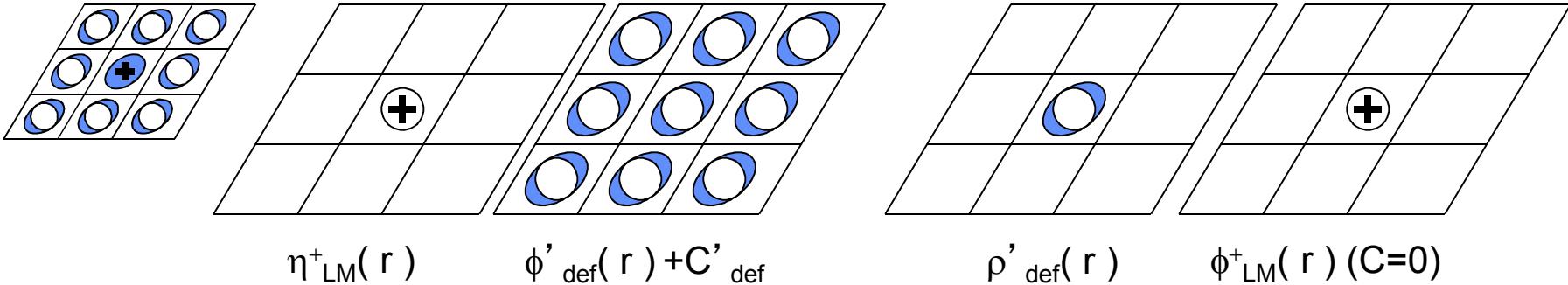
*“Ab initio” computational model – connect model to physics
Calculations with rigorous control of charge boundary conditions*

(i.e., not jellium-based)

A fixed chemical potential μ_e

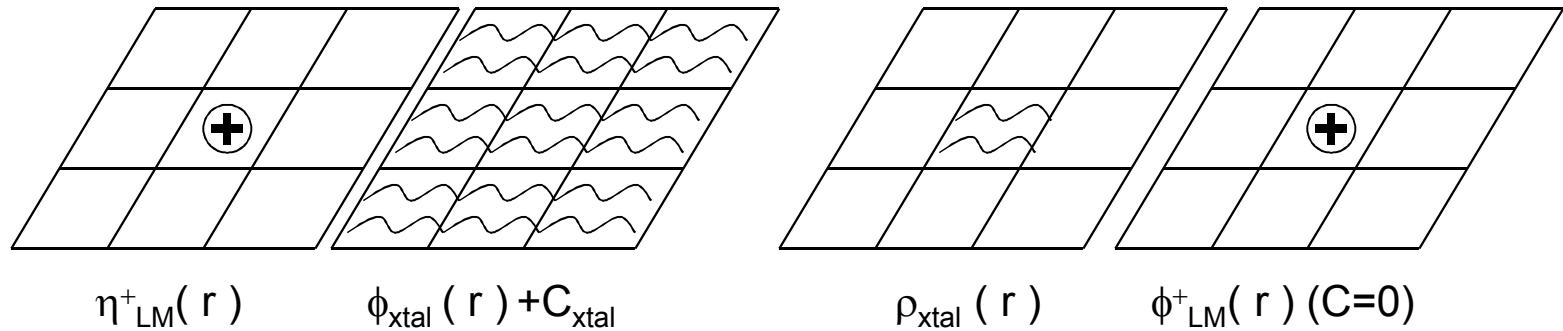
Replace interaction of net charge with periodic defect potential ...

$$E_{\mu_0} = - \int dr \eta^+_{LM} (\phi'_{def} + C'_{def}) + \int_{UC} dr \phi^+_{LM} \rho'_{def}$$



... with crystal potential:

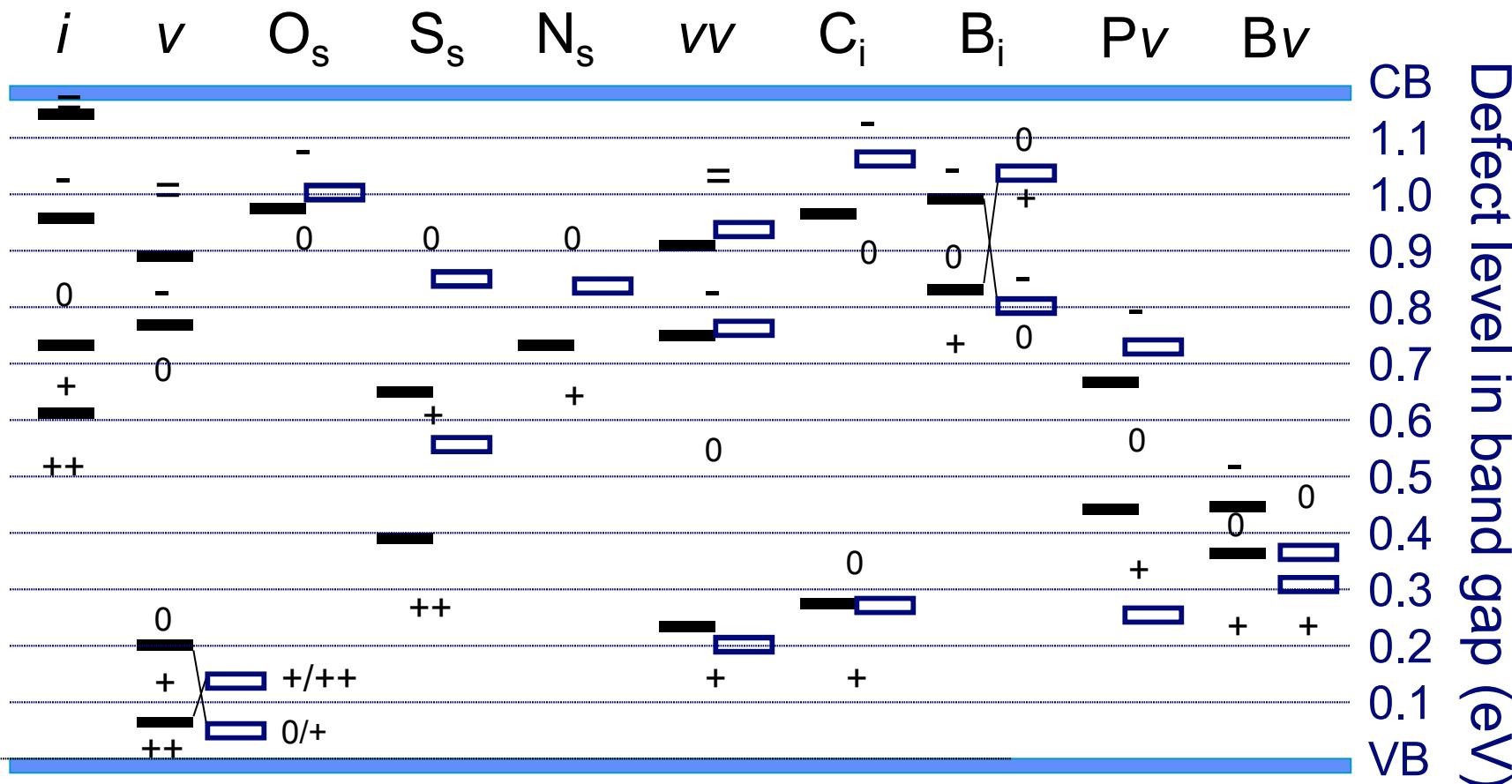
$$+ \int dr \eta^+_{LM} (\phi_{xtal} + C_{xtal}) - \int_{UC} dr \phi^+_{LM} \rho_{xtal}$$



Replace **variable** defect cell C'_{def} , with **fixed** crystal C_{xtal} reference
 Chemical potential equivalent to matching potential at $R=\infty$

Si: DFT/LDA vs. Experimental Levels

Peter A. Schultz, Phys. Rev. Lett. **96**, 246401 (2006).

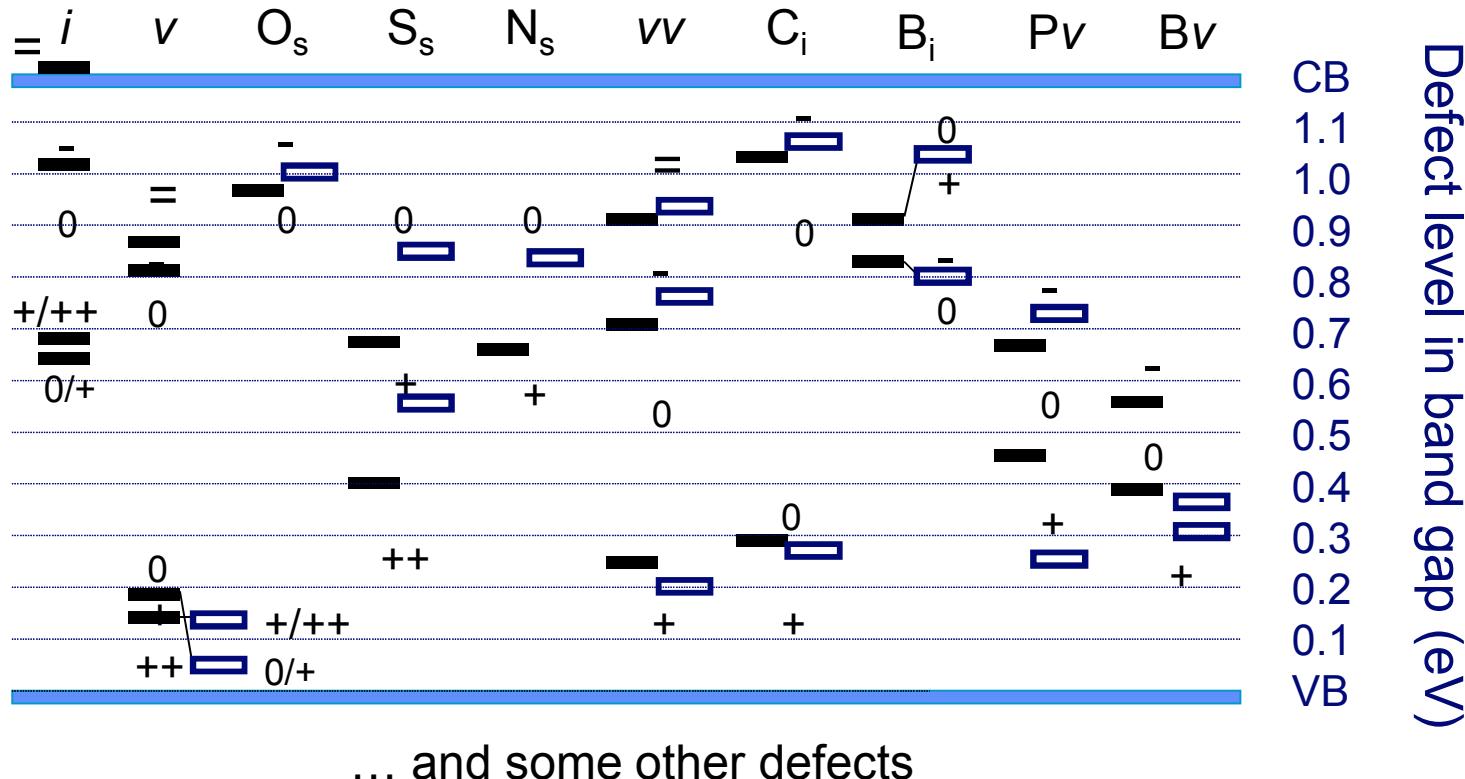


LDA: max error=0.25 eV, mean |error|= 0.10 eV

Intrinsic, first-row, second-row, and complexes across gap
LDA Kohn-Sham gap is only 0.5 eV

Si: DFT/PBE vs. Experimental Levels

P.A. Schultz and A.H. Edwards, NIMB **327**, 2-8 (2014).



