SAND2013-4028C

Modeling charged defects inside DFT band gaps

An improved inside-out perspective

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(With special thanks to Art Edwards at Air Force Research Lab)

SAND2013-XXXX

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, expensive

(2) Quantitative characterization

Predictive simulations, inform coarser models

- not just publishable, but defensible to engineers

Challenges for density functional theory

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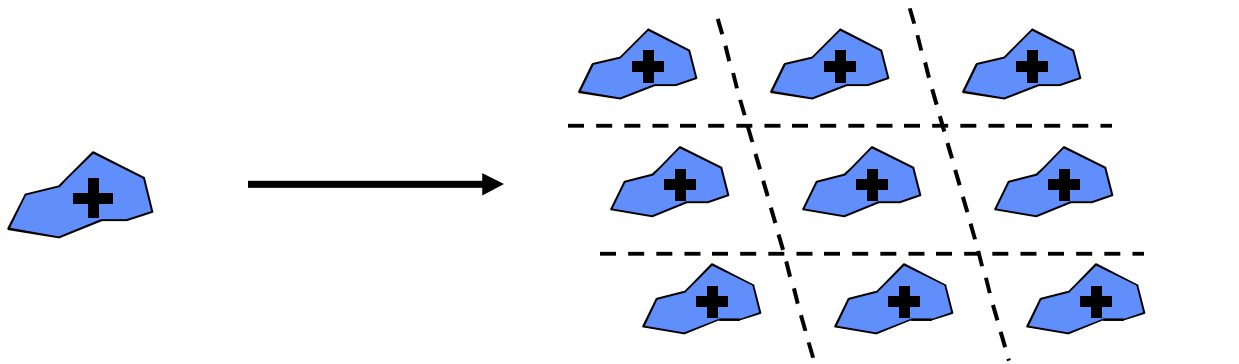
- **Conventional DFT fails for defect levels in semiconductors**
  - (1) Physical accuracy: e.g., “band gap problem”
  - (2) Computational model size limitations
  - (3) Shortage of good data for validation
  - (4) Supercell problem for charged defects:



Finite charged defect

Ill-defined (Coulomb divergence)

Lots of DFT calculations, no robust, predictive method

Radiation damage and defects levels

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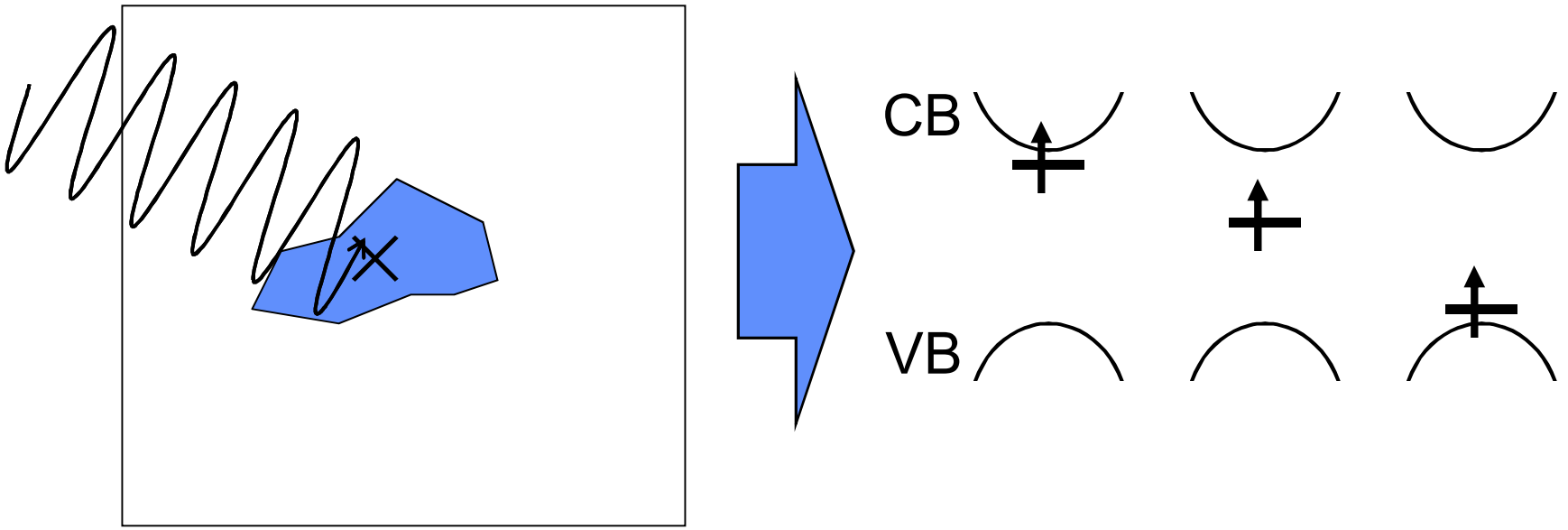
Radiation damage …



produces defects … and introduces electronic transitions

… and we need to quantify these transitions

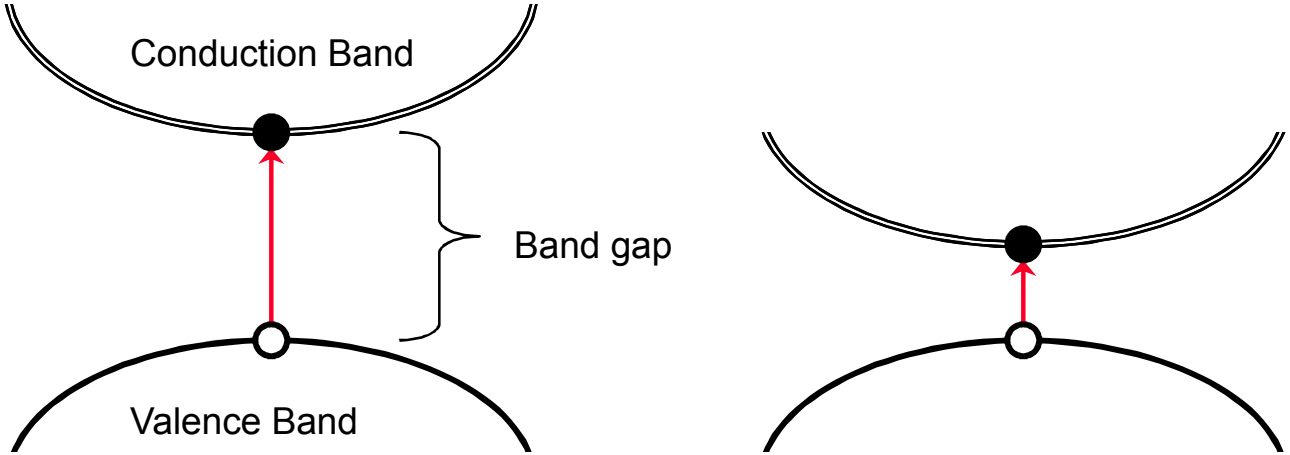
DFT "band gap problem"

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



Experiment

Kohn-Sham (KS) eigenvalue spectrum

The band gap defines the energy scale for defect levels

Fundamental impediment to quantitative predictions?

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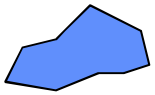
The supercell approximation

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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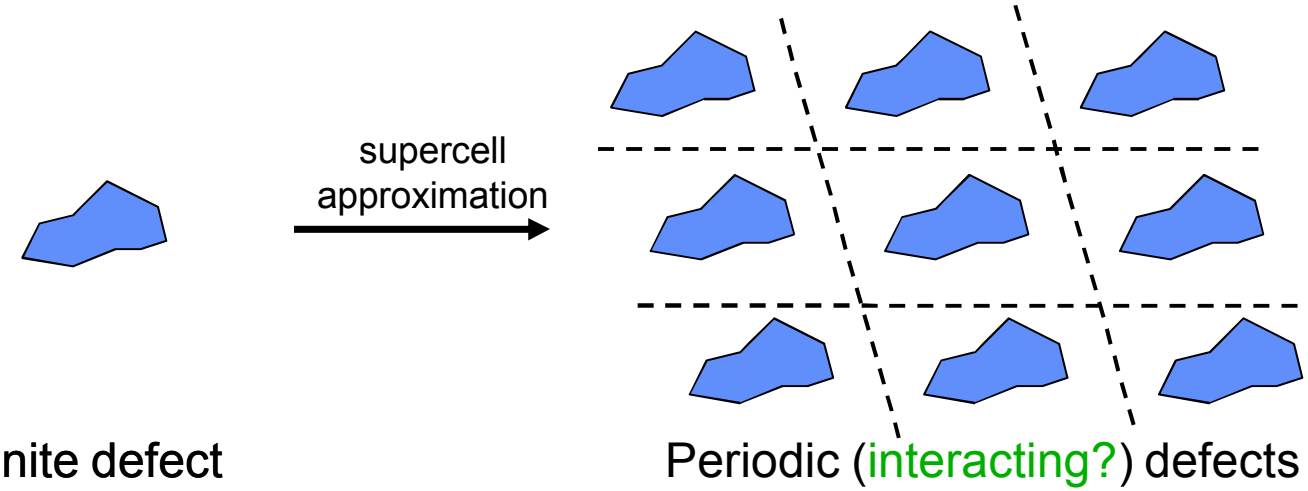

The supercell Idea:
Surround perturbed defect region with enough material to buffer defects.
In the limit of large enough supercells, approach an isolated defect.

The supercell approximation

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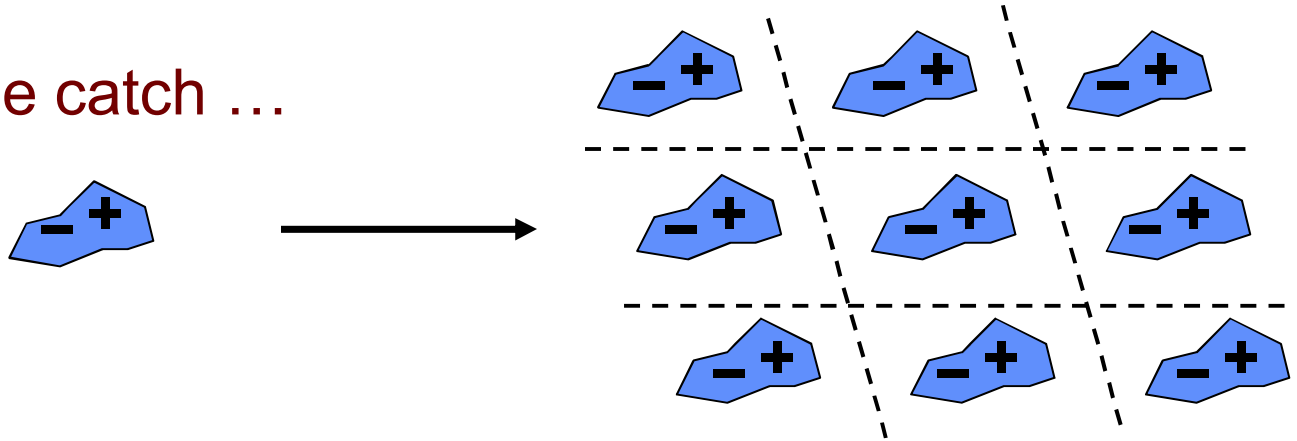
the catch …



Finite defect with dipole

Periodic (interacting) defects

DFT expense limits size of supercell - defects interact

The supercell approximation

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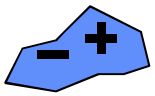
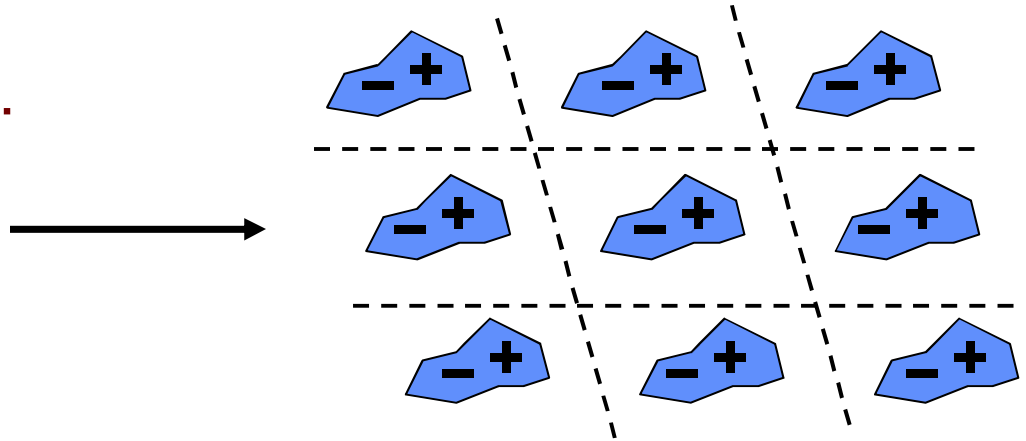
the catch …

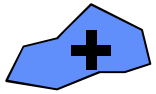


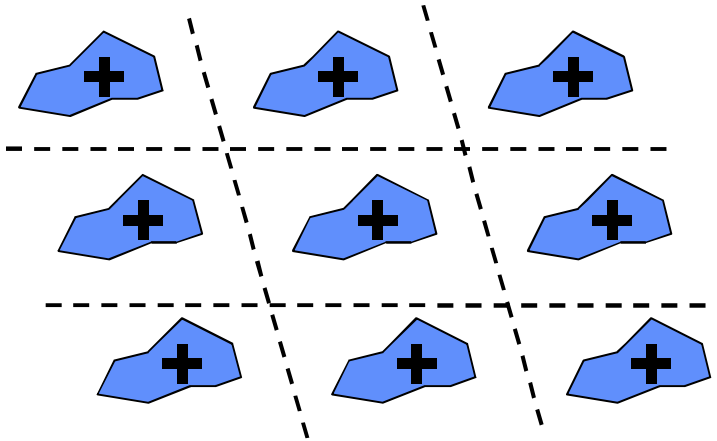


Finite defect with dipole

Periodic (interacting) defects

even worse …





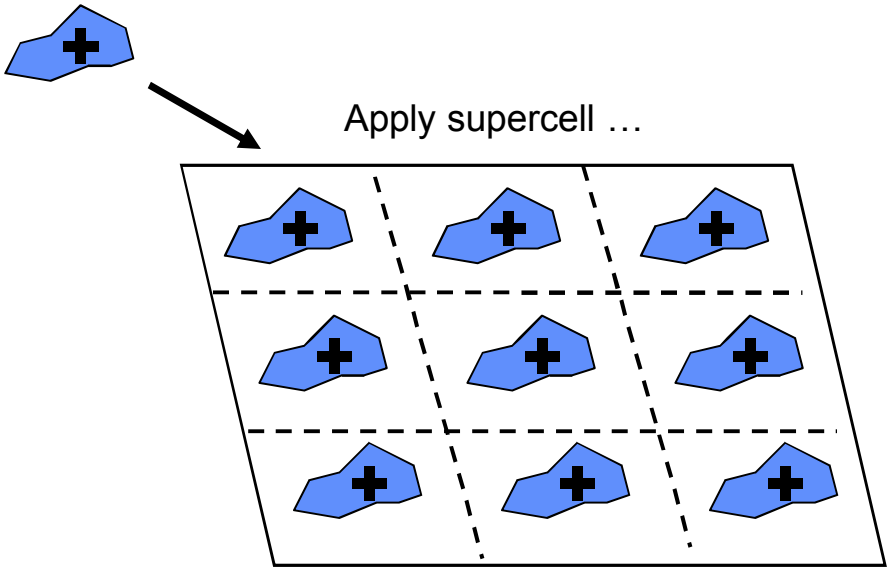
Finite charged defect

Ill-defined (Coulomb divergence)

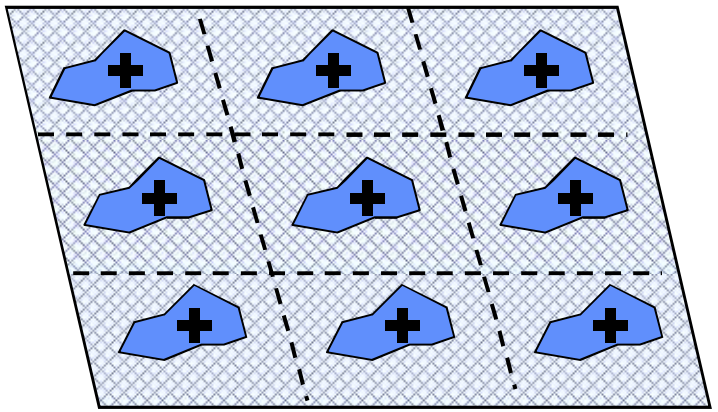
Interactions and divergence are key issues

Jellium to eliminate divergence?