DFT/PBE defect level max error=0.20 eV, mean |error|=0.10 eV
DFT “defect gap” matches experiment (KS gap: 0.6 eV)
Band gap problem not seen in **total-energy-based** defect levels

Computational methods – III-V's

- General purpose DFT code SeqQuest (<http://dft.sandia.gov/Quest>)
 - well-converged (contracted-Gaussian) local orbital basis
 - both LDA and PBE functionals
 - converged norm-conserving pseudopotentials (Ga,In both $Z_{\text{val}}=3,13$)
 - full force relaxed (<1 meV total energies)
 - full FDSM ... robust control of boundary conditions
- Large bulk simulation supercells
 - $a_0=a_0(\text{theory})$; GaAs: 5.60 Å(LDA), 5.63 Å(3d), 5.74 Å(PBE); $a_0(\text{expt})=5.65$ Å
 - Cubic supercells: 64-, 216-, 512-, 1000-site
 - k -sampling: 3^3 for 64-site cells, 2^3 for 216-, 512-, 1000-site cells,
 - fully calibrated polarization model
 - all these computational parameters are tested for convergence

Comparable method that yielded 0.1 eV accuracy in Si

Simple intrinsic defects in GaAs: LDA

P.A. Schultz and O.A. von Lilienfeld, MSMSE 17, 084007 (Dec. 2009).

$216^- = 512^- = 1000$ -site

Verification: cell-converged

LDA-3d = LDA to ≤ 0.1 eV

Verification: PP converged

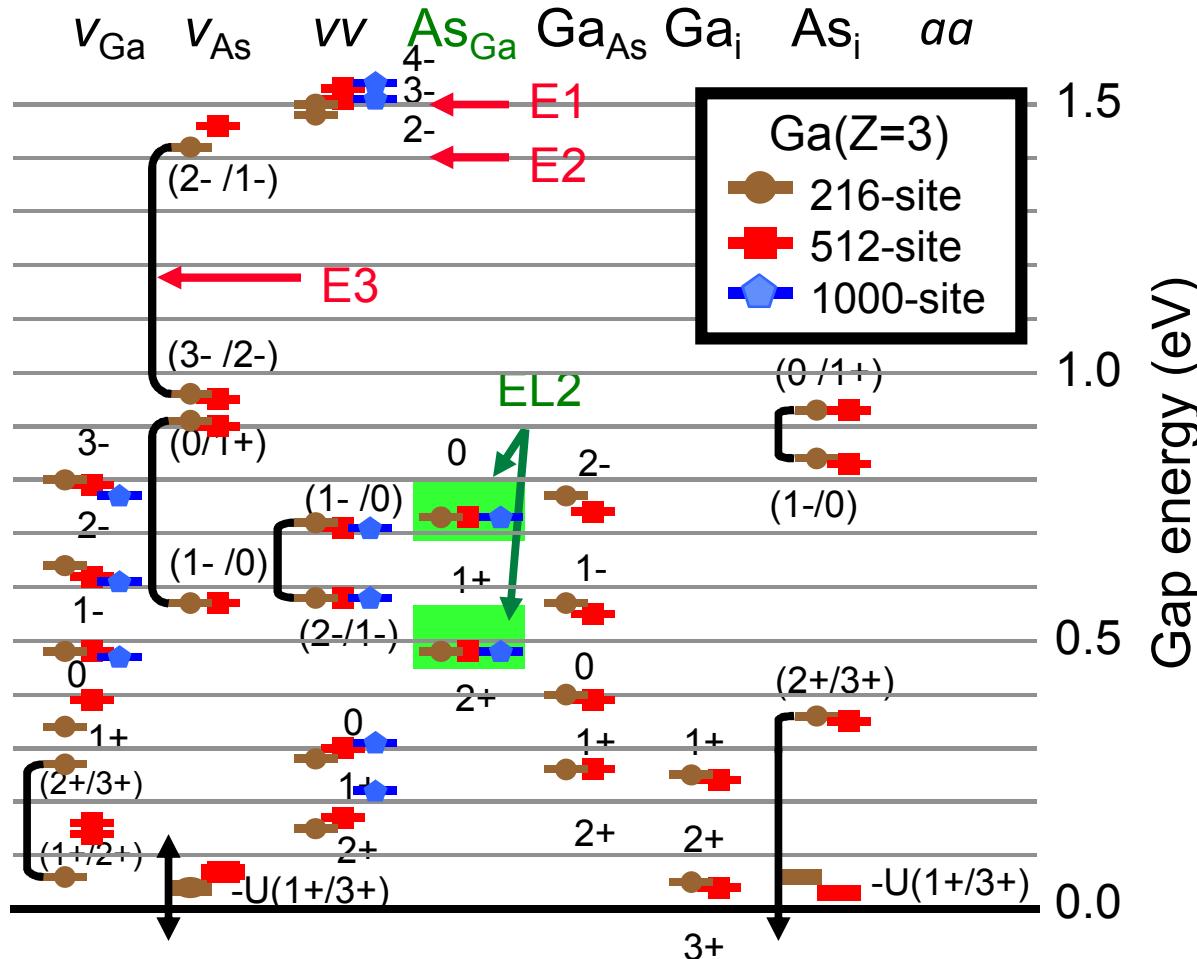
LDA~PBE; spin < 0.05 eV

Verification: functionals

V_{Ga} levels = EL2 levels

V_{As} levels below midgap

Validation: levels < 0.1 eV



DFT+FDSM: Apparent accuracy of ~ 0.1 eV

The GaAs divacancy is the E1-E2 radiation center

P.A. Schultz, J. Phys.: Condens. Matter **27**, 075801 (2015).

Old (experimental) lore, back to 1988:

$E1, E2$ center = $v_{As}(-/0)$, $v_{As}(0/+)$

$E3 = v_{As} + i$

vv is dismissed

Level structure reassigned with DFT:

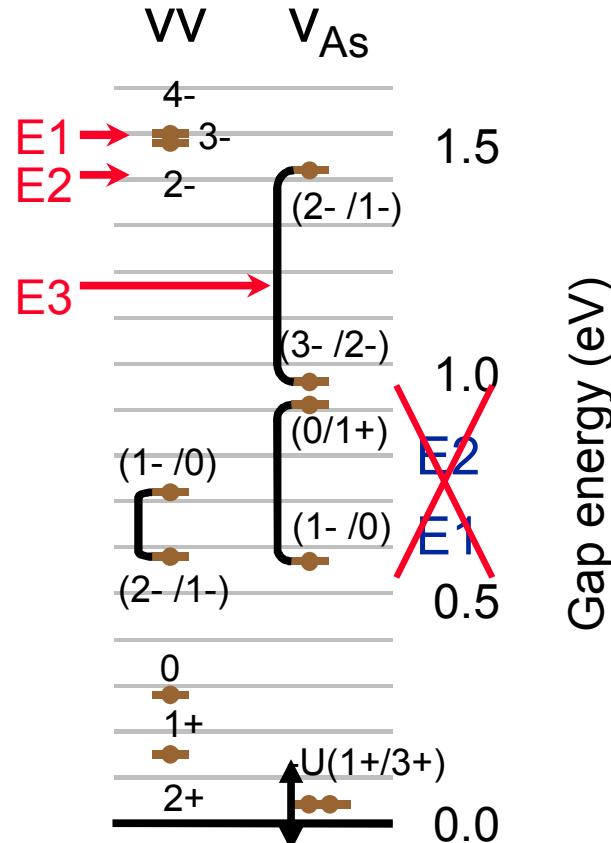
$v_{As}(-/+)$ is mid-gap negative-U (only one level)

$v_{As}(3-/1-)$ is upper-gap -U (one level)

$vv(4-/3-/2-)$ near conduction band

vv is major radiation defect: E1-E2

$v_{As}(3-/1-)$ transition is the E3

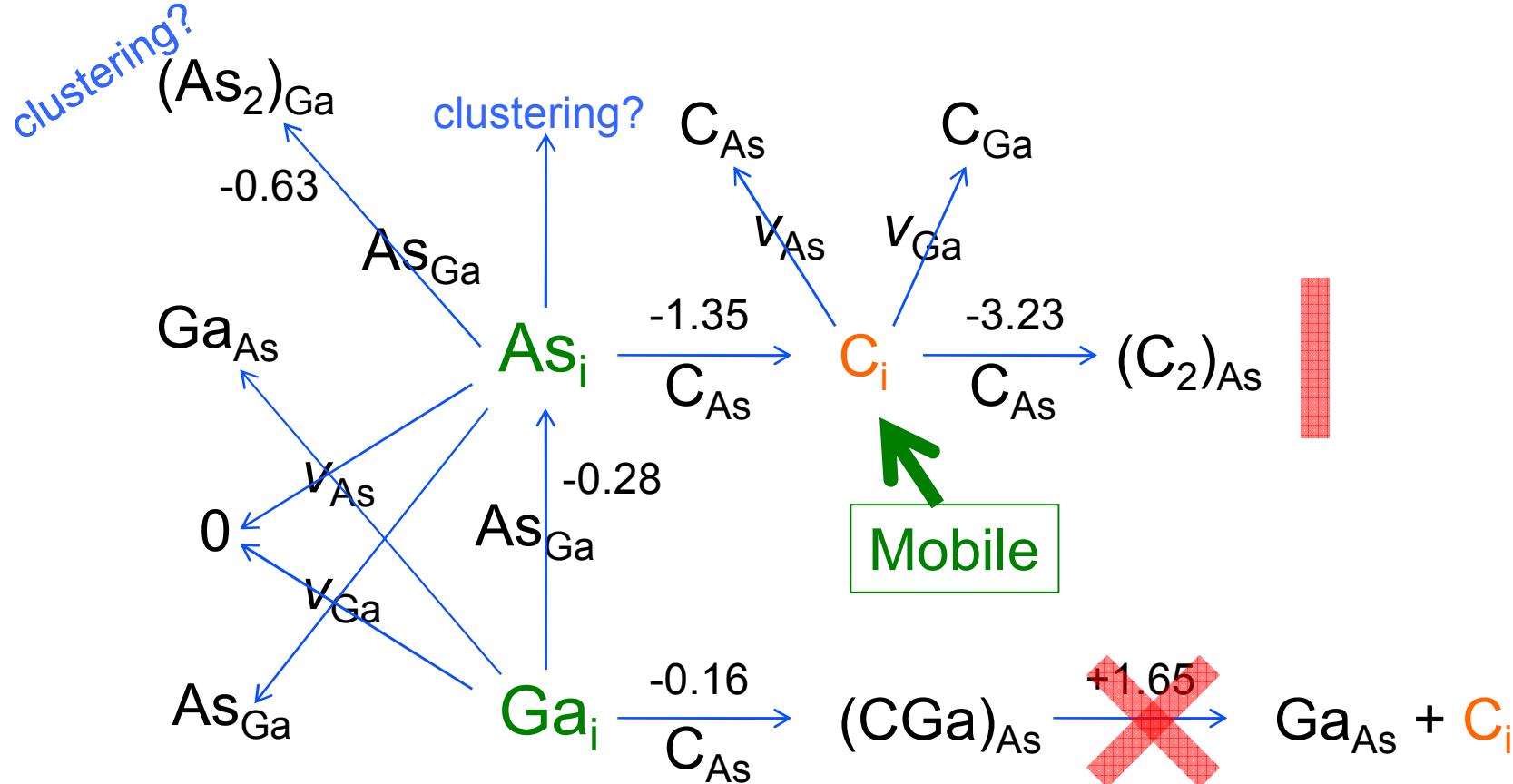


DFT-SeqQuest+FDSM levels good enough to identify defects strictly on *quantitative* defect level calculations

GaAs: C-doped reaction network

P.A. Schultz, J. Res. Eng: Rad. Effects **30**, 257 (201).

SeqQuest, LDA, 216-site, thermodynamic energy with $E_f = VBE$ (p-type)
Reaction networks initiated by identified mobile species: As_i , Ga_i

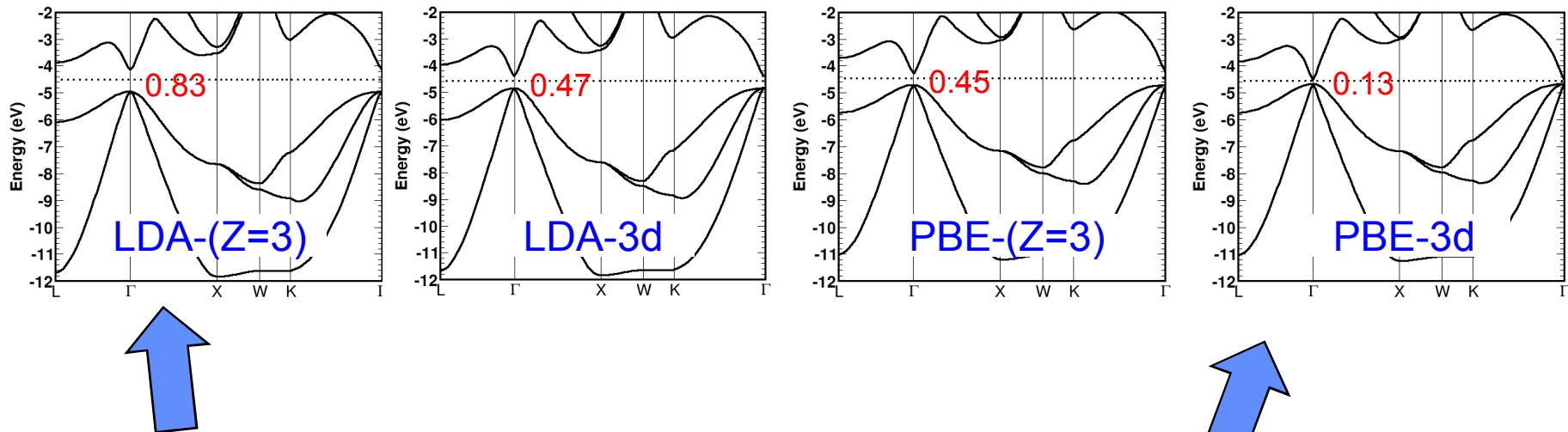


Reliable defect levels means reliable chemistry

GaAs: A theoretical laboratory

P.A. Schultz and A.H. Edwards, NIMB **327**, 2-8 (2014).

Change the Ga pseudopotential and the functional, and the **KS band gap shrinks ...**



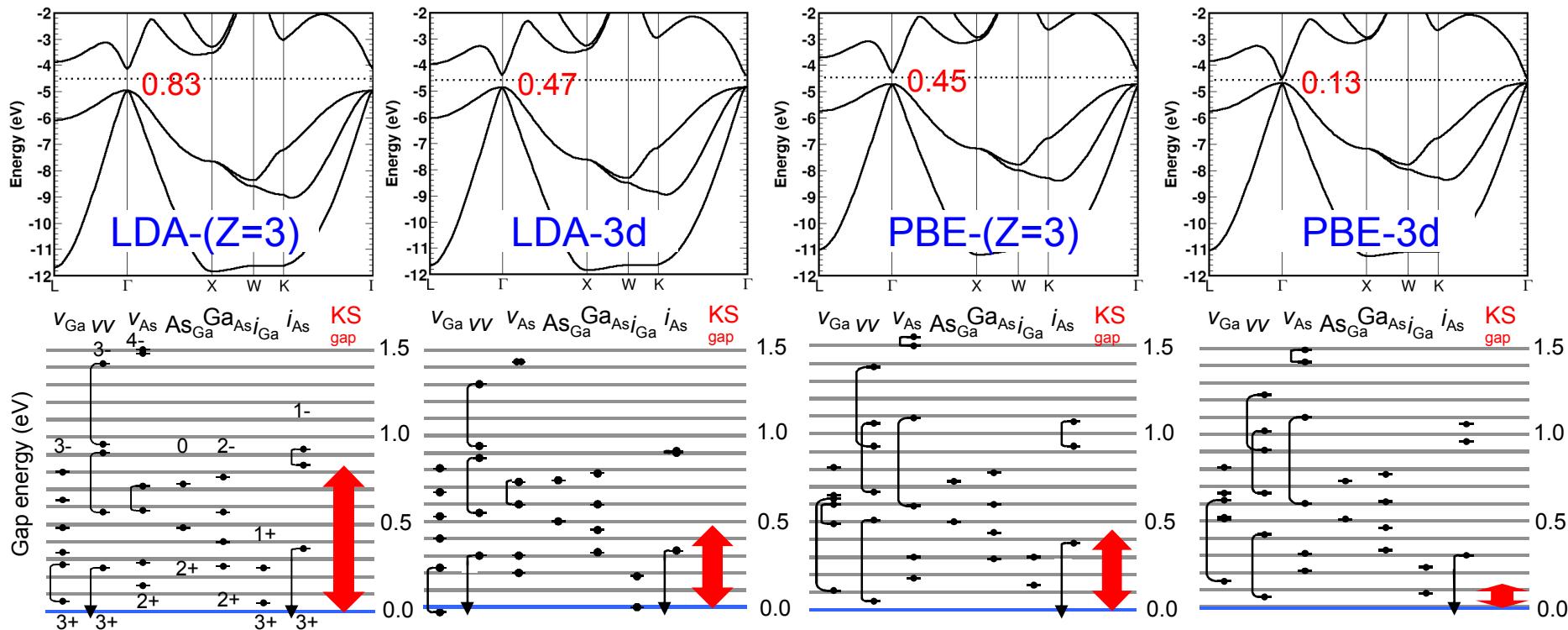
from 0.83 eV, LDA, Ga($Z=3$) pseudopotential (PP) ...

... to 0.13 eV, PBE-3d, Ga($Z=13$) pseudopotential (PP)

GaAs: A theoretical laboratory

P.A. Schultz and A.H. Edwards, NIMB 327, 2-8 (2014).

Change the Ga pseudopotential and the functional, and the **KS band gap** changes ...



... but span of (total-energy-based) defect levels, the “defect band gap”, does not

Defect levels/gap **insensitive** to size of Kohn-Sham gap!

GaAs Computational model lessons

- KS band gap not a problem for Si and GaAs defects
- Defect levels insensitive to size of Kohn-Sham gap!
 - total-energy differences vs. eigenvalue-referenced
 - GaAs is ideal theoretical laboratory for testing methods
- Detailed control of boundary conditions crucial: FDSM works
- Is this unique to Si and GaAs?

Simple intrinsic defects in AlAs: Energy levels

MRS Symposia Proceedings **1370**, (MRS Spring 2011); SAND2012-2938 (April 2012)

Verified cell-convergence

Calibrated: $v_{\text{Al}}^{(\text{u})}$

Checked: As_{Al}

Verified: vv

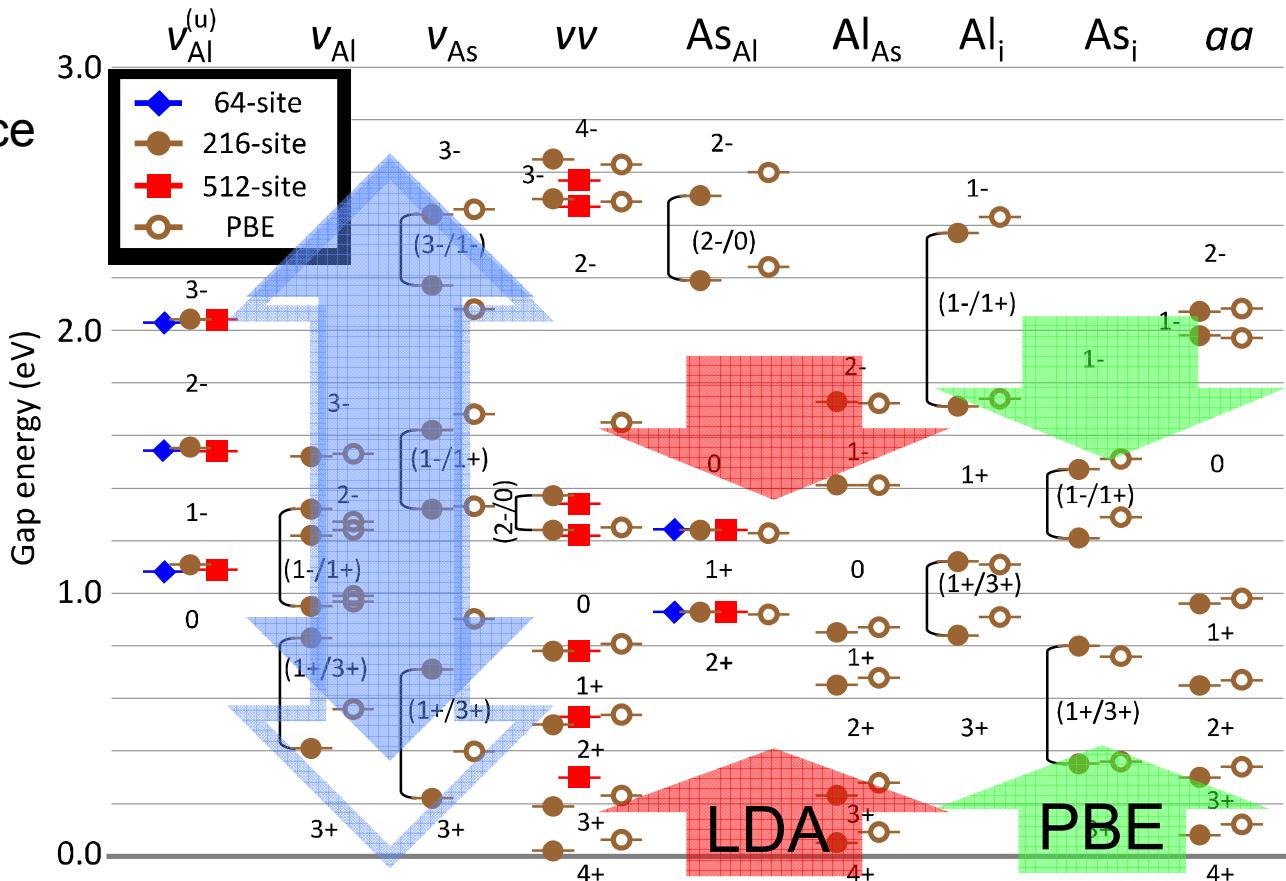
AlAs band gap

KS-LDA: 1.37 eV

KS-PBE: 1.53 eV

Defect span: 2.3 eV

Experiment: 2.16ⁱ eV



Very similar to GaAs defects, with some new features
A reverse band gap problem?