Isolated defect …



Neutralize with flat background charge: "jellium"



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Net charge boundary conditions - jellium

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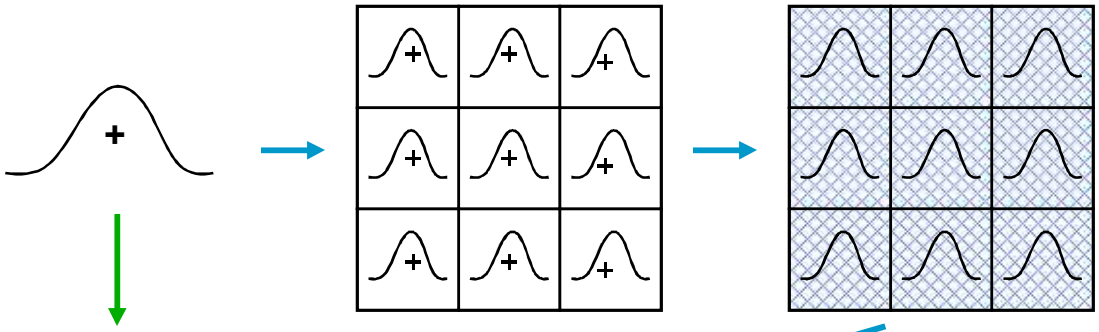
Take isolated charge density…

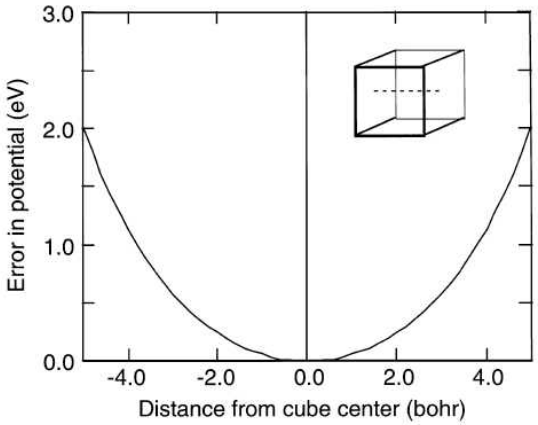
create cubic supercell …

neutralize with "jellium"



Solve Poisson Equation for potential using periodic boundary conditions

Compare exact and jellium potential



Error in electrostatic potential over volume of supercell

Potential error goes as 1/L (length)!

L (Bohr)	Cell size	Median Error (eV)
10.2	8 atoms	2.0 eV
20.4	64	1.0
30.6	216	0.67
40.8	512	0.50
51.0	1000	0.40

Si band gap: 1.2 eV (expt.), 0.5 eV (DFT)

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, PRL **84**, 1942 (2000)]

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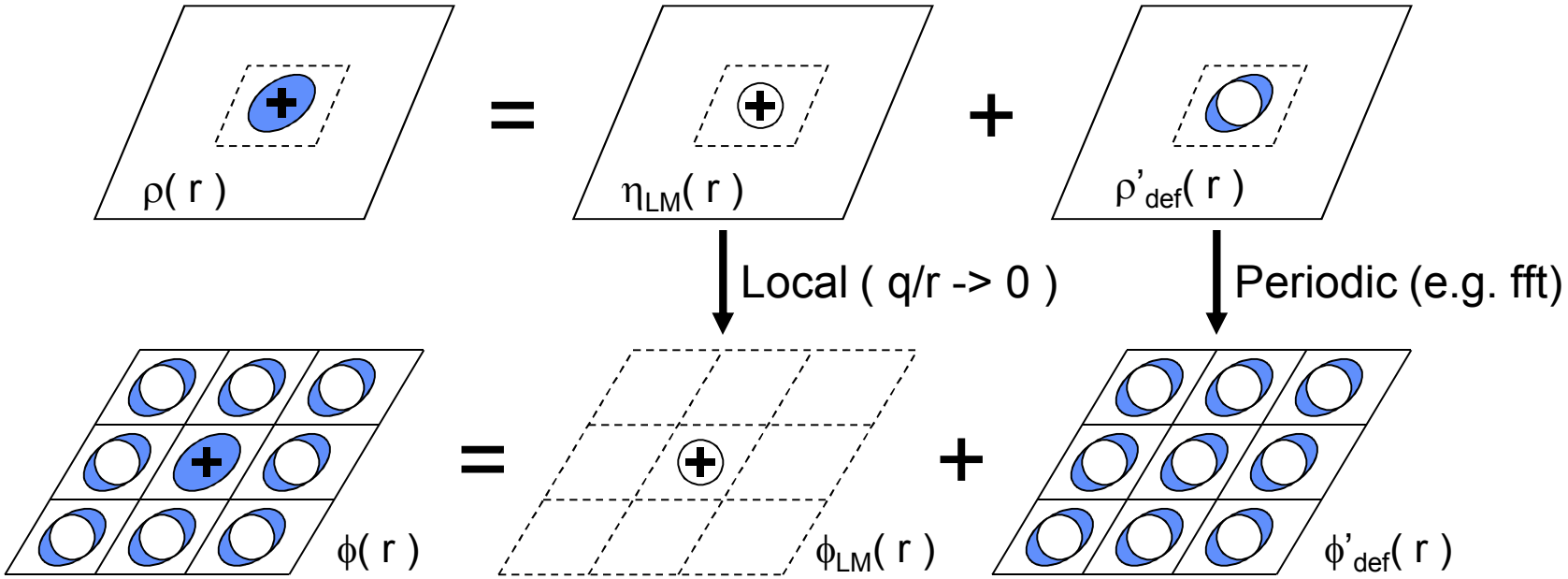
- Solution of Poisson Equation is linear in the density
- LMCC: split total density $\rho(r)$ into two pieces …

  (1) model local density $\eta_{LM}(r)$ matching multipole (charge) of $\rho(r)$

  (2) remainder (momentless) density $\rho'(r) = \rho(r) - \eta_{LM}(r)$

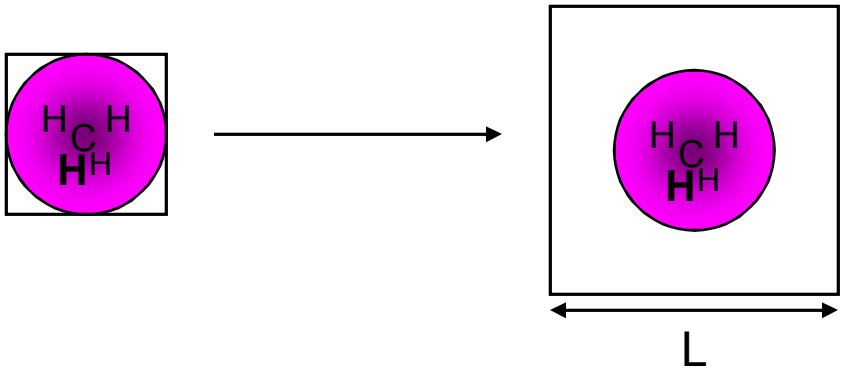


Gives proper $r \to \infty$ asymptotic boundary condition

Avoid (not ignore!) Coulomb divergence

Charged cell convergence - LMCC

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



Charged, no dipole: $CH_4 \rightarrow CH_4[+]$ … Ionization Potential

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

Dipole, no charge: Na–Cl diatomic molecule … Total Energy

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

Dipole, charge: $OH \rightarrow OH[-]$ … 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

LMCC potential in bulk systems

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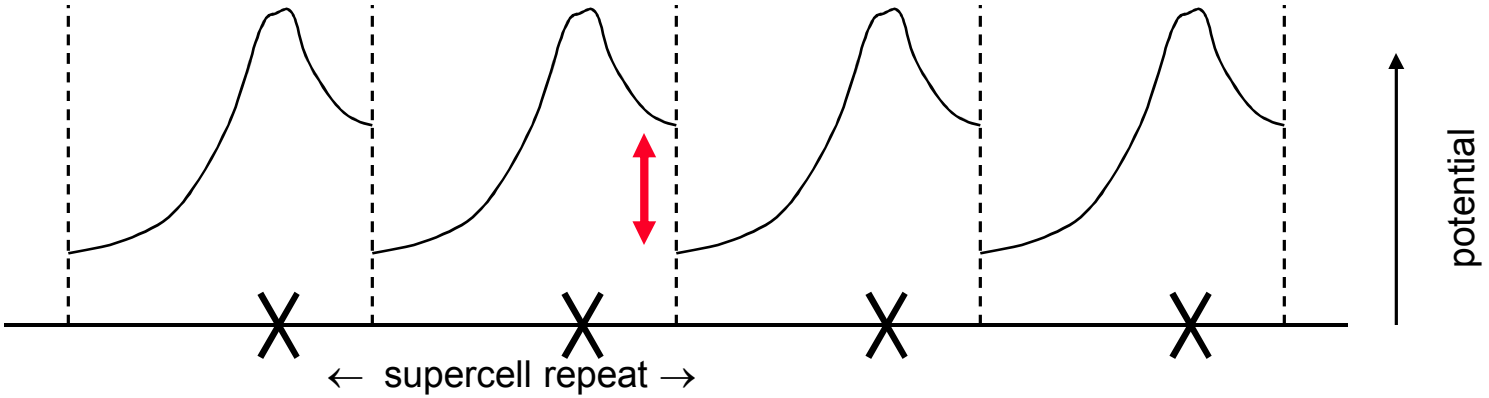
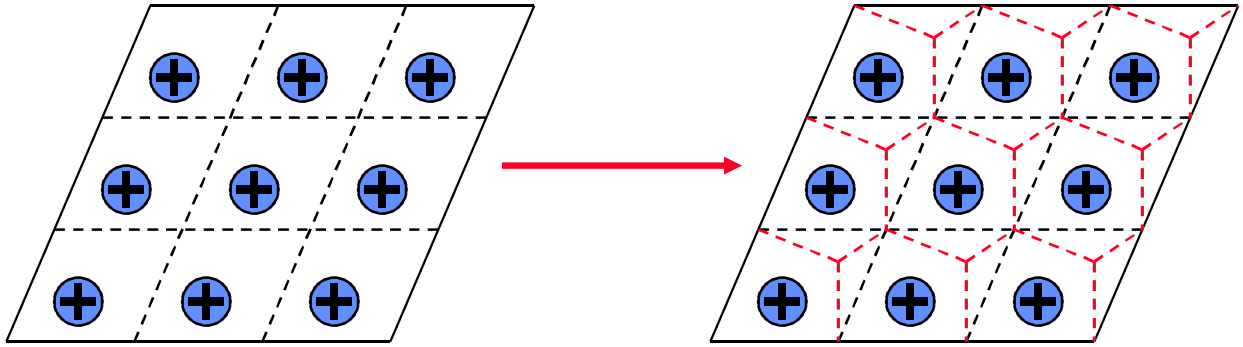
The complication in bulk systems …



Discontinuity in potential from LMCC at supercell boundary!

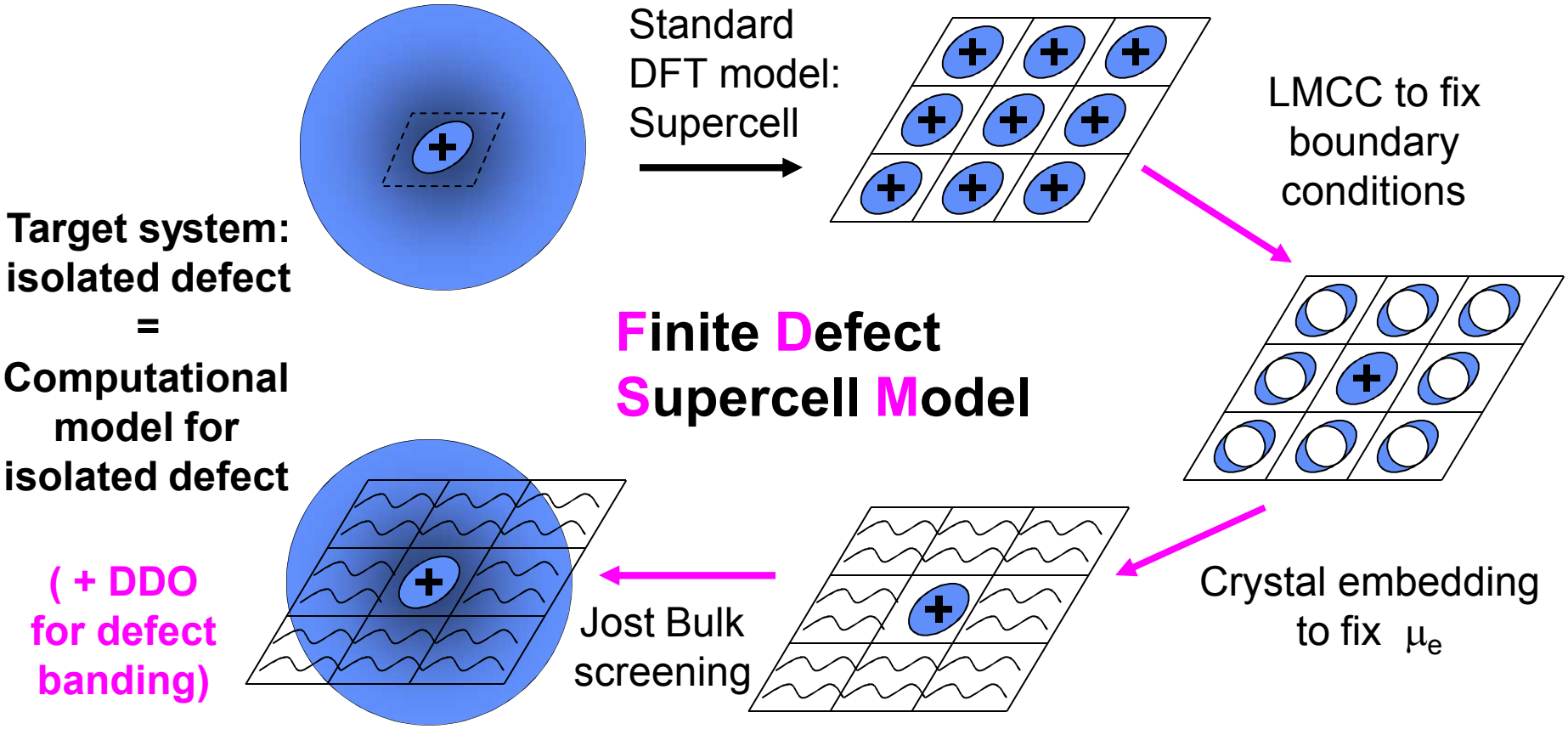
The solution: Wigner-Seitz cells around LMCC positions