GaP intrinsic defects

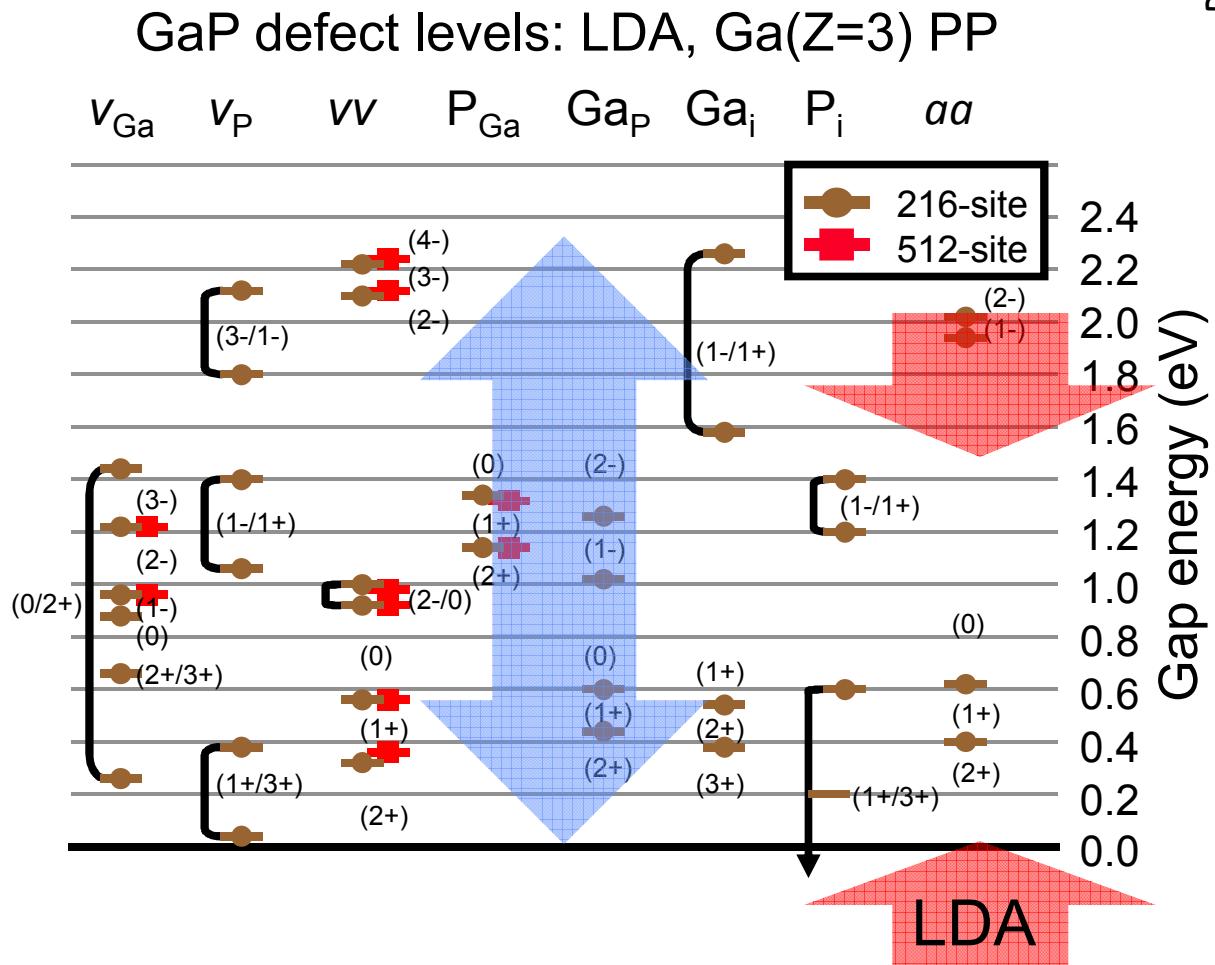
216-site results = 512-site
Verification: cell-converged

GaP band gap

KS-LDA: 1.51ⁱ eV

Defect span: 2.35 eV

Experiment: 2.35ⁱ eV



InP intrinsic defects

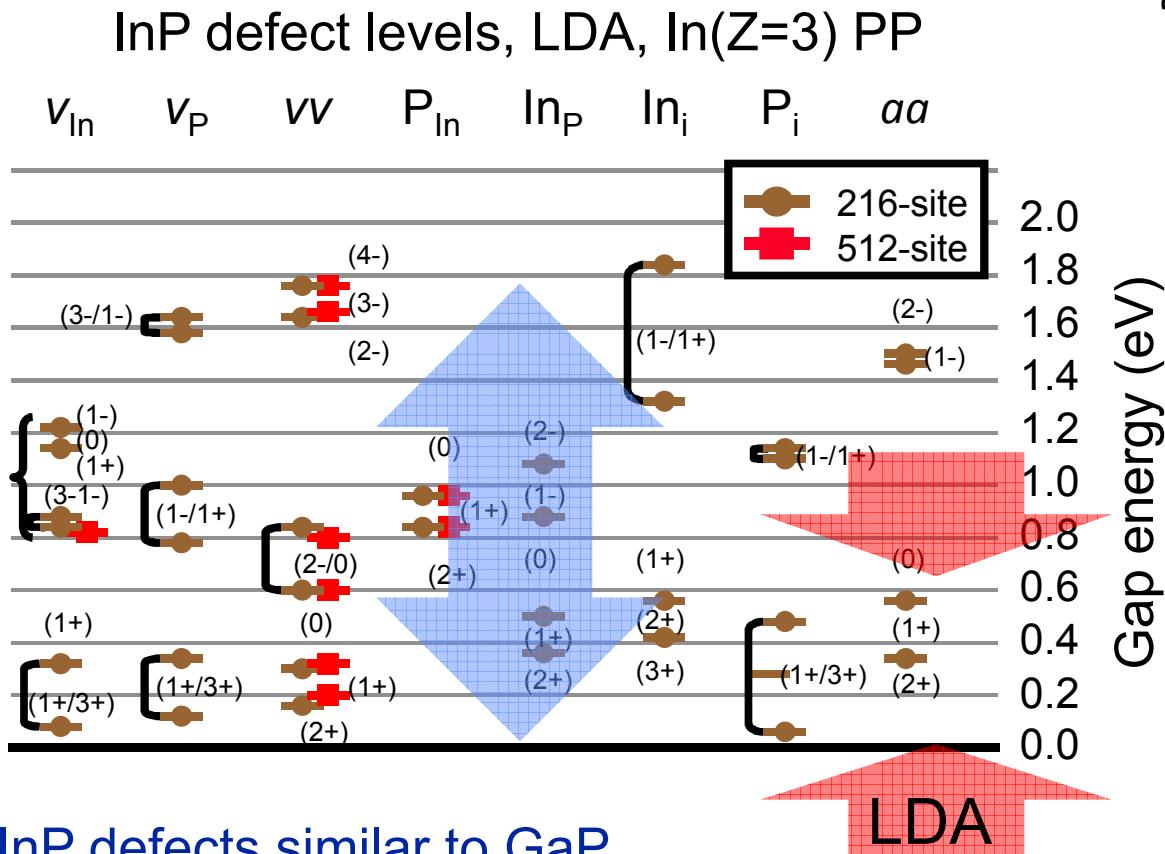
216-site results = 512-site
Verification: cell-converged

InP band gap

KS-LDA: 0.67 eV

Defect span: 1.7 eV

Experiment: 1.42 eV



InP defects similar to GaP
Augurs well for InGaP alloys?

AIP intrinsic defects

A.H. Edwards, H. Barnaby, A.C. Pineda, P.A. Schultz, IEEE-Trans. Nucl. Sci. **60**, 4109 (2013)

216-site results = 512-site
Verification: cell-converged

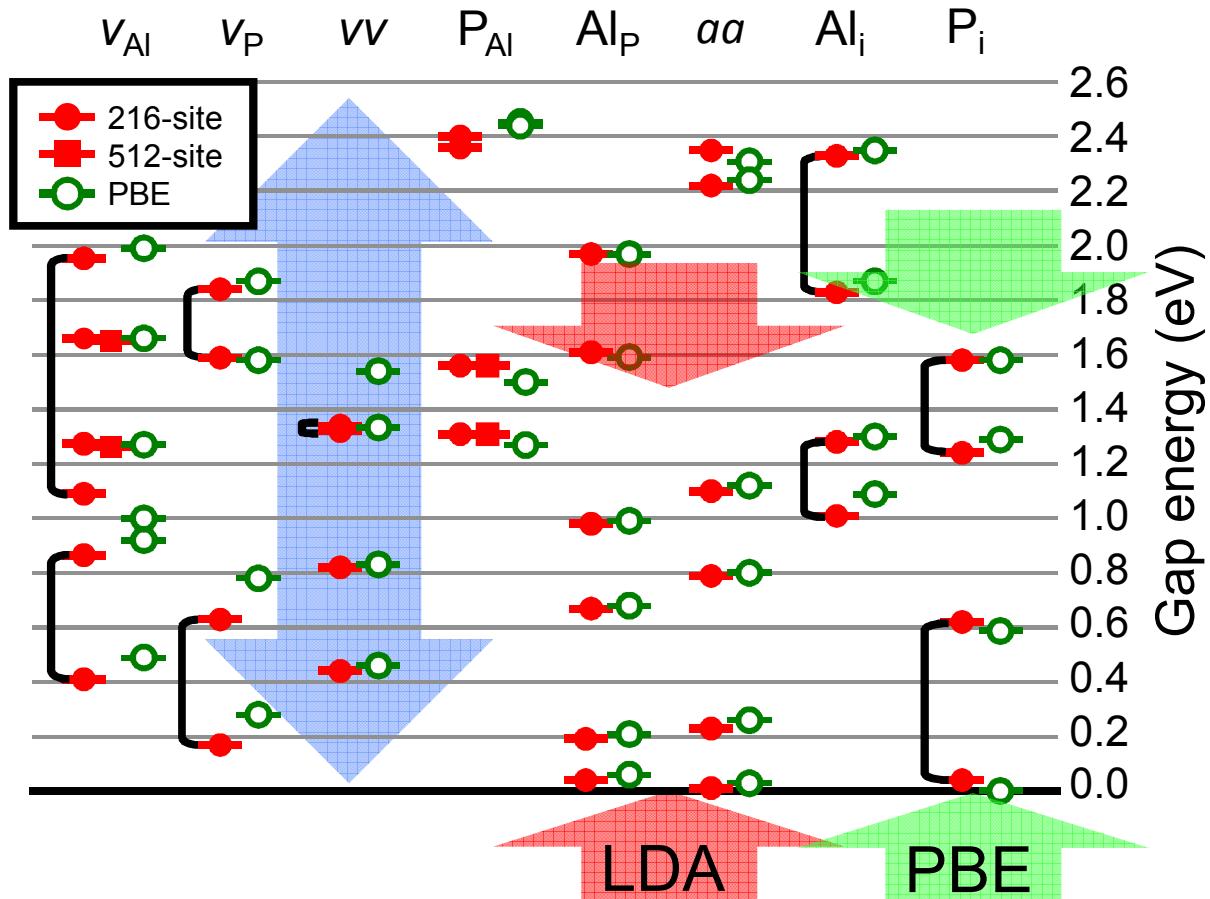
AIP band gap

KS-LDA: 1.48 eV

KS-PBE: 1.67 eV

Defect span: 2.55 eV

Experiment: 2.51 eV



The DFT “Defect band gap”

- Kohn-Sham gap: **outside** bounds of VB to CB *band eigenvalues*
- Defect band gap: **inside** bounds of transition **energies** for defect levels

Band gaps: experiment , Kohn-Sham, DFT defect gap								
Si	1.17 eV		AlAs	2.16 ⁱ eV		AlP	2.51 eV	
	KS	Defect		KS	Defect		KS	Defect
lda	0.49	1.2	lda	1.37	>2.3	lda	1.48	2.55
pbe	0.62	1.2	pbe	1.53	>2.3	pbe	1.67	2.55
GaAs		1.52 eV	GaP		2.35 ⁱ eV	InP		1.42 eV
KS		Defect	KS		Defect	KS		Defect
lda	0.83	1.54	lda	1.51	2.35	lda	0.67	1.7
lda-3d	0.47	1.52	lda-3d	1.47	2.35	lda-3d	0.66	1.7
pbe	0.45	1.50	pbe	1.74	2.35	pbe	0.47	1.7
pbe-3d	0.13	1.50	pbe-3d	1.52	n/c	pbe-3d	0.46	n/c

Total energy defect gap insensitive to Kohn-Sham gap
Defect band gap matches (overshoots?) experiment

Other examples

IV-IV: 3C-SiC (cubic)

GGA/PBE KS Gap: 1.38 eV

Defect Gap (PBE): ~2.7

Experimental Gap: 2.40

II-VI: CdTe (3d-valence)

LDA KS Gap: 0.81 eV

PBE KS Gap: 0.69 eV

Defect Gap (LDA&PBE): ~1.6

Experimental band gap: 1.60

Close correlation of the **defect gap** with **experiment band gap**

What about a crystal that is not tetrahedral, and a large gap?

CsI defect level spectrum - DFT

R. M. Van Ginhoven and P.A. Schultz, J.Phys.: Cond. Matter **25**, 495504 (2013)

250-site results = 432-, 686-site

Verification: cell-converged

v_I levels match experiment

Validation of accuracy

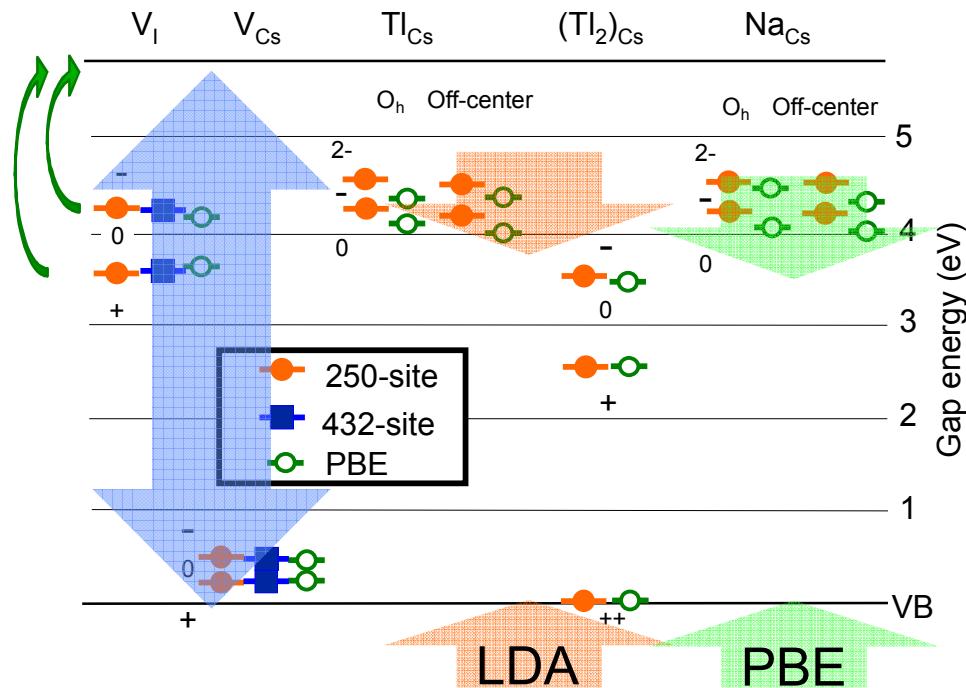
CsI band gap

KS-LDA: 3.80 eV

KS-PBE: 3.58

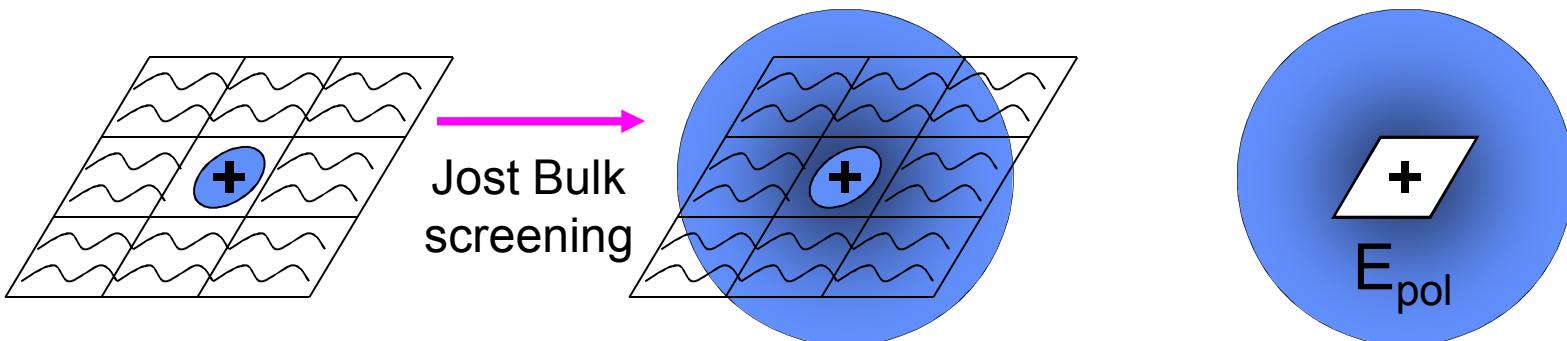
Defect span: >5.8 eV

Experiment: 6.3 eV



Not a band *gap* problem, a *band edge problem*—
where are they cf. total energy defect levels?

The polarization model



For extrapolation to bulk, need energy of screening outside of supercell: E_{pol}

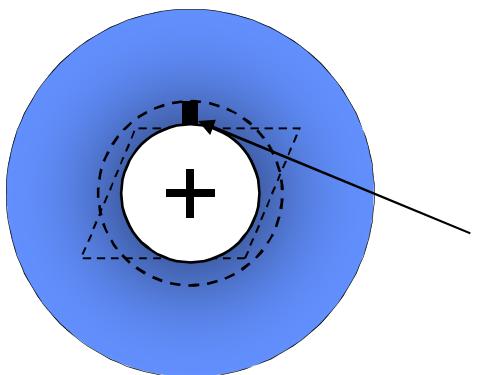
Jost model: $E_{pol} = \frac{(1 - 1/\epsilon_0) q^2}{R_{jost}}$

$$R_{jost} = R_{vol} - R_{skin}$$

q = charge on defect

$$R_{jost} = R_{vol} - R_{skin}$$

R_{vol} = radius of volume sphere

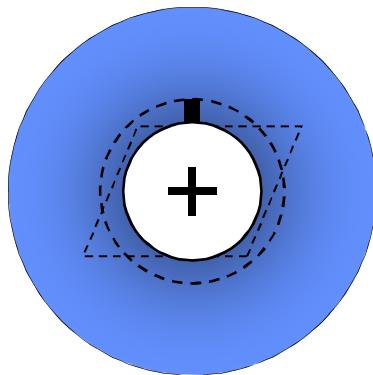


Two parameters for any material

R_{skin} = unscreened volume **inside** cell.
fit: = 1.3-1.7 Bohr

ϵ_0 = static dielectric constant - expt
Si GaAs InP GaP AlAs InAs
11.8 13 12.5 11.2 10.1 15.15

How big is bulk screening?



$$E_{\text{pol}} = \frac{(1 - 1/\epsilon_0) q^2}{R_{\text{jost}}}$$

Defects mostly converged at 64-site cells

E_{pol} mostly insensitive to ϵ_0 at 10-15, use GaAs (LDA)

Charge $q = +1, -1 \quad +2, -2 \quad +3, -3 \quad +4, -4$

Screening: 1.09 eV 4.36 eV 9.81 eV 17.43 eV

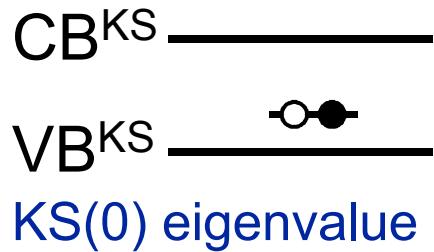
This is lower bound on classical screening energy

Bulk classical screening outside defect is **huge**
 Key insight to understanding KS gap vs. defect gap

How is a good defect band gap possible?

Conventional picture:

Defect state depicted as eigenvalue inside KS eigenvalue gap

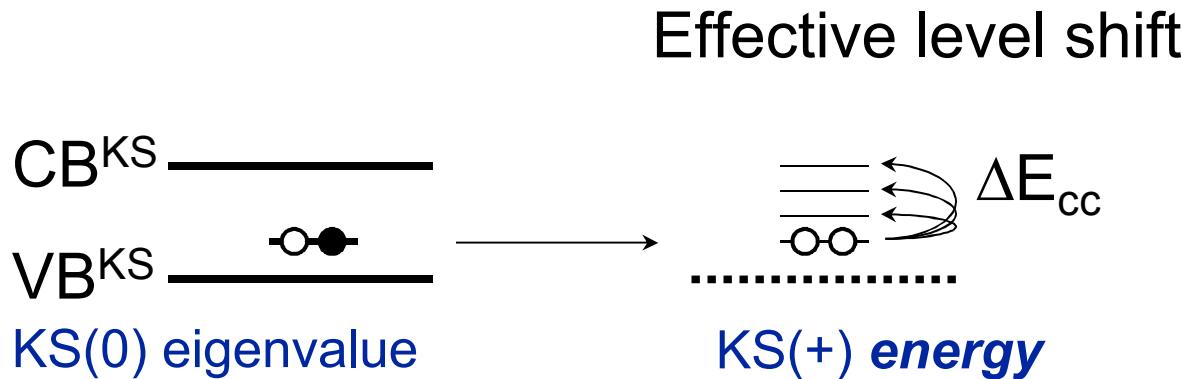


Sham and Kohn [Phys. Rev. 145, 561 (1966)]

the KS eigenfunctions and eigenenergies are auxiliary functions of the KS equations, and “must *not* be interpreted as corresponding to elementary excitations.”

How is a good defect band gap possible?

What about:
final state effects?



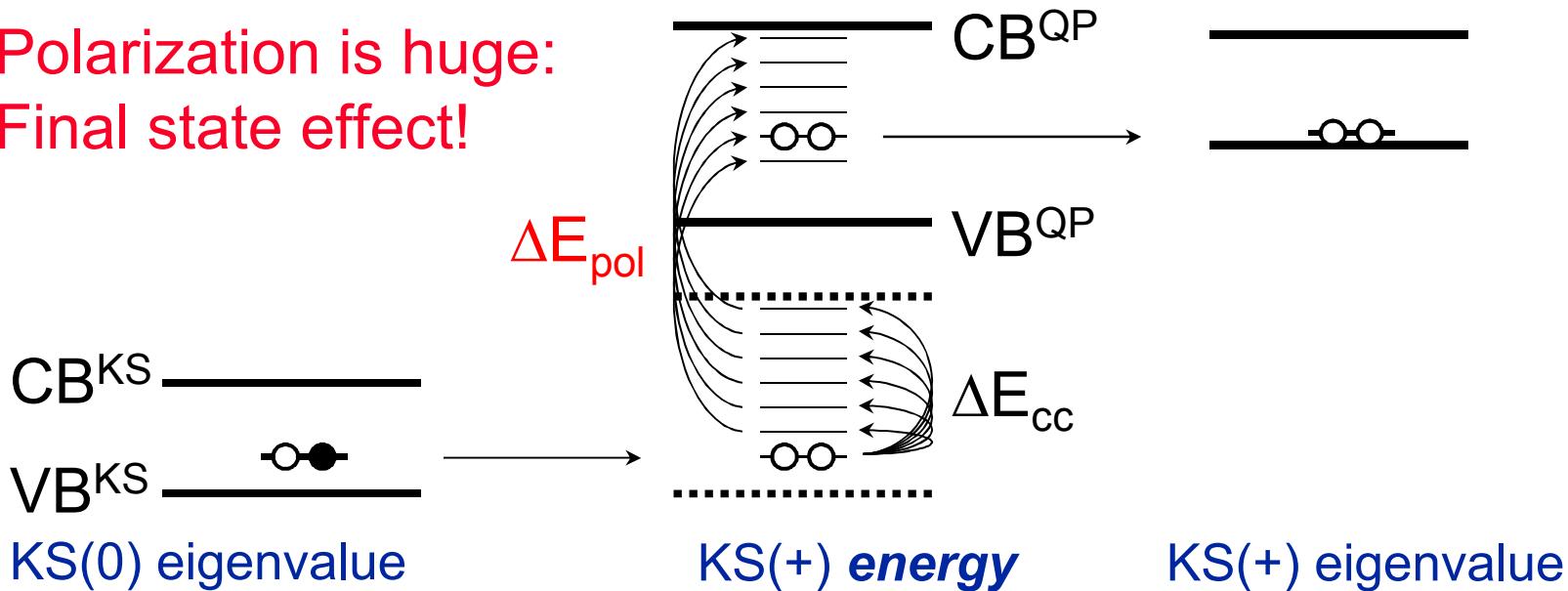
Central cell electronic relaxation (quantum): ΔE_{cc}

Sham and Kohn [Phys. Rev. 145, 561 (1966)]

the KS eigenfunctions and eigenenergies are auxiliary functions of the KS equations,
and “must *not* be interpreted as corresponding to elementary excitations.”