With Wigner-Seitz local volume, LMCC potential is continuous

A supercell theory of defect energies

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



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

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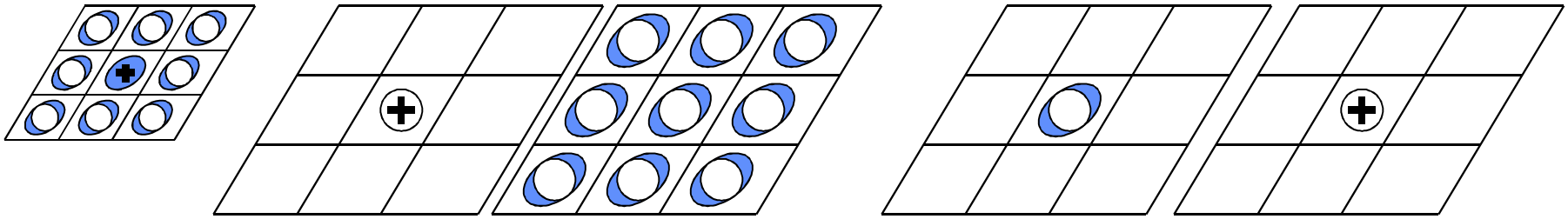
A fixed chemical potential μ_e

Replace interaction of net charge with periodic defect potential …

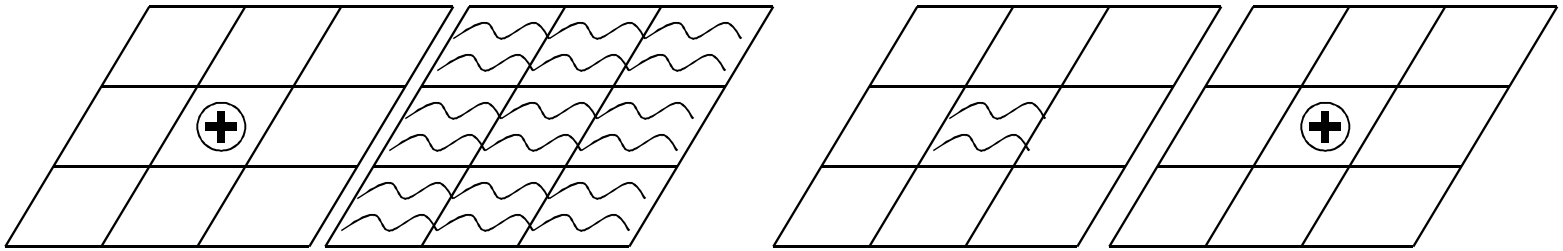
$$E_{\mu 0} = -\int dr\ \eta^{+}_{LM}\,(\phi'_{def} + C'_{def}) + \int_{UC} dr\ \phi^{+}_{LM}\ \rho'_{def}$$



$\eta^{+}_{LM}(r)$ $\phi'_{def}(r) + C'_{def}$ $\rho'_{def}(r)$ $\phi^{+}_{LM}(r)\ (C=0)$

… with crystal potential:

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



$\eta^{+}_{LM}(r)$ $\phi_{xtal}(r) + C_{xtal}$ $\rho_{xtal}(r)$ $\phi^{+}_{LM}(r)\ (C=0)$

Replace ***variable*** defect cell C'_{def}, with ***fixed*** crystal C_{xtal} reference

Chemical potential equivalent to matching potential at R=∞

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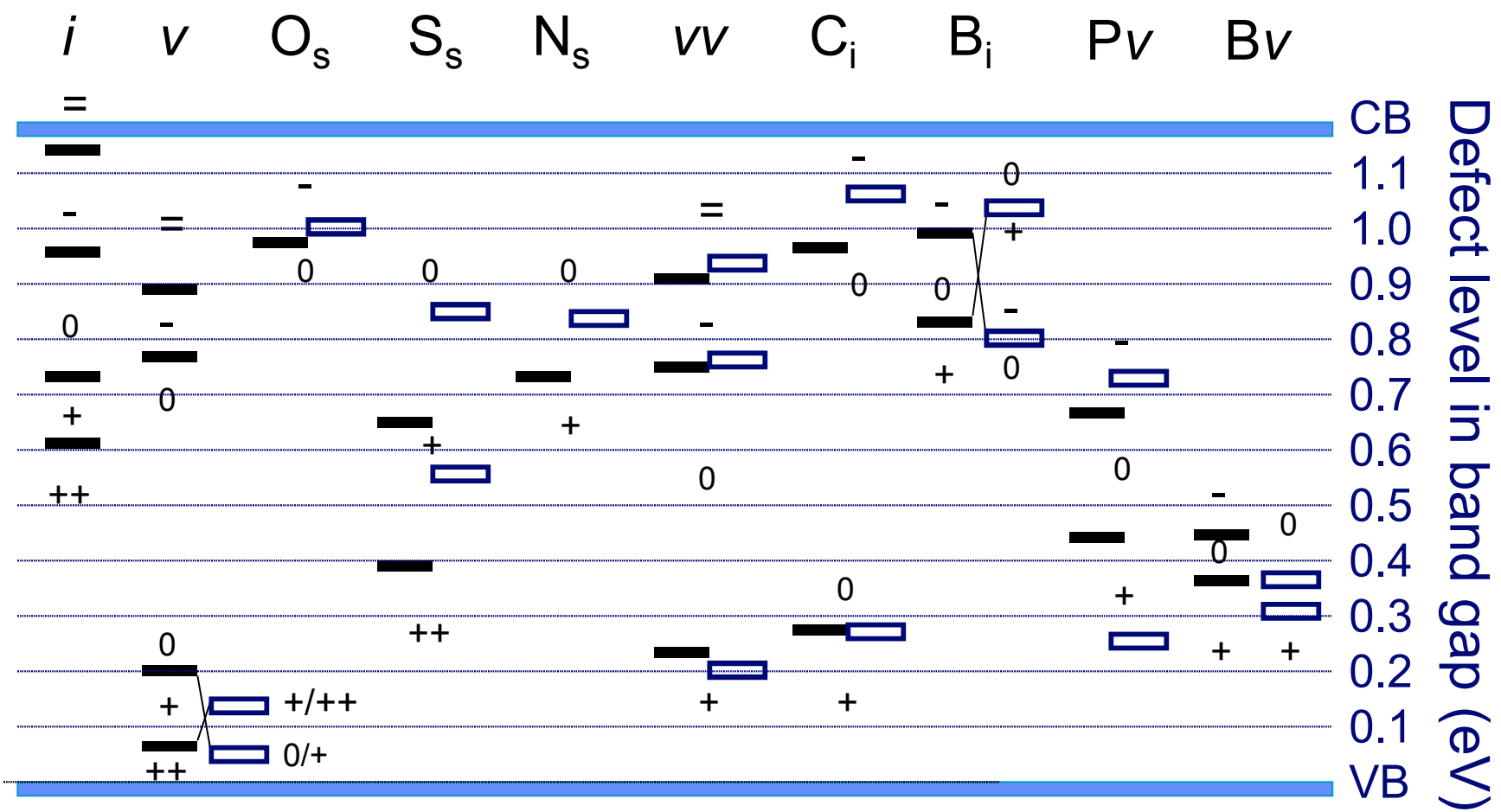
Si: DFT/LDA vs. Experimental Levels



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

Problems: Boron interstitial (negative-U), *v*acancy (0/+/2+)

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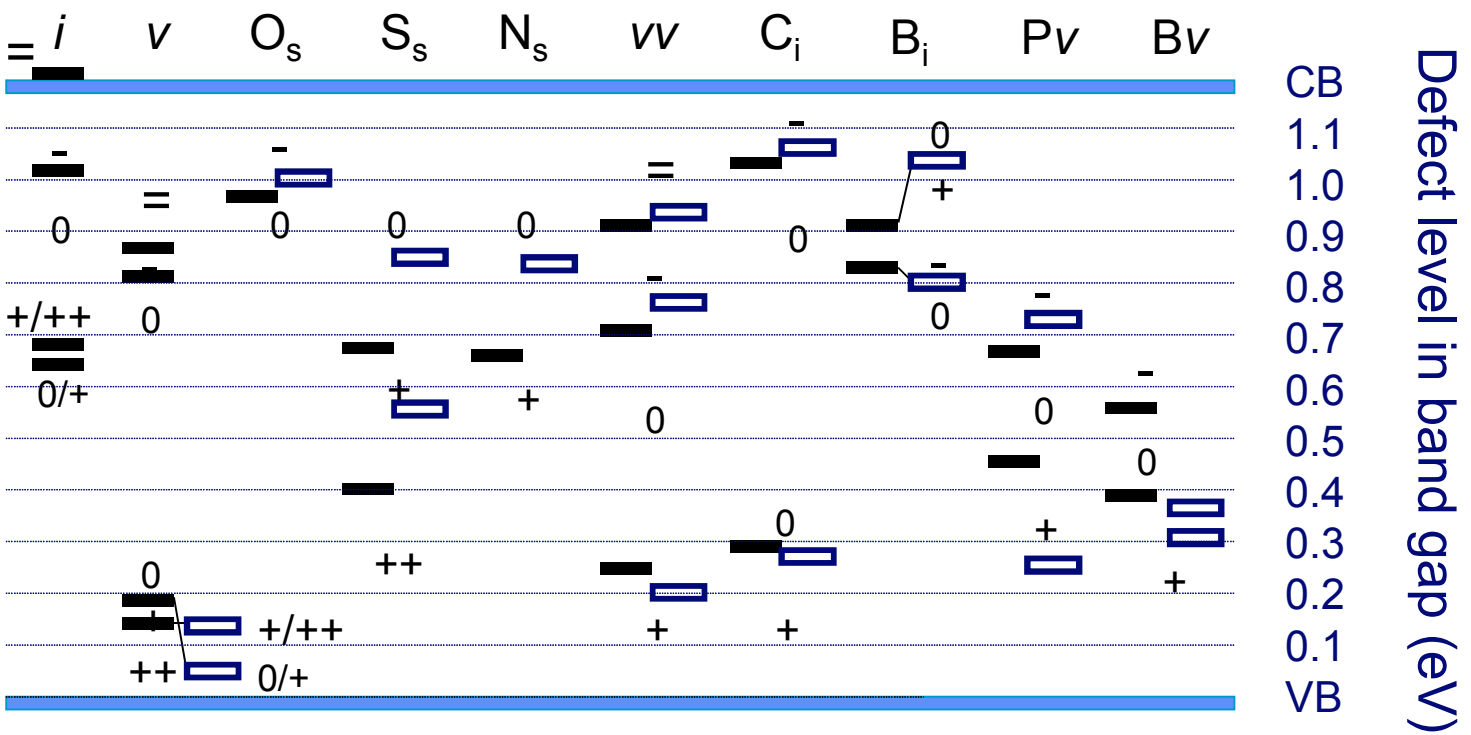
Si: DFT/PBE vs. Experimental Levels



… and some other defects

DFT "defect gap" matches experiment.
DFT/PBE defect level max error=0.20 eV, mean |error|=0.10 eV
Band gap problem not seen in **total-energy-based** defect levels

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Computational methods – III-V's

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- **General purpose DFT code SeqQuest** (http://dft.sandia.gov/Quest)
  - –well-converged (Gaussian-based) local orbital basis
  - –both LDA and PBE functionals
  - –converged norm-conserving pseudopotentials (Ga,In both Z_{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(theory); GaAs: 5.60Å(LDA), 5.63Å(3d), 5.74Å(PBE); a_0(expt)=5.65 Å)
  - –Cubic supercells: 64-, 216-, 512-, 1000-site
  - –***k***-sampling: 3^2 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 to Si that yielded 0.1 eV accuracy

Simple intrinsic defects in GaAs: LDA

Peter A. Schultz

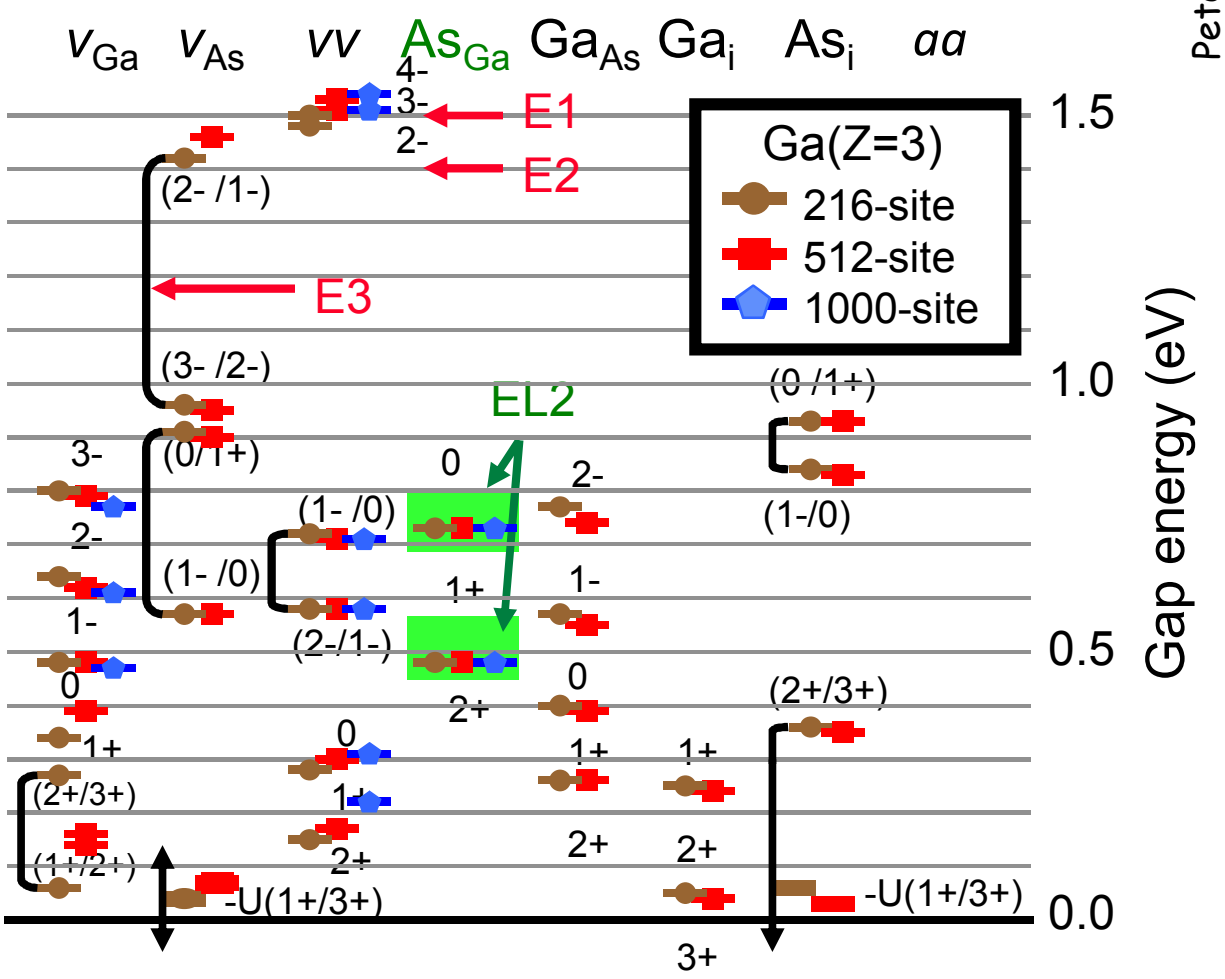
P.A. Schultz and O.A. von Lilienfeld, MSMSE **17**, 084007 (Dec. 2009).

216- = 512- = 1000-site
Verification: cell-converged

LDA-3d = LDA to ≤0.1eV
Verification: PP converged

LDA~PBE; spin <0.05 eV
Verification: functionals

As_{Ga} levels = EL2 levels
v_{Ga} levels below midgap
Validation: levels < 0.1 eV



DFT+FDSM: Apparent accuracy of ~0.1 eV

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The GaAs divacancy is the E1-E2 radiation center

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Old (experimental) lore, back to 1988:

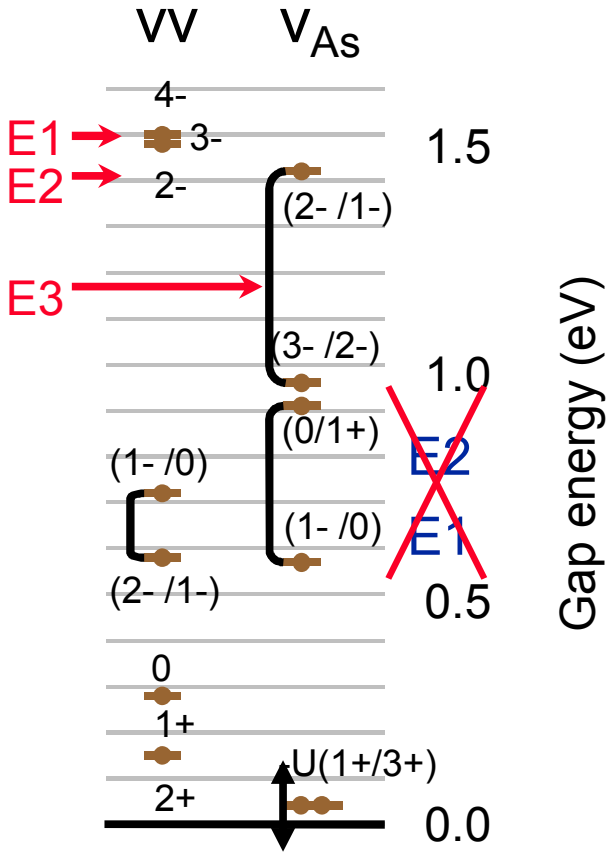
- E1, E2 center = v_{As}(-/0), v_{As}(0/+)
- E3 = v_{As} + *i*
- *vv* is dismissed

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

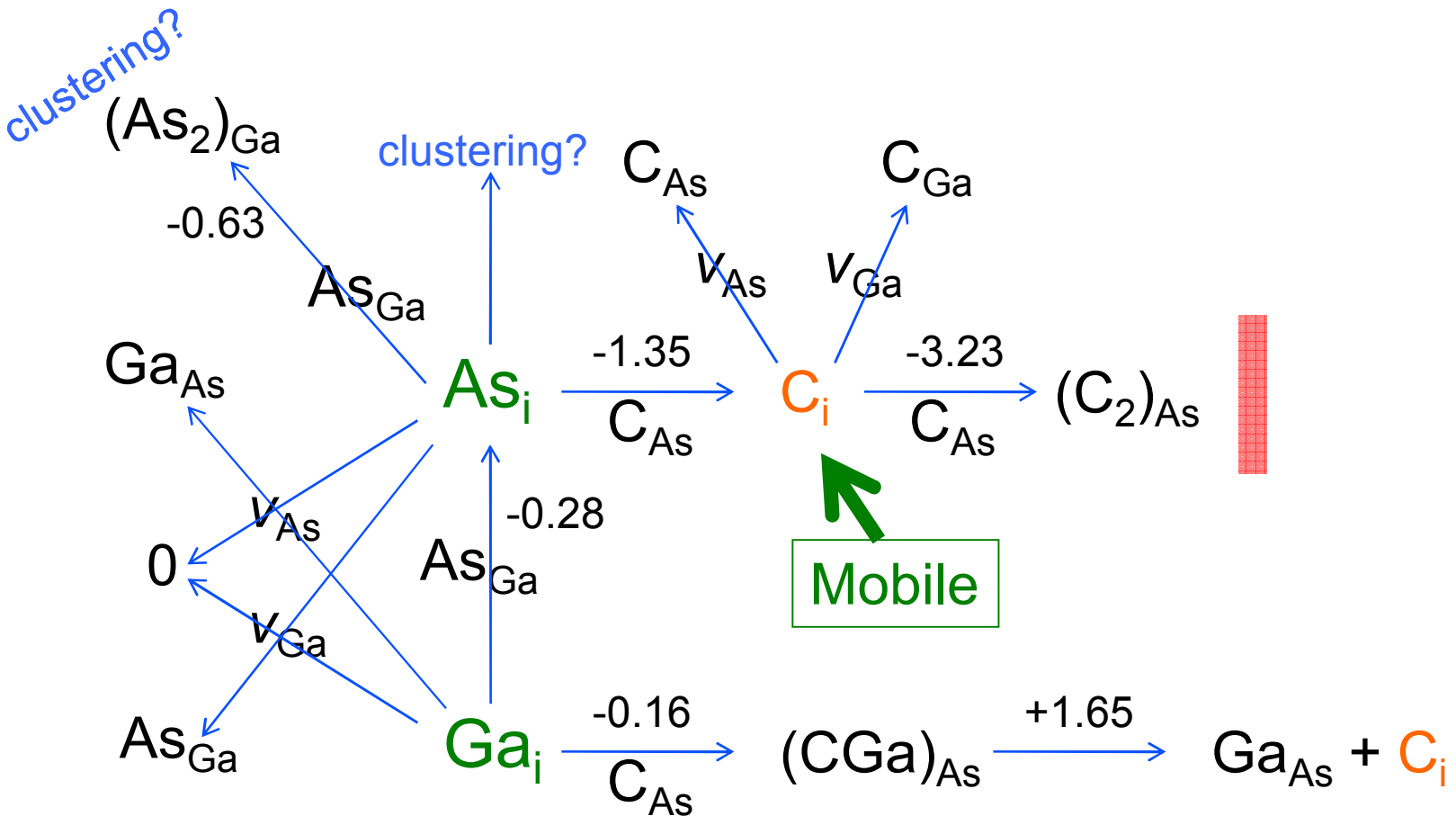
v_{As}(3-/1-) transition is the E3



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

GaAs: C-doped reaction network

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



Reliable defect levels means reliable chemistry

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Simple intrinsic defects in GaAs: LDA

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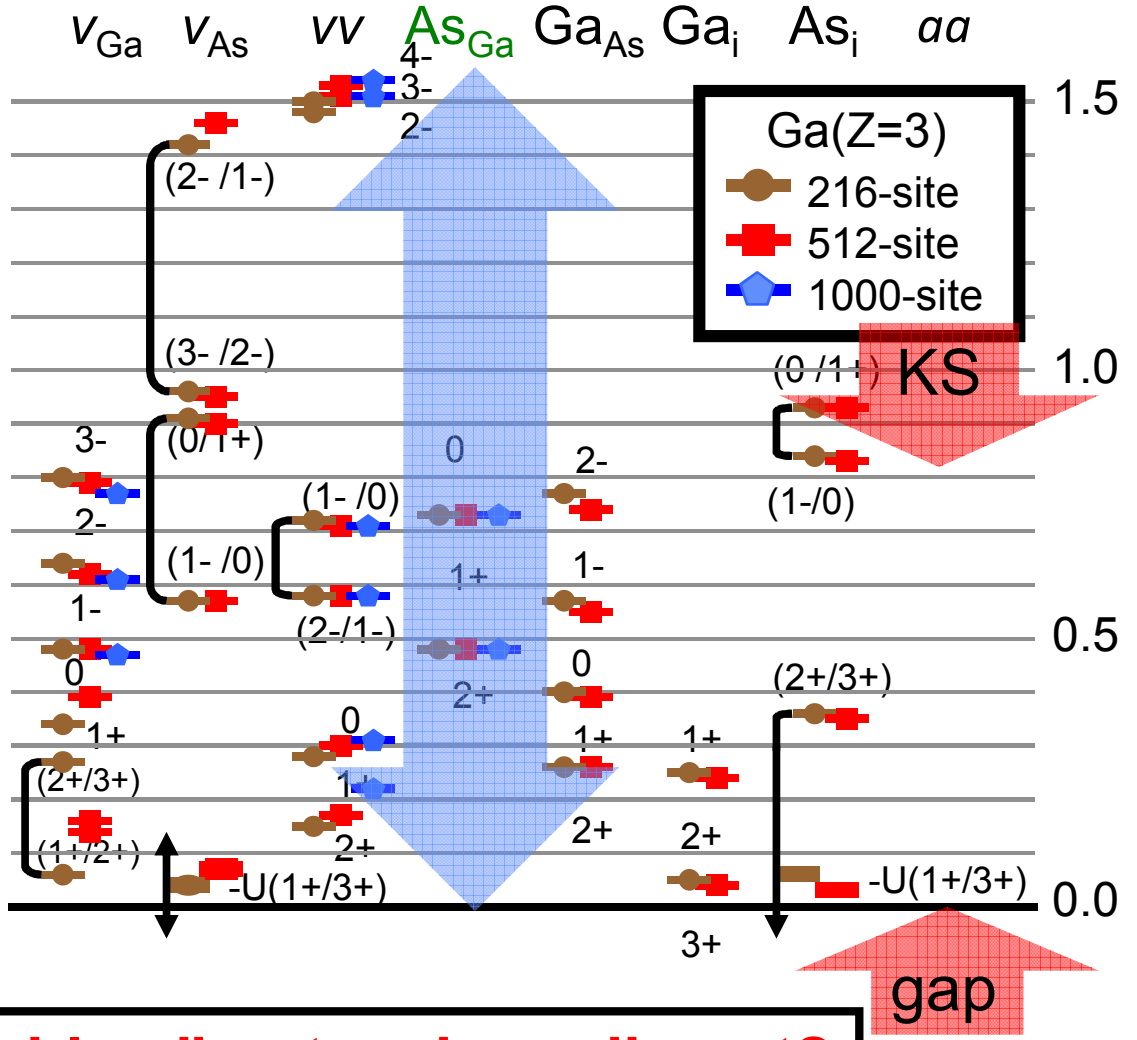

Band gap

Kohn-Sham: 0.83 eV

Defect span: 1.54 eV

Experiment: 1.52 eV

"Band gap problem" not an impediment?

GaAs defect levels: LDA-3d

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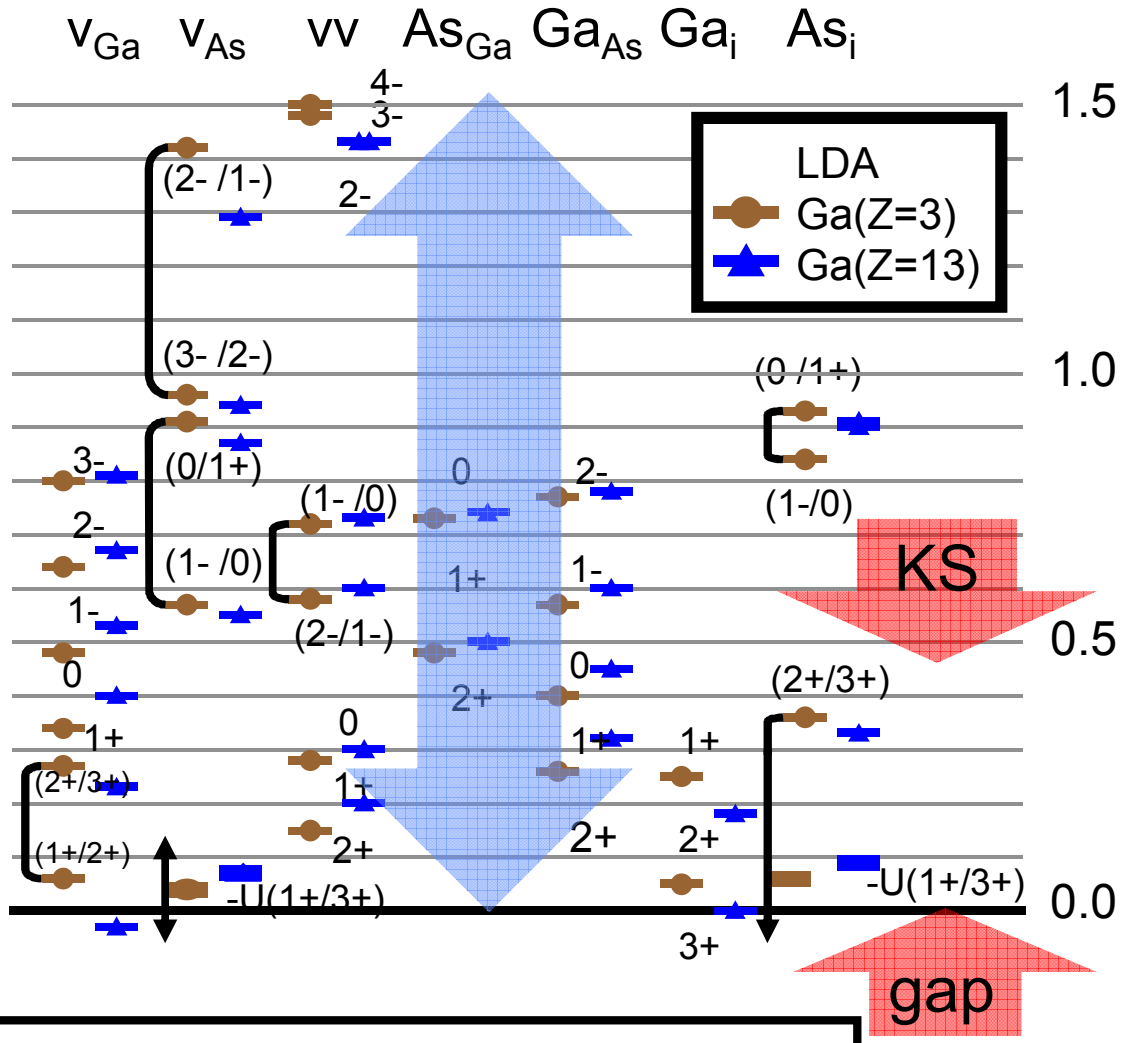