How is a good defect band gap possible?

Polarization is huge:
Final state effect!



Central cell relaxation (quantum): ΔE_{cc}

Long range screening (classical): $\Delta E_{\text{pol}} > E_g$

Defect levels bounded by (screened) quasiparticle gap, not eigenvalue gap

Sham and Kohn [Phys. Rev. 145, 561 (1966)]

the KS eigenfunctions and eigenenergies are auxiliary functions of the KS equations, and “must *not* be interpreted as corresponding to elementary excitations.”

Not only eigenvalues but eigenstates are meaningless

Conclusions

- **Total energy** DFT defect levels not constrained by KS band gap problem
- Semilocal DFT+FDSM - quantitative (~0.1 eV) for defect levels in semiconductors
- **Defect band gap** is good predictor of experimental band gap
- KS interpretation of band gap is not-even-wrong for defect levels
 - Sham and Kohn's ignored warning about misinterpreting KS eigenvalues
- **Rigorous charge boundary conditions** more crucial than KS band gap
 - **band edge problem** — where are they? — is the more serious question
- Path to better functionals: “fixing” using KS gap as primary metric is misguided
- **Diligence in credibility — verification/validation/UQ — crucial to predictive DFT**

Thanks to Arthur H. Edwards (AFRL) and also Renee M. Van Ginhoven (AFRL/RDHEC)

----- Supporting slides -----

A supercell theory of defect energies

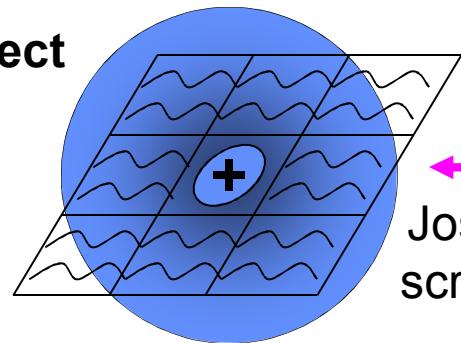
Peter A. Schultz, Phys. Rev. Lett. **96**, 246401 (2006).

Target system:
isolated defect

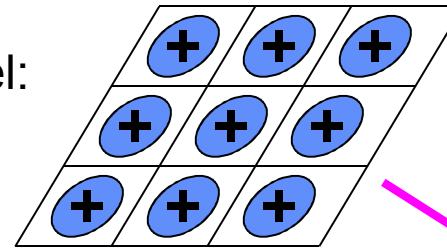
=

**Computational
model for
isolated defect**

(+ DDO
for defect
banding)

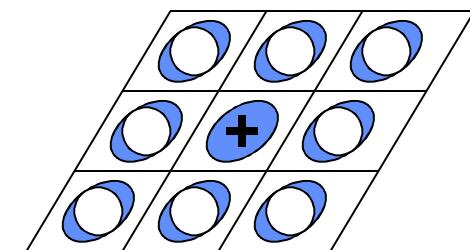


Standard
DFT model:
Supercell

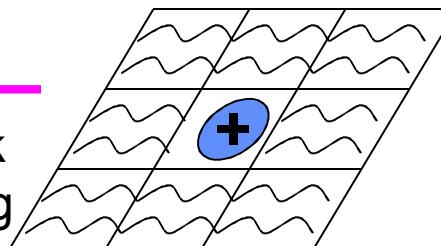


LMCC to fix
boundary
conditions

Finite Defect Supercell Model



Jost Bulk
screening

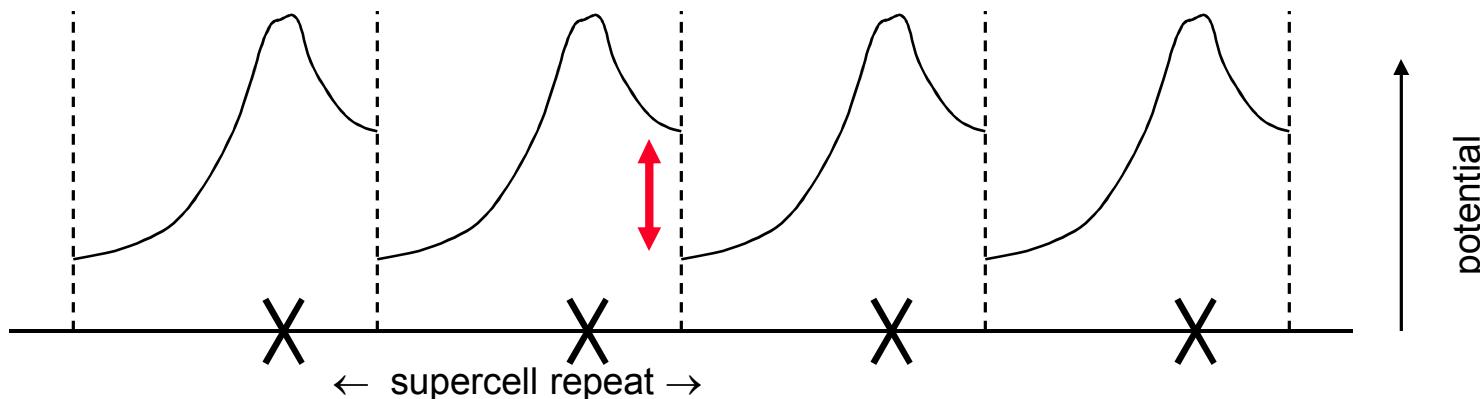


Crystal embedding
to fix μ_e

FDSM: *Ab initio* computational model – connect model to physics
Calculations with rigorous control of charge boundary conditions

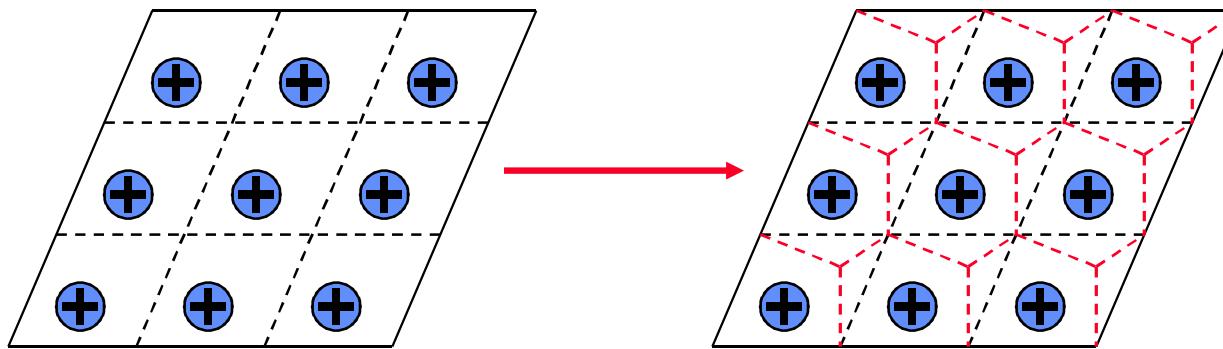
LMCC potential in bulk systems

A complication in bulk systems ...



Discontinuity in potential from LMCC at supercell boundary!

... is solved by using Wigner-Seitz cells around LMCC positions



With Wigner-Seitz local volume, LMCC potential is continuous

The electron chemical potential μ_e

- Standard E_{form} of charged defects needs electron reservoir:

$$E_{\text{form}}(q) = E_{\text{defect}}(q) - E_{\text{xtal}}(0) - \sum N_i \mu_i + q \mu_e$$

linked

- Supercells with charge: $\phi_{\text{def}}(r) = \phi_{\text{pbc}}(r) + C_{\text{def}}$

Periodic potential $\phi_{\text{def}}(r)$ only known to within a constant C_{def}

$C_{\text{def}} = \text{fcn}\{\text{defect type, configuration, cell shape, cell size, ...}\}$

$E_{\text{defect}}(q)$ has qC_{def} term in its internal energy

- Standard ad hoc workarounds unsatisfactory - unquantitative

- matching VB,CB edge, band structure features, average potentials ...
- Issue: renormalizing infinities, defect modified bands, band-bending, ...
- calibration uncertainty of “few tenths of eV” (Garcia & Northrup) - best case

Needed a more rigorous scheme to fix electron reservoir

Defect energy and level calculation

Finite Defect Supercell Model Formation Energy

$$E_{\text{form}}(q) = E_{\text{defect}}(q) - E_{\text{xtal}}(0) - \sum N_i \mu_i + E_{\mu_0}(q) + E_{\text{pol}}(q)$$