Band gap
- Kohn-Sham: 0.47 eV
- Defect span: 1.52 eV
- **Experiment: 1.52 eV**

LDA-3d: KS gap shrinks, defects ~same

GaAs defect levels: PBE

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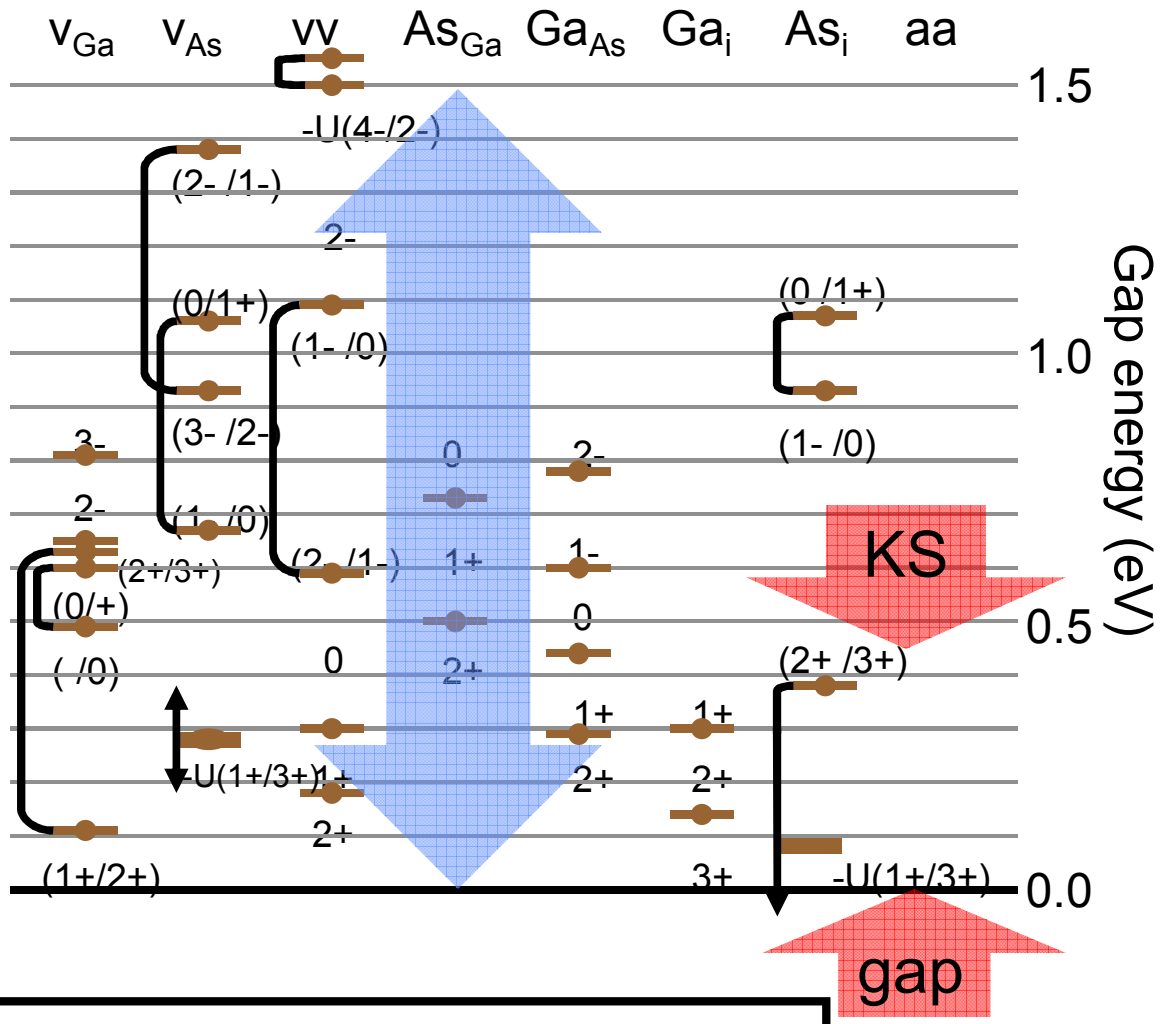
Band gap
- Kohn-Sham: 0.45 eV
- Defect span: 1.50 eV
- **Experiment: 1.52 eV**



PBE Kohn-Sham gap is even smaller …

GaAs defect levels: PBE-3d

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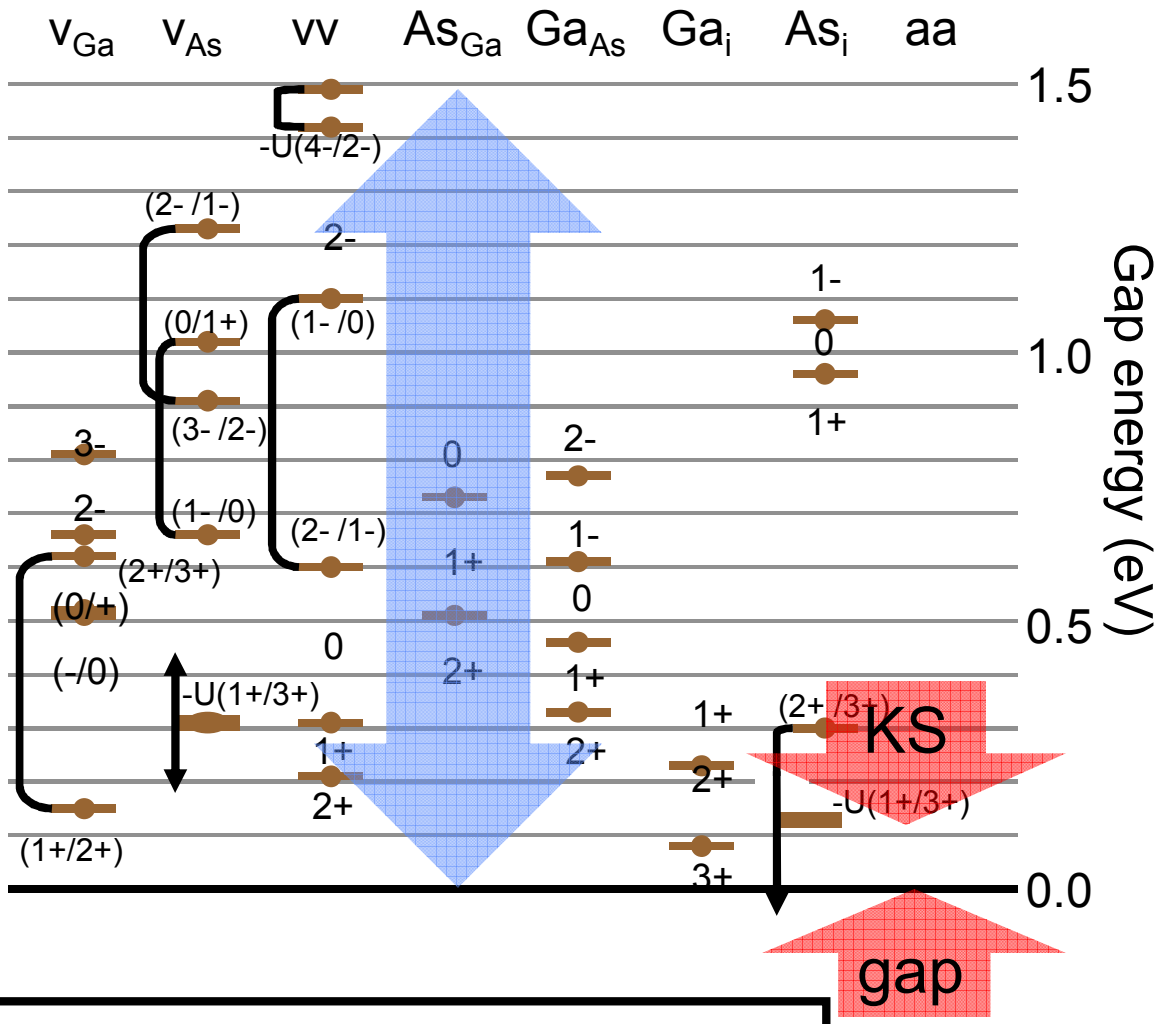

Band gap

Kohn-Sham: 0.13 eV

Defect span: 1.50 eV

Experiment: 1.52 eV

… with 3d-valence, KS gap is very small

GaAs Computational model lessons

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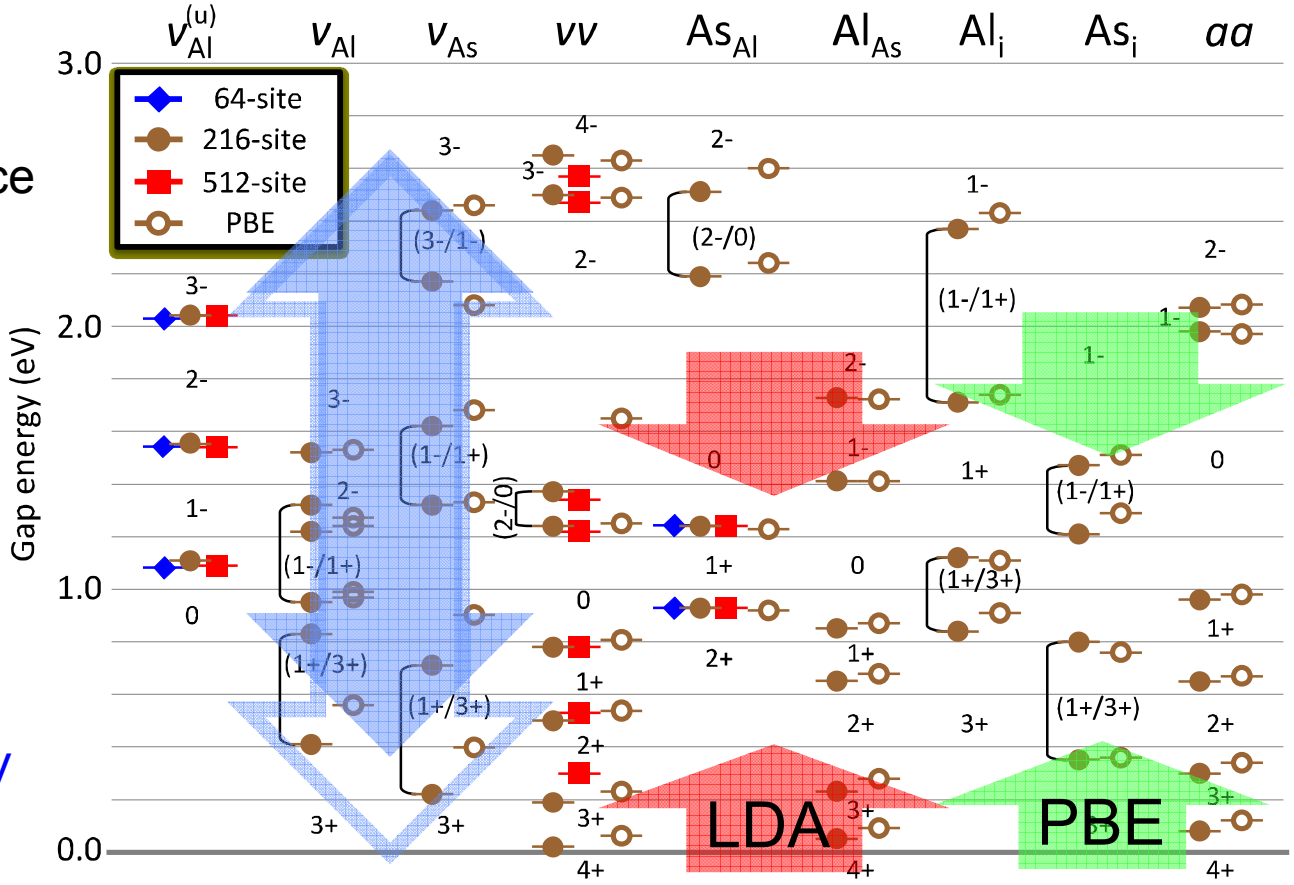
- KS band gap not a problem for Si and GaAs defects
- Defect levels insensitive to size of Kohn-Sham gap!
  - total-energy differences vs. eigenvalue-referenced
  - GaAs is ideal theoretical laboratory for testing methods
- Detailed control of boundary conditions crucial: FDSM works
- Is this unique 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: $v_{Al}^{(u)}$
- Checked: As_{Al}
- Verified: *vv*

Band gap
- KS-LDA: 1.37 eV
- KS-PBE: 1.53 eV
- Defect span: 2.3-2.7 eV
- **Experiment: 2.16[i] eV**



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

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GaP intrinsic defects

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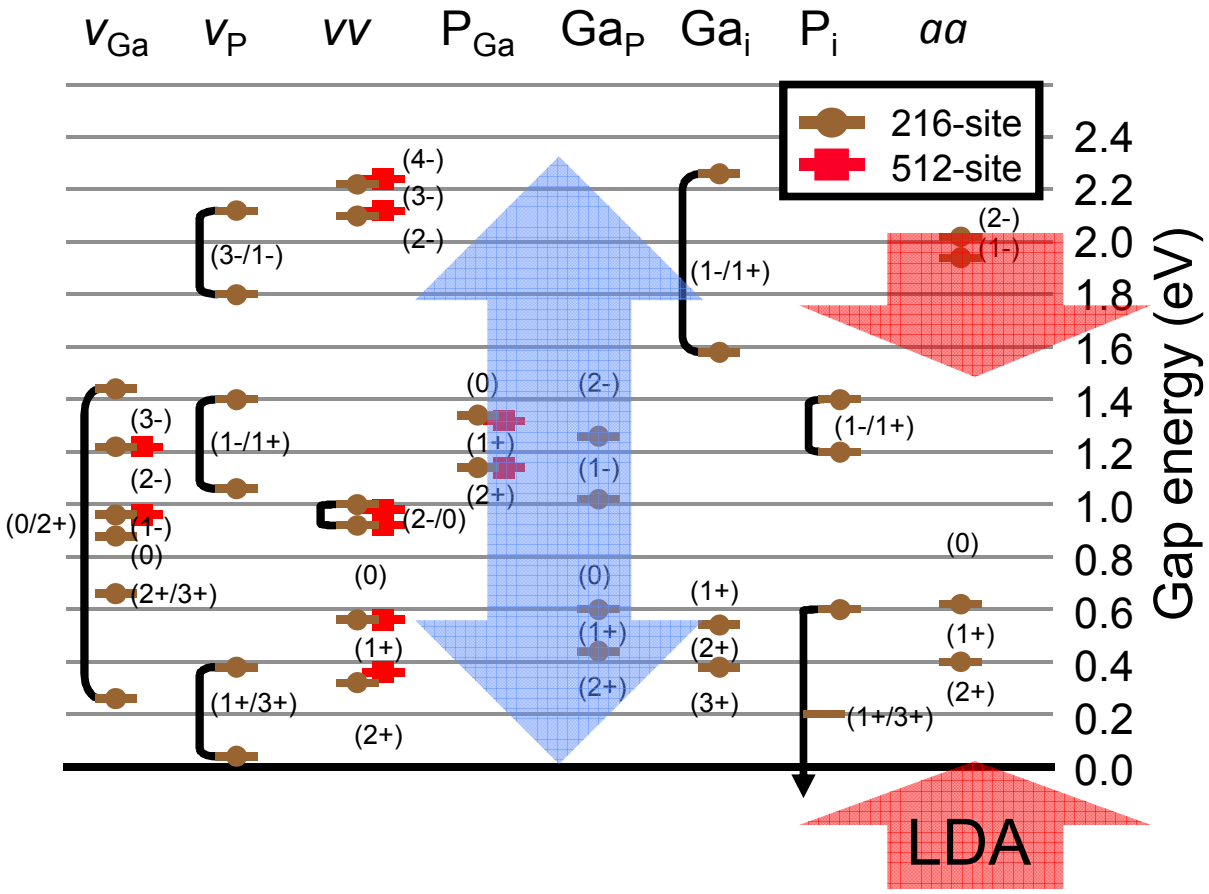
216-site results = 512-site
Verification: cell-converged

GaP band gap
KS-LDA: 1.51 eV
Defect span: 2.35 eV
Experiment: 2.35 eV

GaP defect levels: LDA, Ga(Z=3) PP



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InP intrinsic defects

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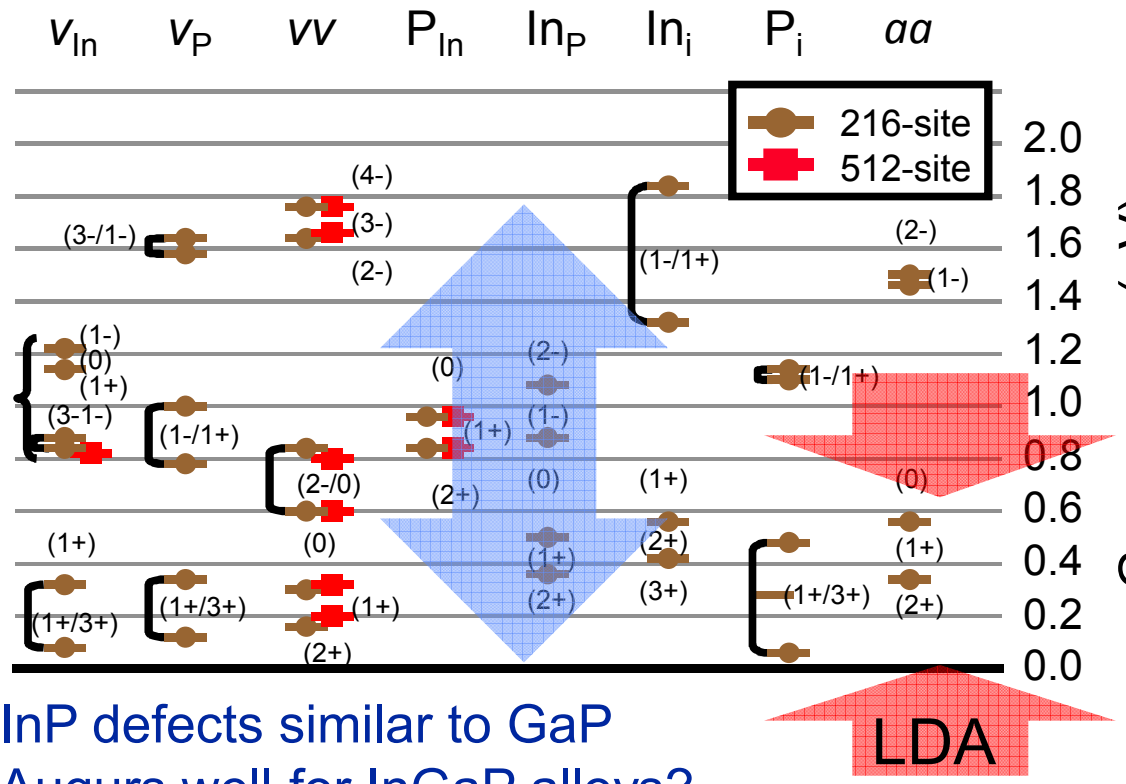
216-site results = 512-site
Verification: cell-converged

InP band gap
KS-LDA: 0.67 eV
Defect span: 1.7 eV
Experiment: 1.42 eV

InP defect levels, LDA, In(Z=3) PP



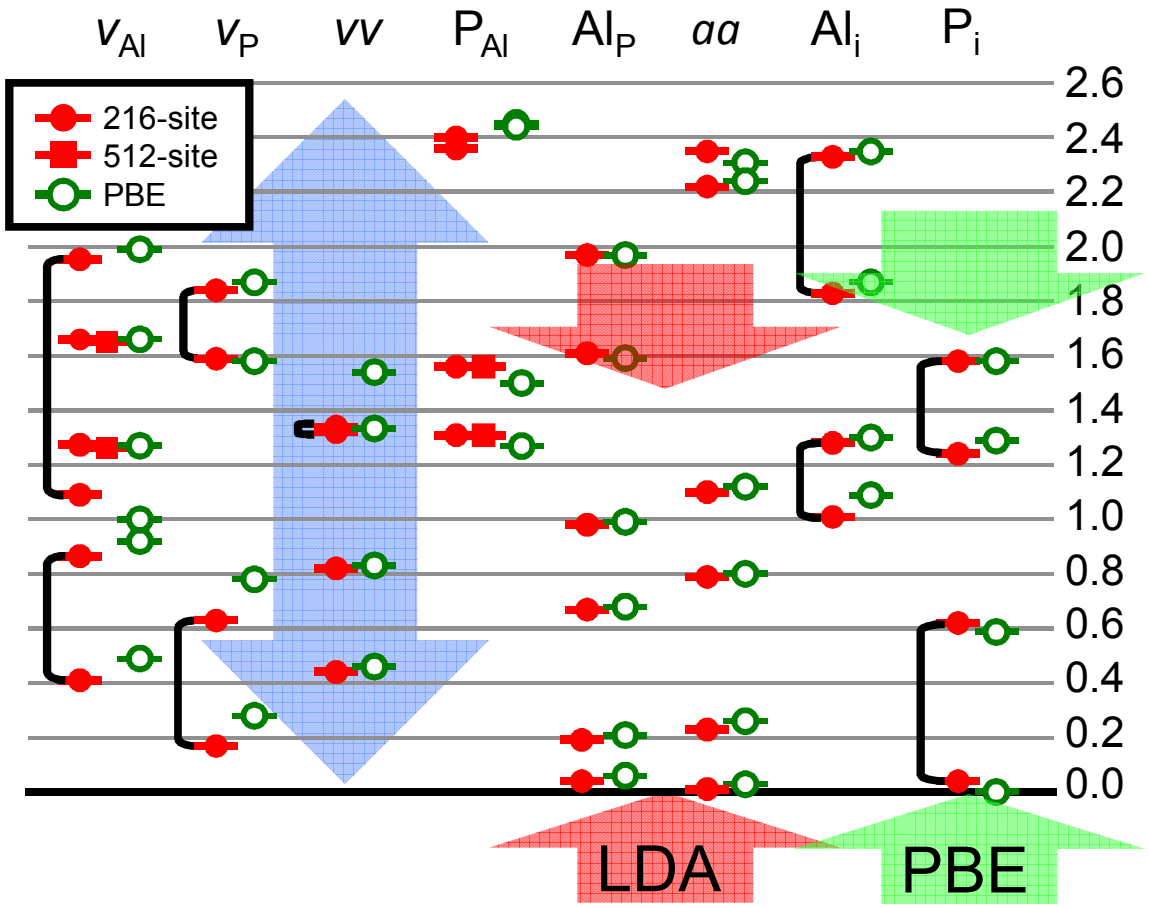
InP defects similar to GaP
Augurs well for InGaP alloys?

AlP intrinsic defects

Peter A. Schultz

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

AlP band gap
KS-LDA: 1.48 eV
KS-PBE: 1.67 eV
Defect span: 2.55 eV
Experiment: 2.51 eV



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The DFT "Defect band gap"

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- Kohn-Sham gap: CB to VB energy, *outside* bounds of *band eigenvalues*
- Defect band gap: *inside* bounds of transition *energies* for local defects

Band gaps: **experiment**, Kohn-Sham, DFT defect span

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 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

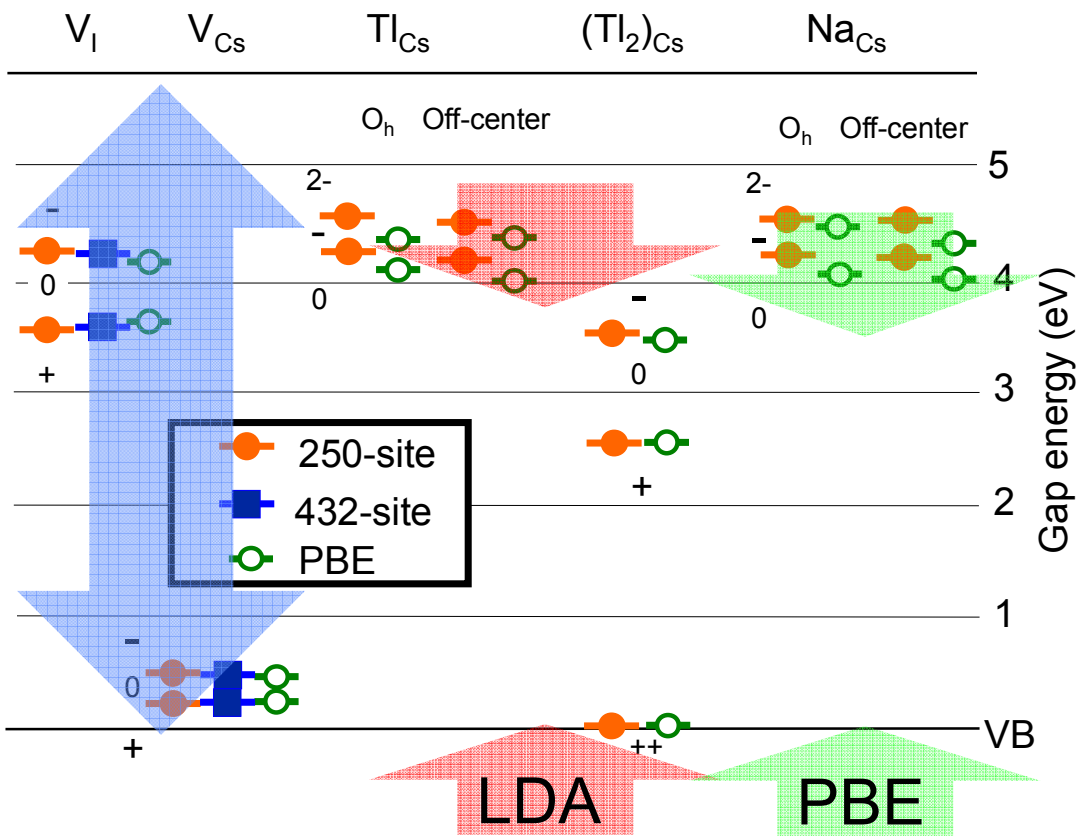
CsI defect level spectrum

Thanks: R. M. Van Ginhoven (PNNL), unpublished results

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: 0.63 eV



(... and not only tetrahedral crystals)

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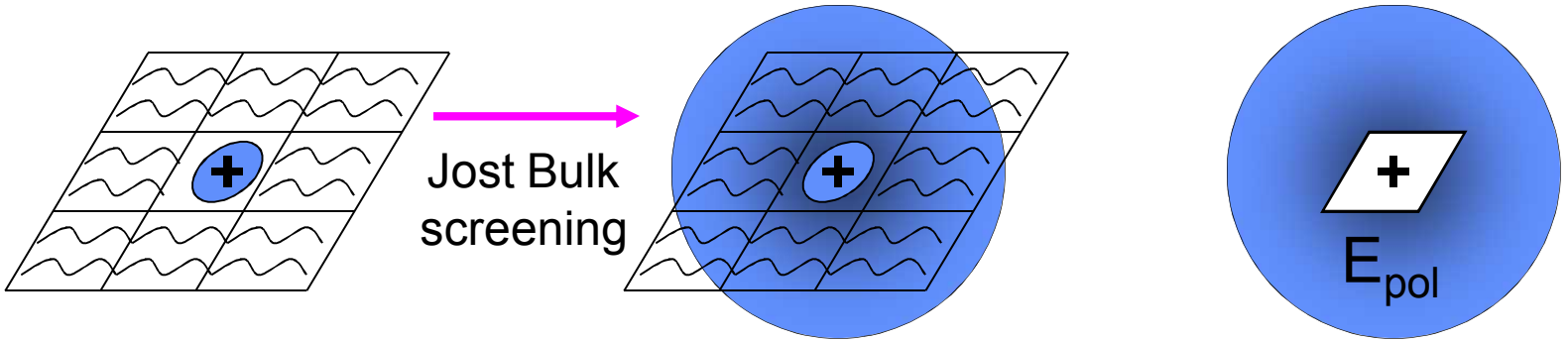
The polarization model



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

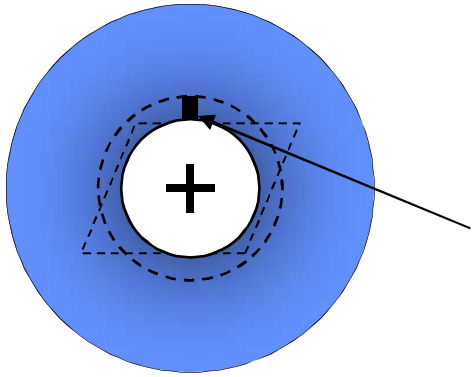
Jost model: $E_{pol} = \frac{(1 - 1/\varepsilon_0)\, q^2}{R_{jost}}$

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

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: =1.4-1.7 Bohr

ε_0 = static dielectric constant - expt

Si	GaAs	InP	GaP	AlAs	InAs
11.8	13	12.5	11.2	10.1	15.15

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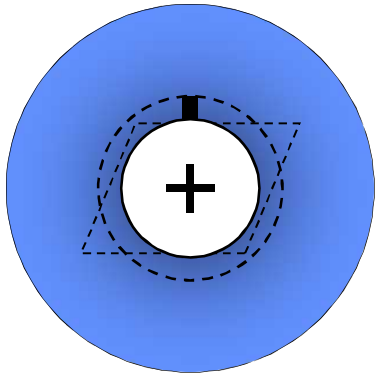
How big is bulk screening?



$$E_{pol} = \frac{(1 - 1/\varepsilon_0)\, q^2}{R_{jost}}$$

Defects mostly converged at 64-site cells
Formula mostly insensitive to ε_0 at 10-15, use GaAs

Charge:	+1,-1	+2,-2	+3,-3	+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**
This is key to understanding KS gap *vs.* defect gap

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How is a good defect band gap possible?

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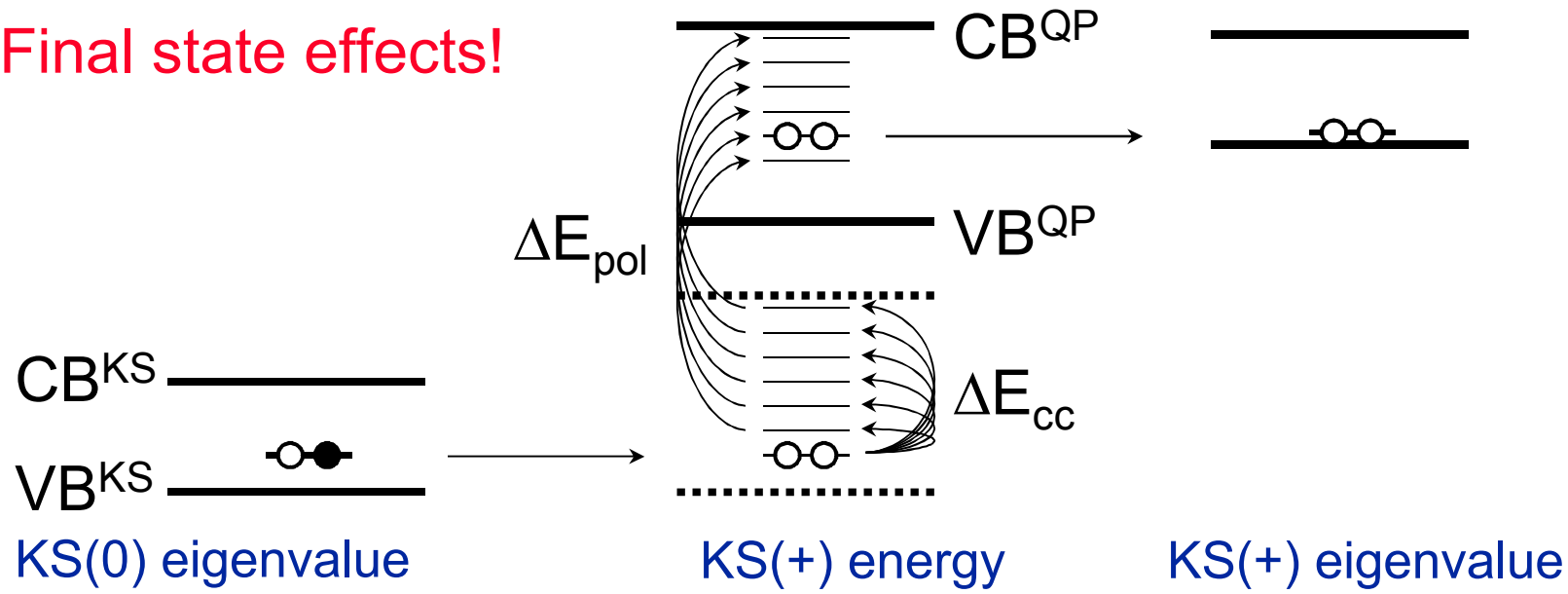
Final state effects!