$E_{\text{defect}}(q)$: DFT energy with LMCC potential

$- E_{\text{xtal}}(0) - \sum N_i \mu_i$: match number of each type of atom

$E_{\mu_0}(q)$: fix chemical potential μ_e to common electron reservoir

$E_{\text{pol}}(q)$: bulk polarization response

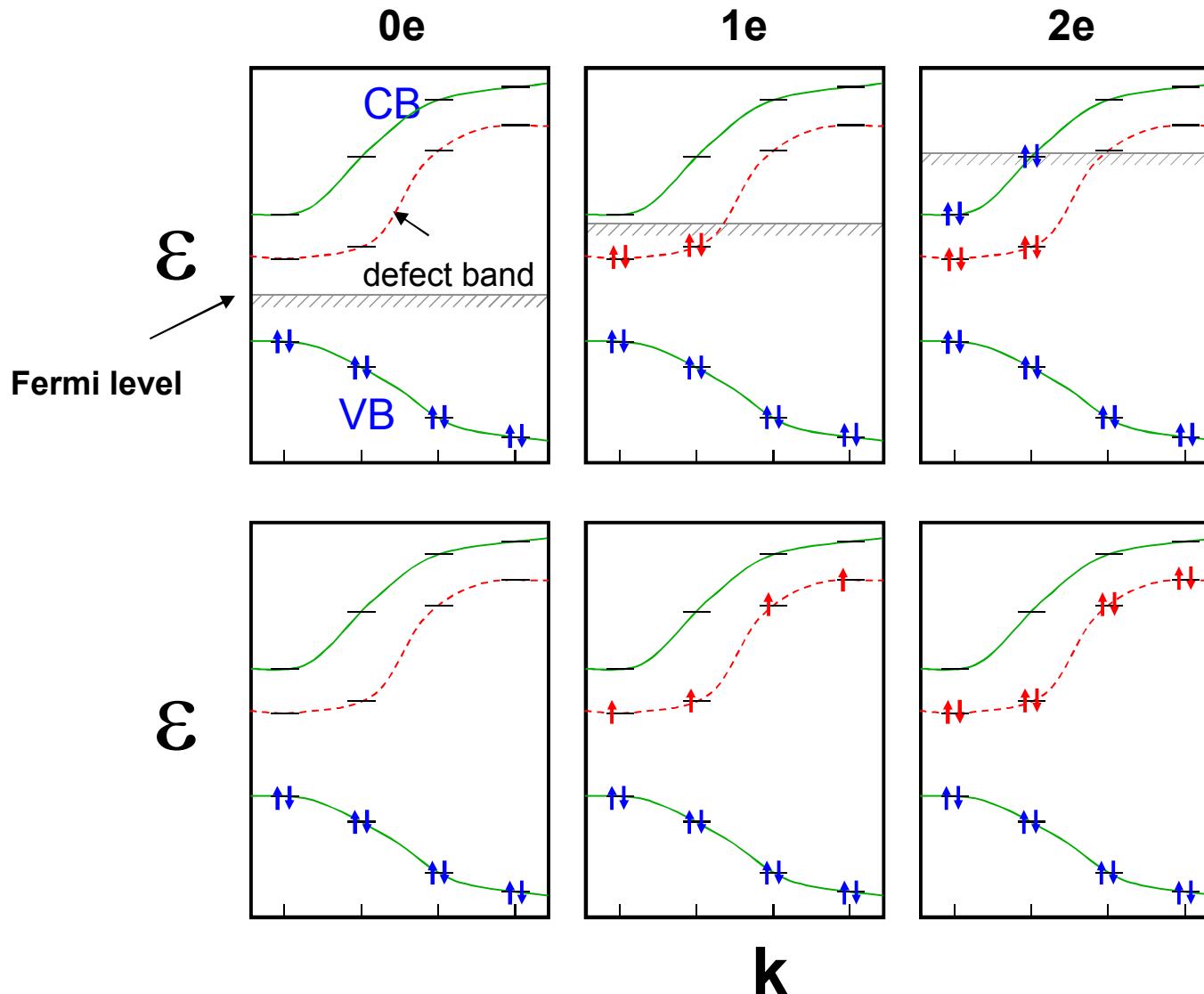
Defect level calculation

$$\Delta E(q/q-1) = E_{\text{form}}(q) - E_{\text{form}}(q-1)$$

Need to set spectrum vs. VB/CB by single marker.

All defect levels for all defects then fixed by continuity.

Defect banding: Discrete Defect Occupations



Charged cell convergence - Jellium

PHYSICAL REVIEW B

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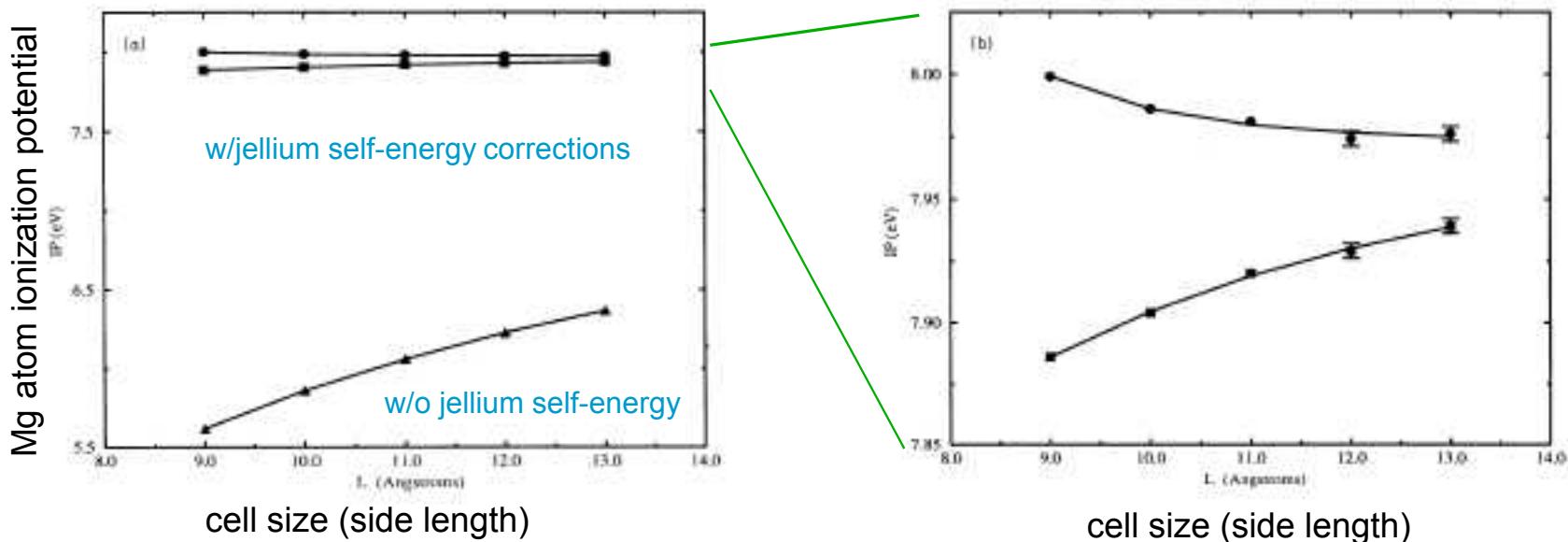
Periodic boundary conditions in *ab initio* calculations

G. Makov and M. C. Payne

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, United Kingdom

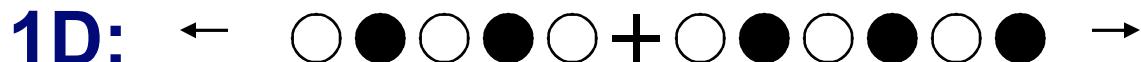
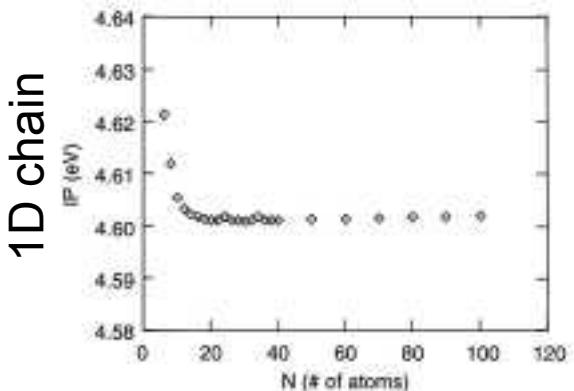
(Received 19 July 1994)

Figure 3

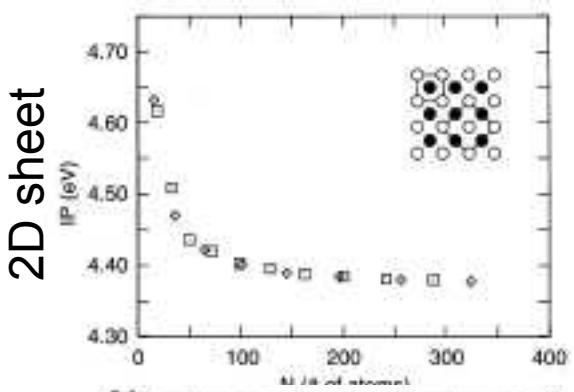


Variation in computed total energy due to incorrect charge potential

LMCC: NaCl - Cl vacancy ionization



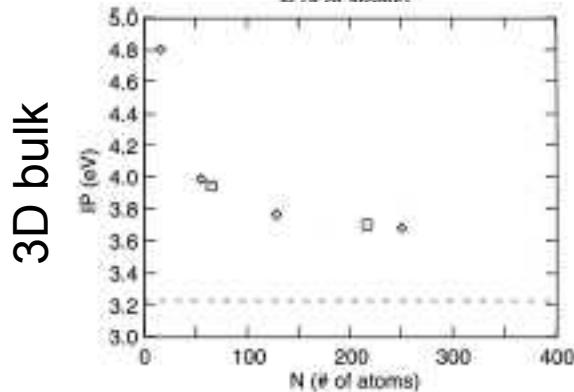
Supercell size dependence due to polarization.
Larger supercell \rightarrow more polarization
Apparent L^{-3} scaling = 1D classical dielectric screening



2D: single-layer 2D square sheet (polar&non-polar)

Apparent L^{-2} scaling = 2D classical dielectric screening

Insensitive to cell type, polar vs. non-polar



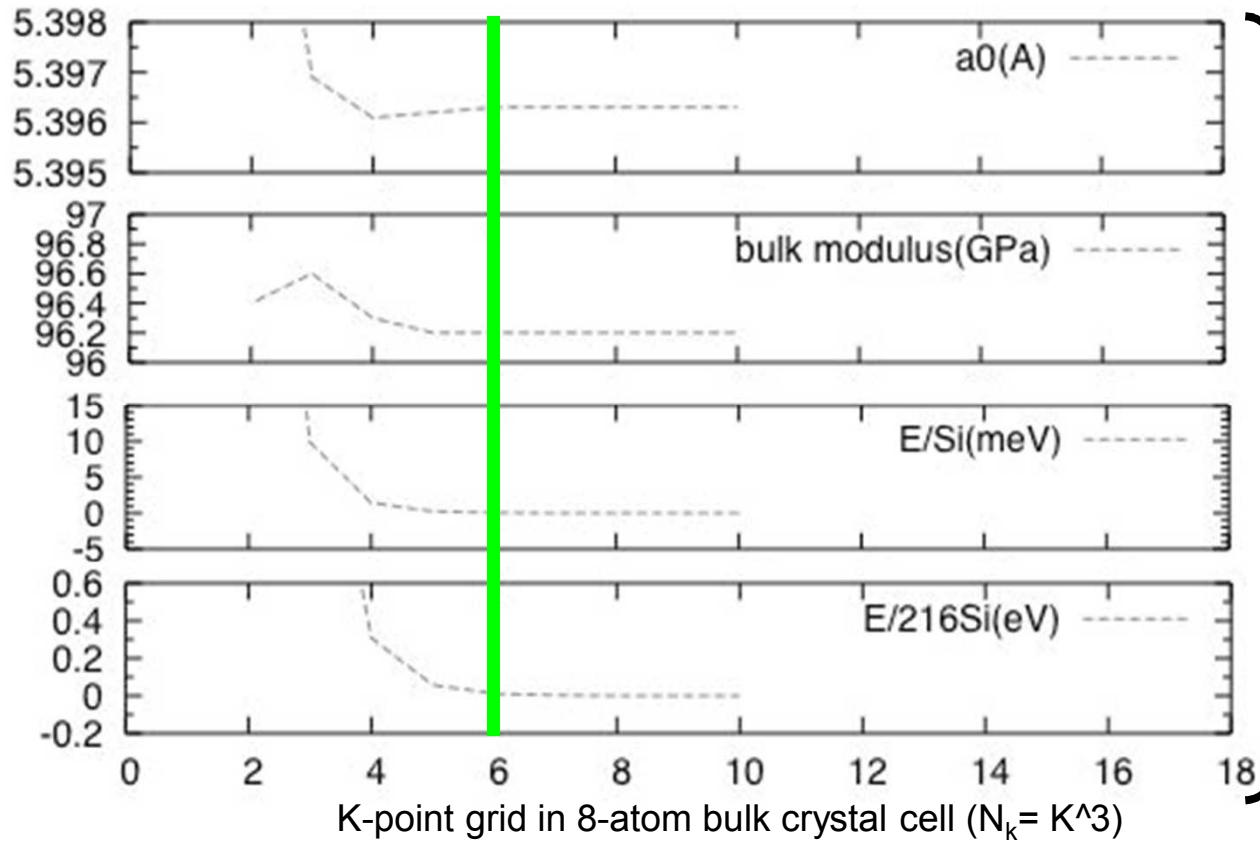
3D: bulk-layer 3D square sheet (fcc&sc cells)