Central cell relaxation (quantum): ΔE_{cc}
Long range screening (classical): $\Delta E_{pol} > E_g$
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

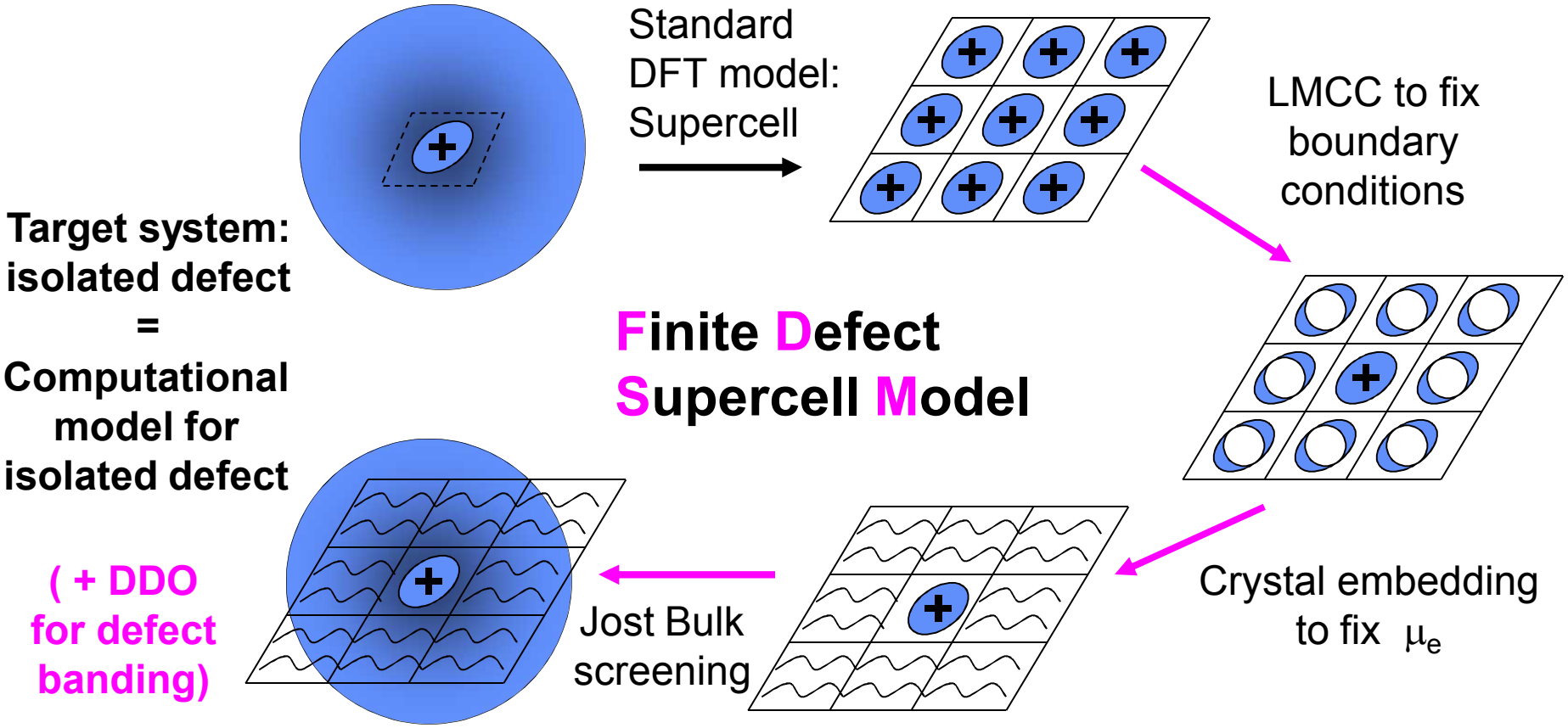
- Ab initio *computational model* – reconstruct computational model from roots
  - crucial to bridge "gap" between model (DFT code) and reality (defects)
  - rigorous, explicit control of boundary conditions is essential: FDSM works
- Semilocal DFT+FDSM - quantitative (~0.1 eV) for defect levels in semiconductors
  - the "band gap problem" is not a limitation (for these systems)
  - defect gap is surprisingly? good estimator of experimental gap
- But neither is this a complete solution (yet)
  - where are the band edges?
  - LDA and PBE limitations (vdW, localized states, highly correlated …)
- KS interpretation of band gap is not-even-wrong for defects
- LDA,PBE already describe defects (very) well
- Path to better functionals: "fixing" KS gaps as primary goal may be wrong

Thanks to: Arthur H. Edwards (AFRL), Renee M. Van Ginhoven (PNNL)

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

A supercell theory of defect energies

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



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

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The electron chemical potential μ_e

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

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

linked

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

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

C_{def} = fcn{defect type, configuration, cell shape, cell size, …}

$E_{defect}(q)$ 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

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Finite Defect Supercell Model Formation Energy

$$E_{form}(q) = E_{defect}(q) - E_{xtal}(0) - \Sigma N_i \mu_i + E_{\mu 0}(q) + E_{pol}(q)$$

$E_{defect}(q)$: DFT energy with LMCC potential
$- E_{xtal}(0) - \Sigma N_i \mu_i$: match number of each type of atom
$E_{\mu 0}(q)$: fix chemical potential μ_e to common electron resevoir
$E_{pol}(q)$: bulk polarization response

Defect level calculation

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

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

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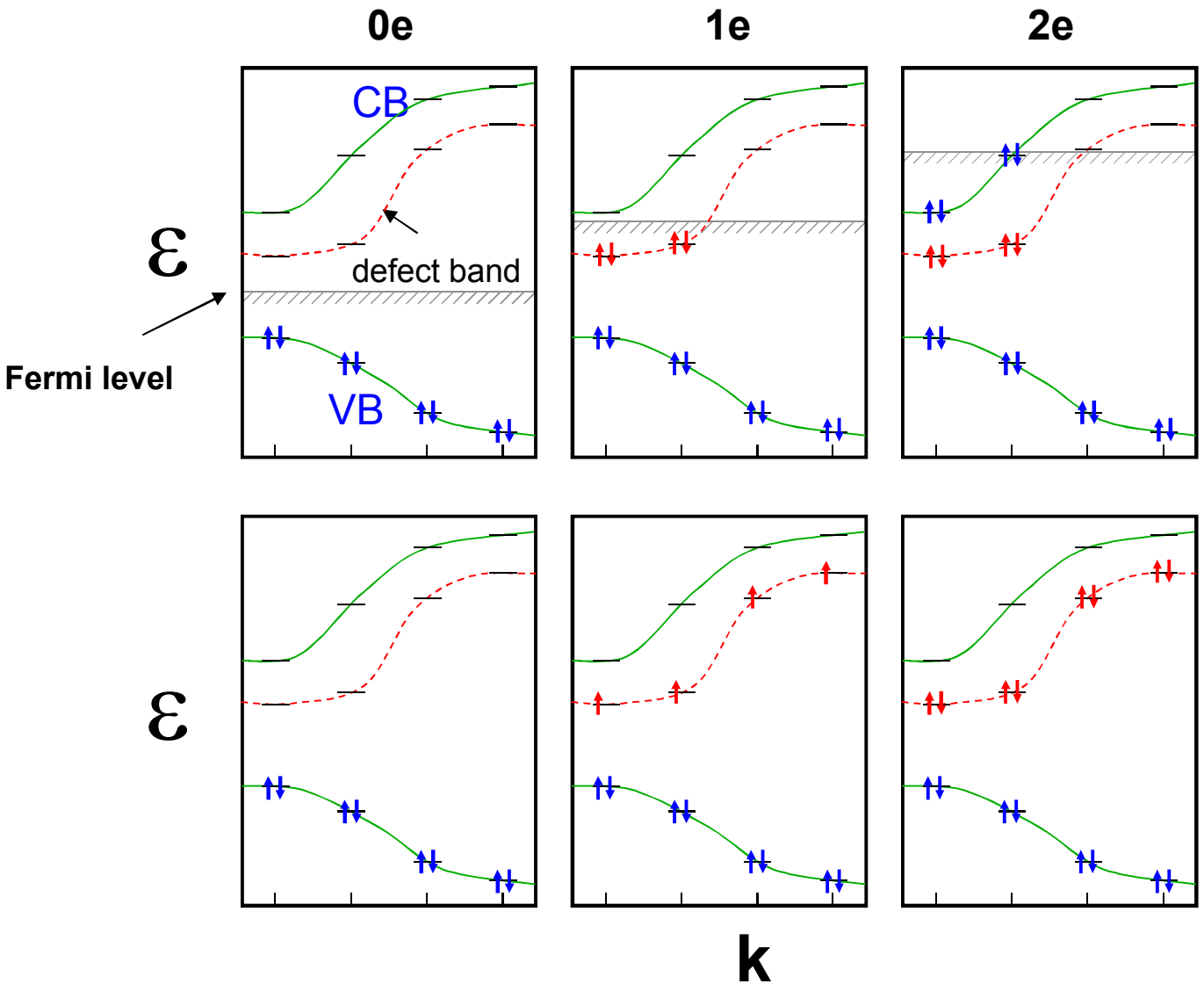

Standard methods: metallic, poor model of defect.

DDO: valid model of defect state with 0,1,2 electrons

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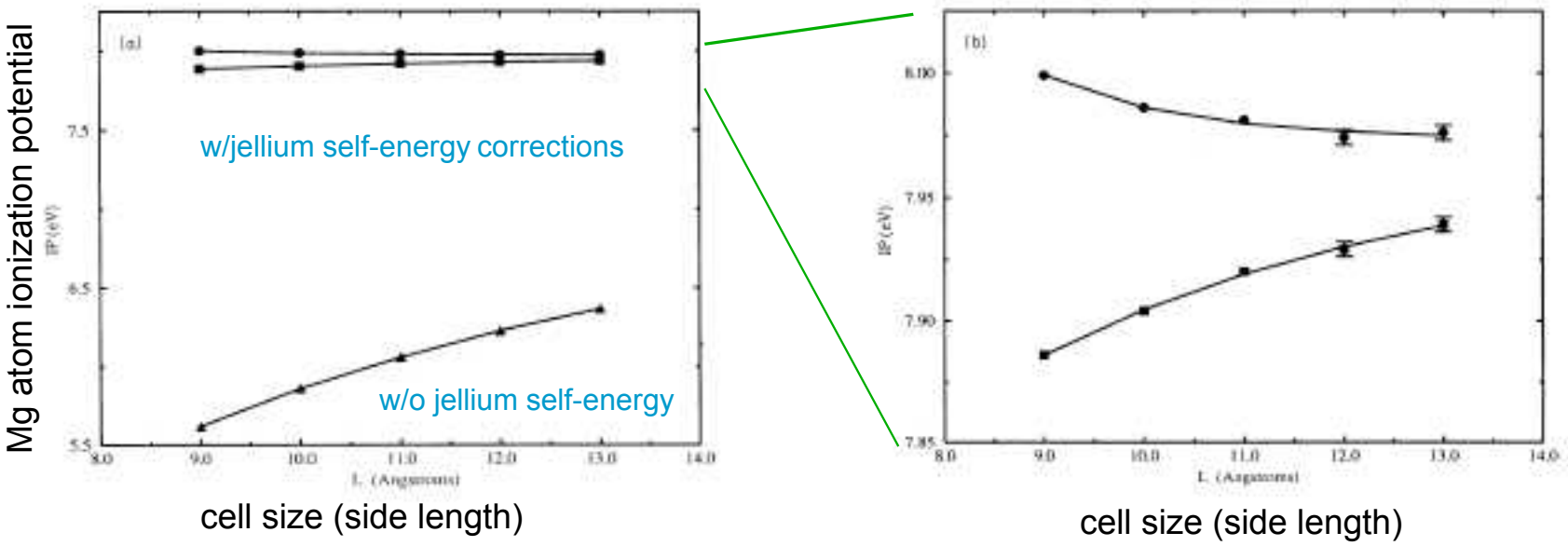
Charged cell convergence - Jellium

PHYSICAL REVIEW B VOLUME 51, NUMBER 7 15 FEBRUARY 1995-I

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

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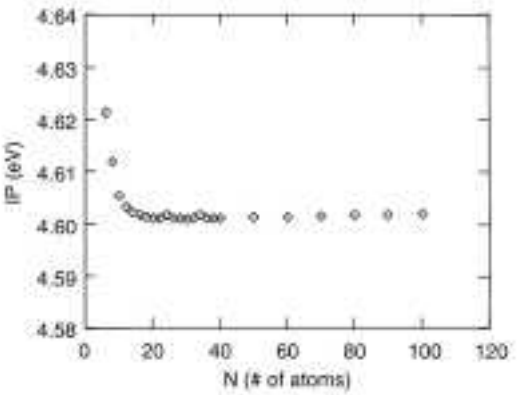
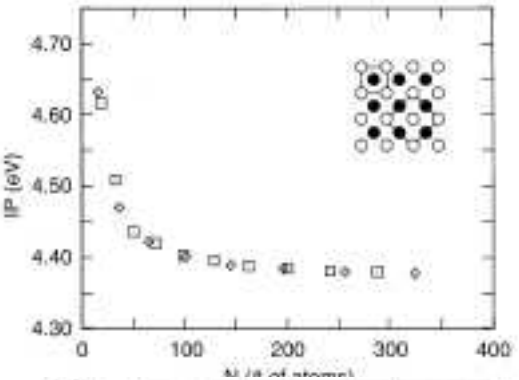
1D chain



1D: ← ○●○●○+○●○●○● →

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

2D sheet

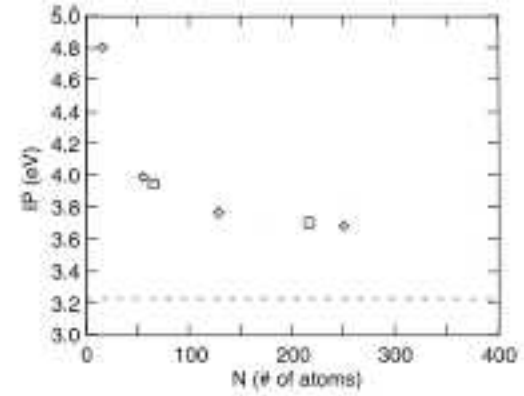


2D: single-layer 2D square sheet (polar&non-polar)

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

Insensitive to cell type, polar vs. non-polar

3D bulk



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

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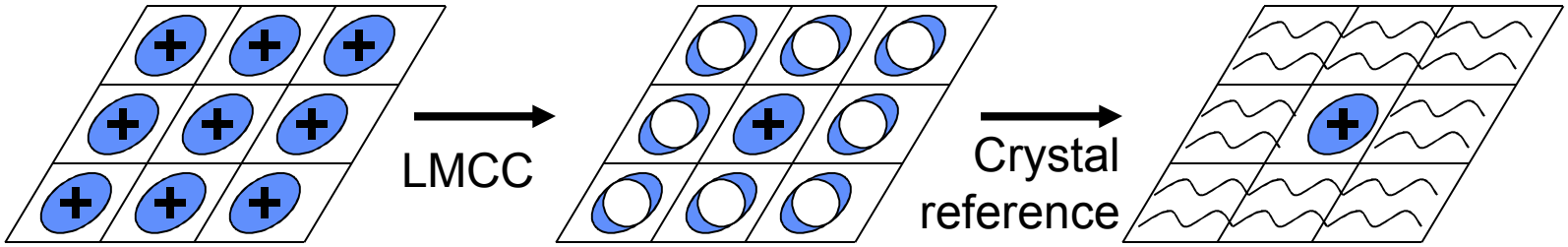
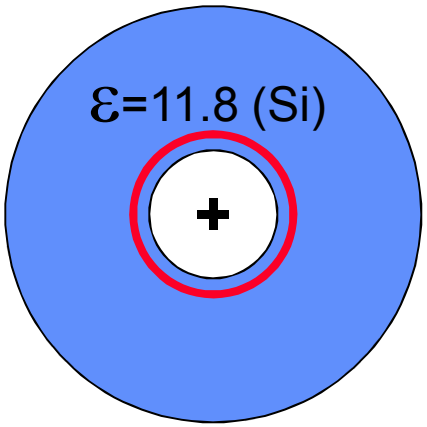
Bulk polarization in a dielectric medium



Ill-posed b.c.