Apparent L^{-1} scaling = 3D classical dielectric screening

Strictly screening due to large supercell volume

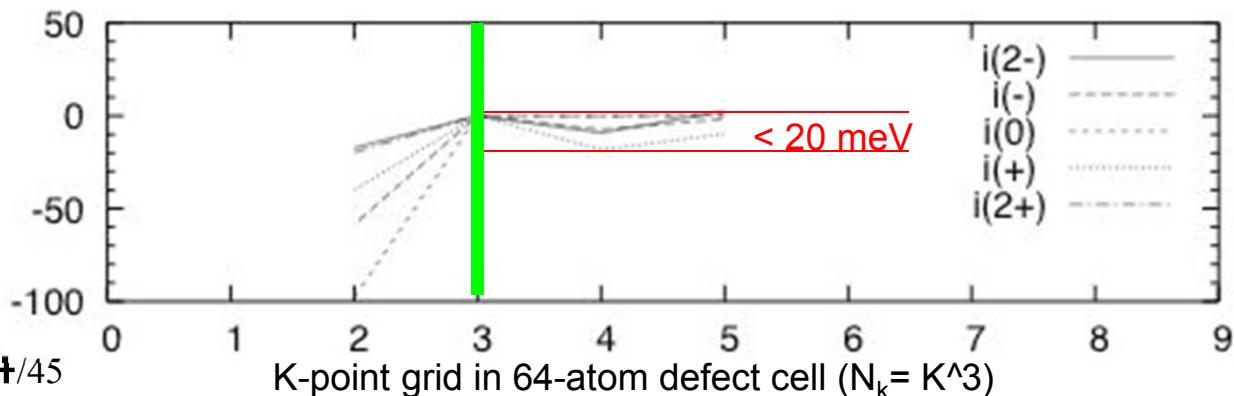
Insensitive to cell shape

BZ convergence: Si self-interstitial



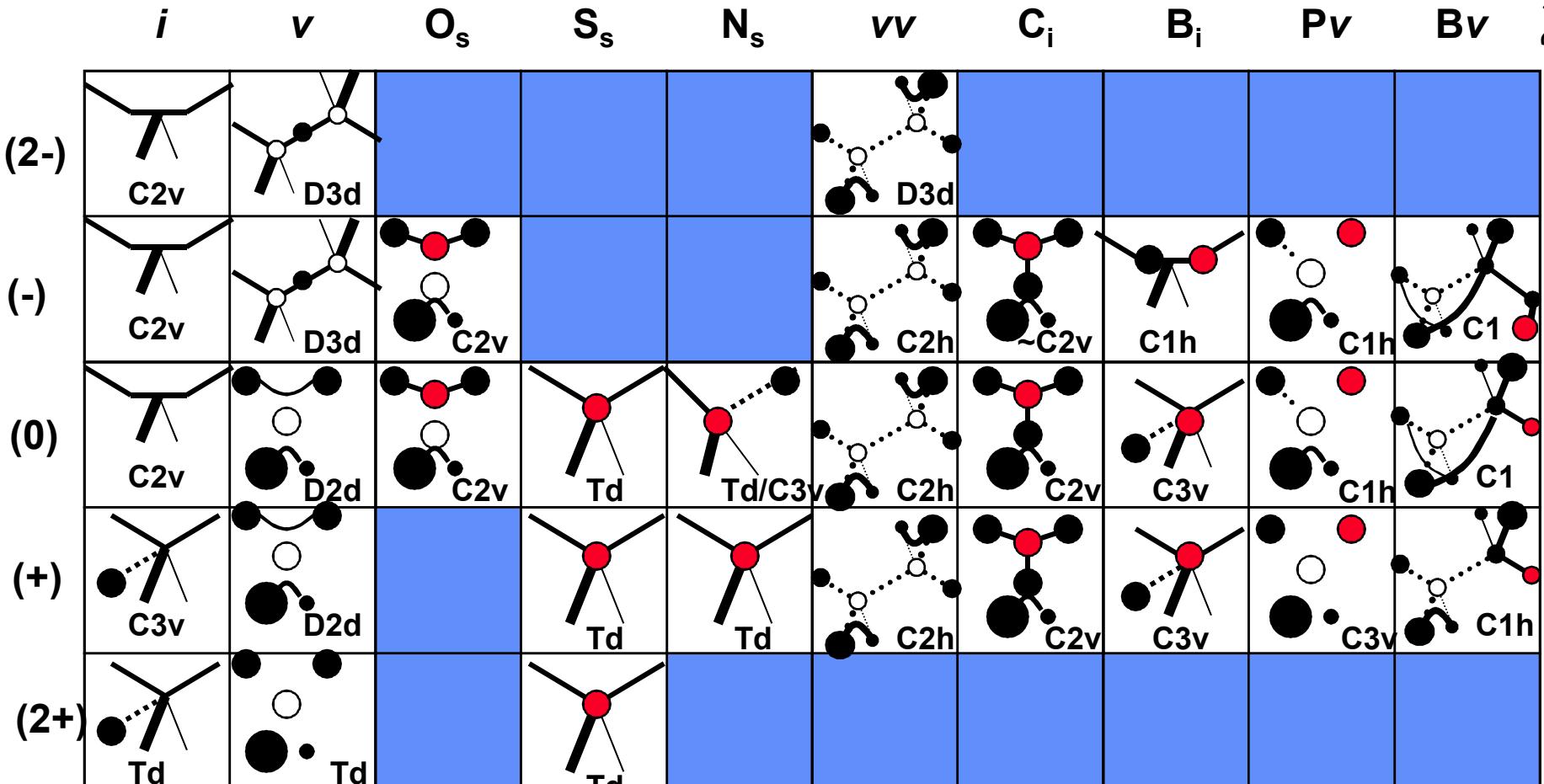
Bulk properties ($a_0, B, E/Si, E_{tot}$) converge quickly:
at 6^3 k w/8-cell
= 3^2 k w/64-cell
= 2^3 k w/216-cell

Defect energies should not vary faster than bulk, IF computational model is valid.



Interstitial formation energies in 64-site cell vary < 20 meV
{10 meV w/o $i(+)$ } beyond equivalent of 6^3 k-grid in 8-site.

Silicon defect structures



GGA: $E(C2v) < E(D3d)$ for $v(-)$

Si: new P-v and B-v charge states

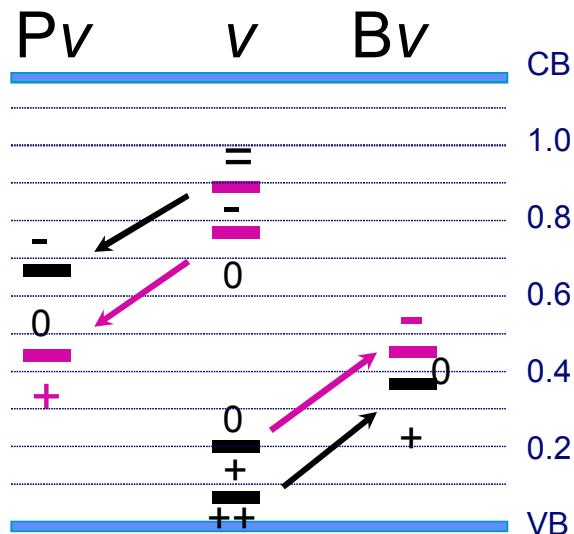
- Silicon level calculations - over 15 defects with levels

$i(=/-/0/+/++), v(=/-/0/+/++), vv(=/-/0/+), C_i(-/0/+), B_i(-/0/+), Pv, Bv$

O_s (A-center), O_i , N_s , S_s , v_2O , v_2O_2 , H_i , vP_2 , v_2P , ...

DFT “defect band gap” matches experiment (1.2 eV)

DFT: mean $|error| = 0.10$ eV, max error~0.2 eV



Task: Theory quantified $v(=/-)$, $v(-/0)$

Discovery: Theory predicted $Pv(+)$ and $Bv(-)$

“Absolute prediction”

new levels >0.4 eV from band edge

validation error: 0.2

$Pv(0/+)$ subsequently confirmed in experiment
[Larsen, et al PRL 97, 106402 (2006)]

VALIDATION is key to quantitative DISCOVERY - GaAs is ALL discovery

Calibrating the polarization model: v_{Ga}

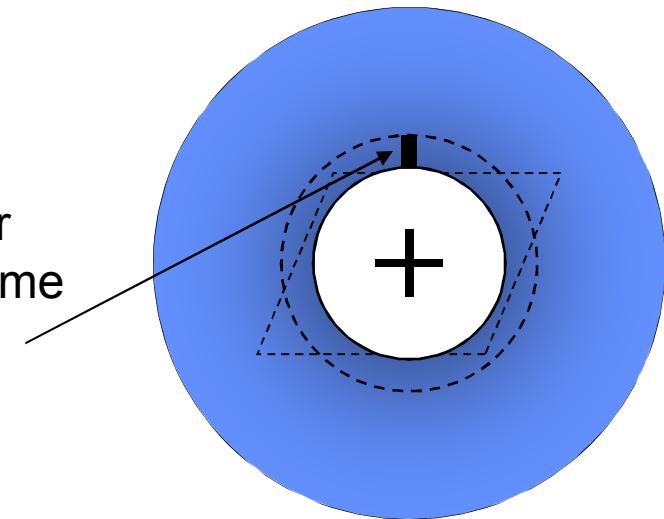
Jost model:

$$E_{\text{pol}} = \frac{(1 - 1/\epsilon_0) q^2}{R_j}$$

$$R_j = R_{\text{vol}} - R_{\text{skin}}$$

R_{skin} accounts for unscreened volume **inside** supercell

Need ϵ_0 (use 13), and R_{skin} (fit)



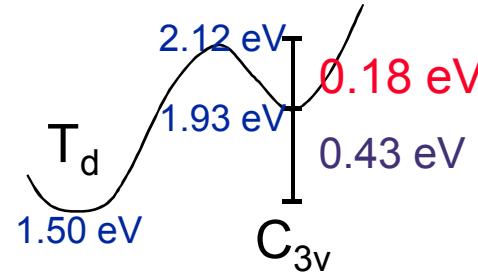
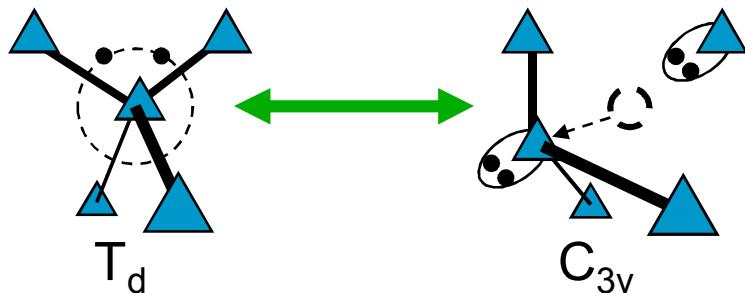
Why use v_{Ga} ?

Need higher charge states (0 to -3), best if not strongly distorted (near T_d)

Energy(eV)	$v_{\text{Ga}}(0)$	$E(2/-1)-E(1/0)$	$E(3/-2)-E(2/-1)$	$a\text{As}: E(0/+)-E(+/2+)$
64-site	2.81	0.167	0.174	0.231
216-site	2.69	0.168	0.152	0.246
512-site	2.75	0.162	0.141	0.252

GaAs EL2 and the As antisite

EL2 = antisite $\text{As}_{\text{Ga}}(0)$



216-site =
512-site
(~ 64-site)

	Experiment -EL2	SeqQuest/FDSM - As_{Ga}
EL2(0/1+)	E_c -0.74 eV	E_c -0.81 eV
EL2(1+/2+)	E_v +0.54 eV	E_v +0.48 eV
Splitting:	0.24 eV ($E_g = 1.52$)	0.25 eV
EL2*	no donor states	no donor states
Reorientation:	~0.3 eV	~0.2 eV

Verification: 64-216-512-1000-site supercell results match

Validation: DFT matches experiment for EL2 w/in 0.1eV