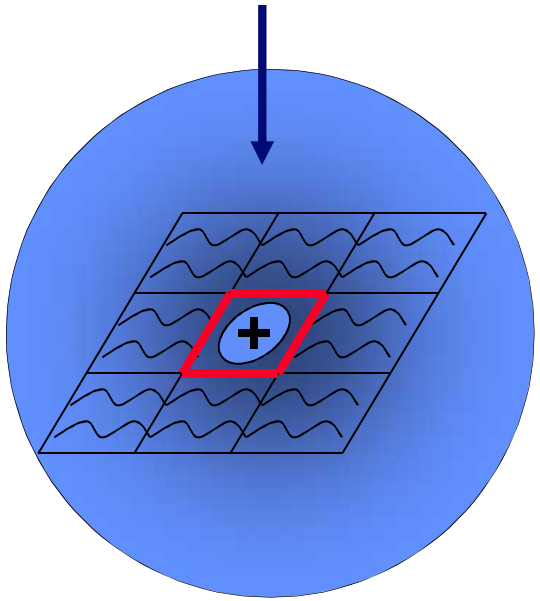
Variable μ_e

Bulk polarization?



Jost model (1934):

E_{jost} = response of dielectric to charge q in a cavity (I.e., our defect supercell)



$E_{pol}(q) = (1-1/\varepsilon_0)(q^2/2R_{jost})$

Bulk polarization included through classical dielectric theory

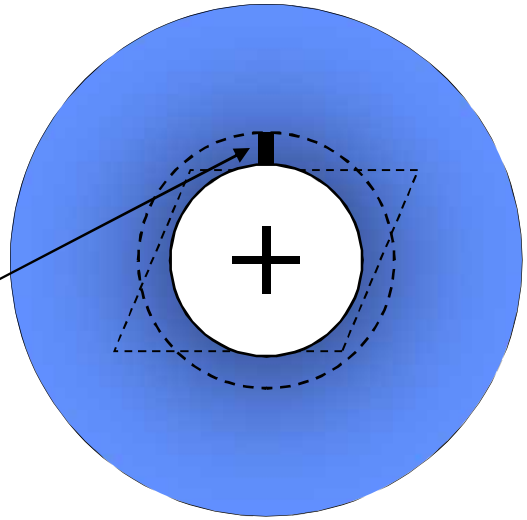
Calibrating the polarization model: v_{Ga}

Jost model:

$$E_{pol} = \frac{(1 - 1/\varepsilon_0)\, q^2}{R_j}$$

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

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_{Ga}(0)	E(2-/1-)-E(1-/0)	E(3-/2-)-E(2-/1-)	aAs: 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

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Silicon defect structures

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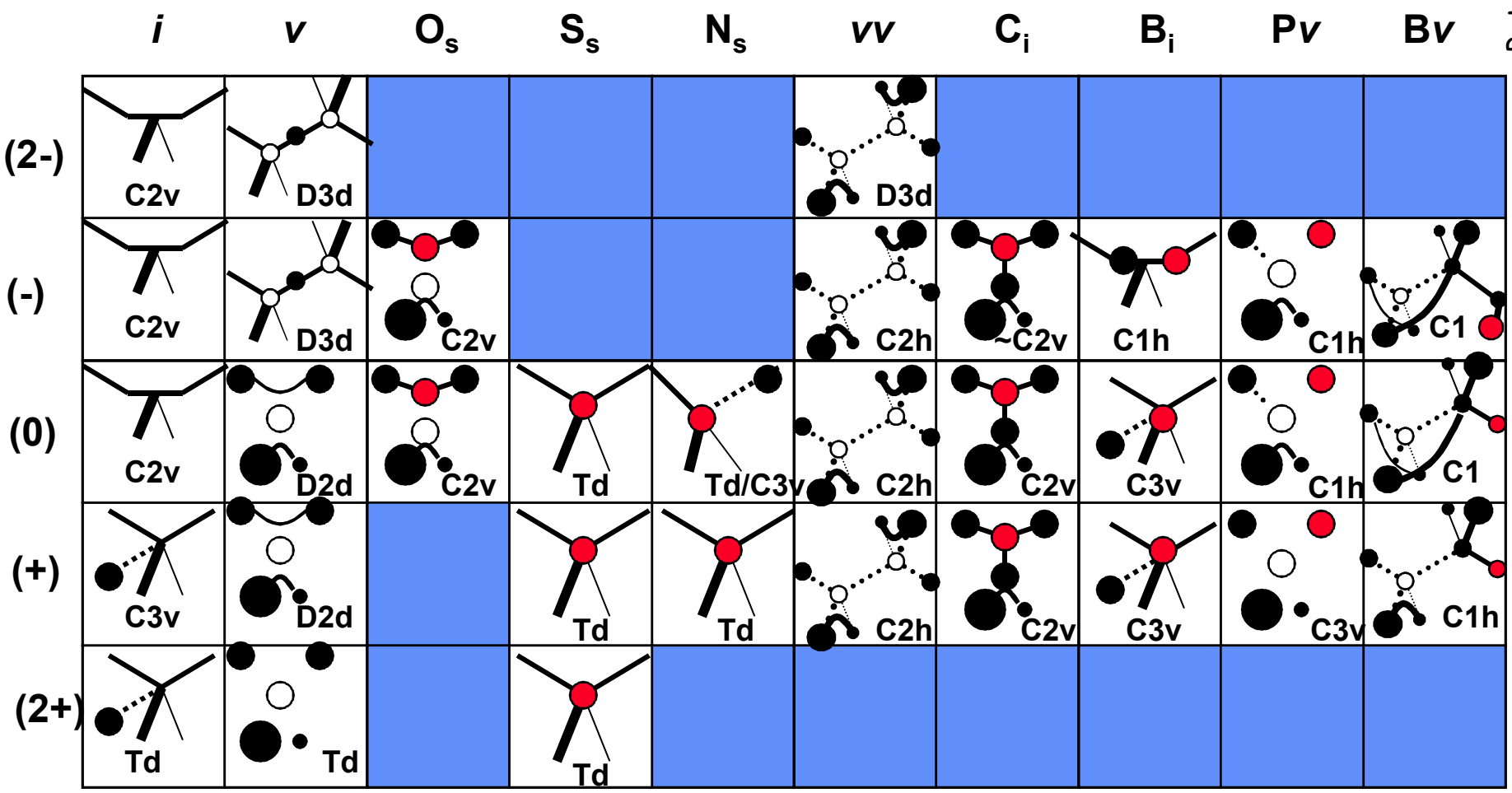

GGA: E(C2v) < E(D3d) for *v*(-)

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

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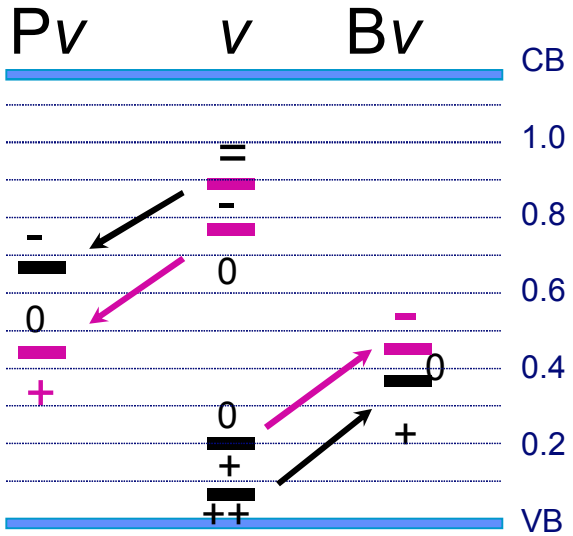
- Silicon level calculations - over 15 defects with levels

  i(=/-/0/+/++), *v(=/-/0/+/++)*, *vv(=/-/0/+)*, C_i(-/0/+), B_i(-/0/+), P*v*, B*v*
  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
P*v*(0/+) subsequently confirmed in experiment
[Larsen, et al PRL 97, 106402 (2006)]

VALIDATION is key to quantitative DISCOVERY - GaAs is ALL discovery

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GaAs EL2 and the As antisite

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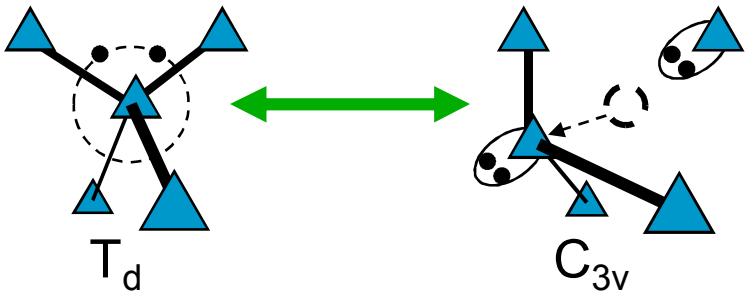
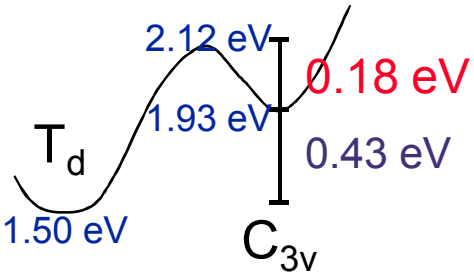
EL2 = antisite $As_{Ga}(0)$





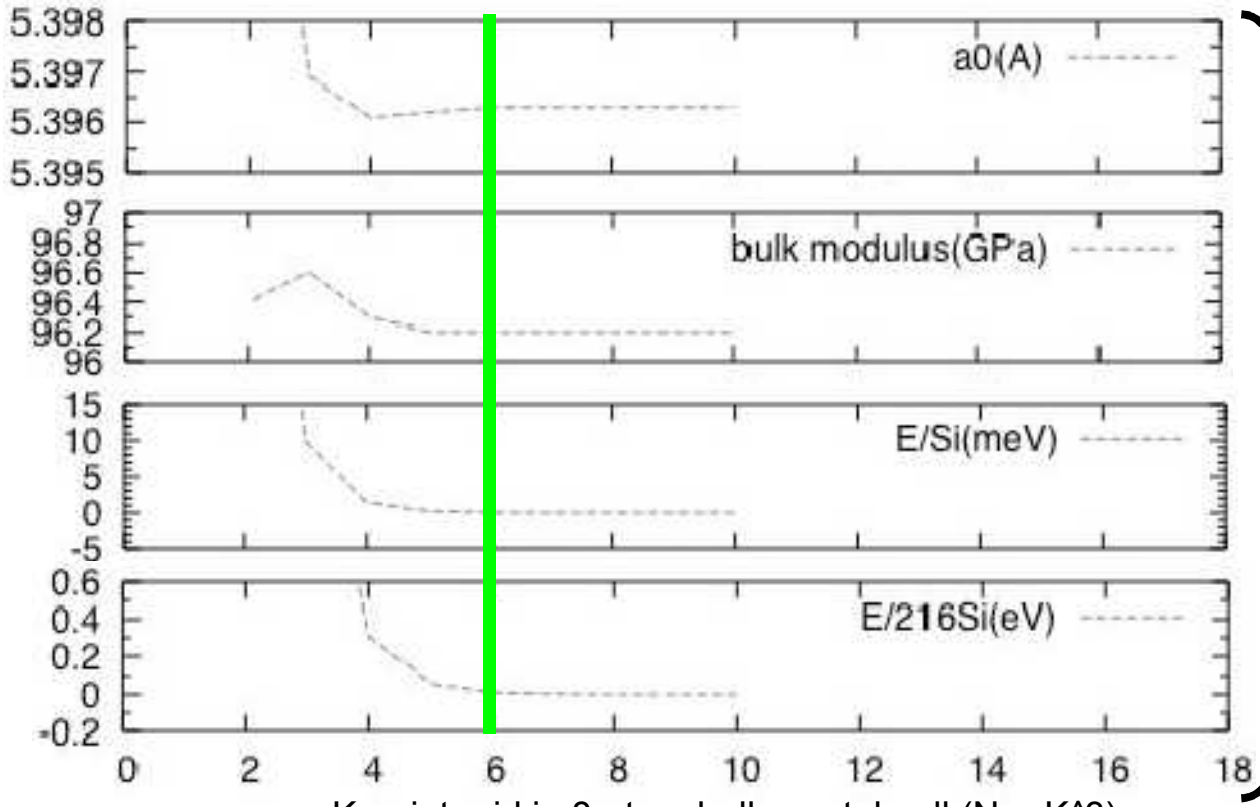
216-site =
512-site
(~ 64-site)

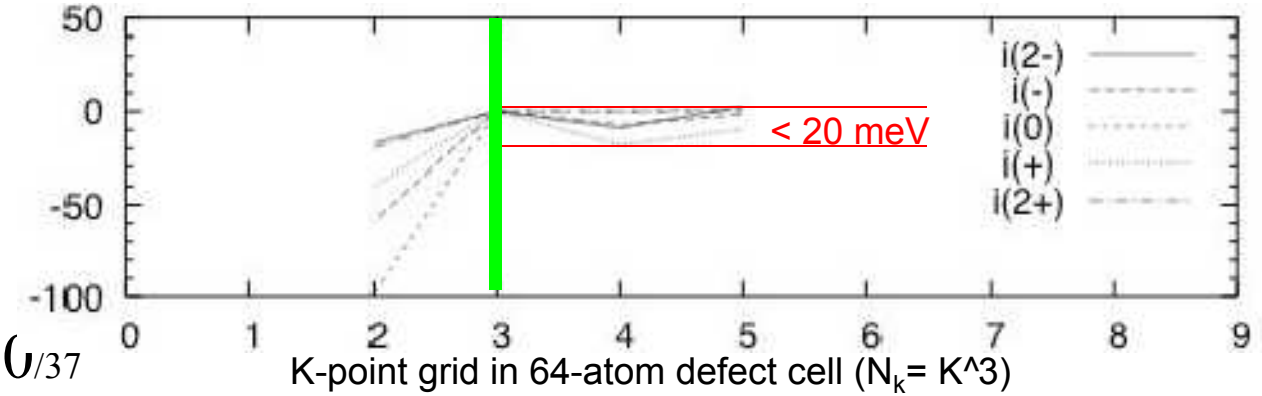
	Experiment -EL2	**SeqQuest/FDSM - As_{Ga}**
EL2(0/1+)	E_c -0.74 eV	E_c -0.81 eV
EL2(1+/2+)	E_v+0.54 eV	E_v +0.48 eV
Splitting:	0.24 eV (E_g=1.52)	0.25 eV
EL2*	no donor states	no donor states
Reorientation:	~0.3 eV	~0.2 eV

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

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

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.

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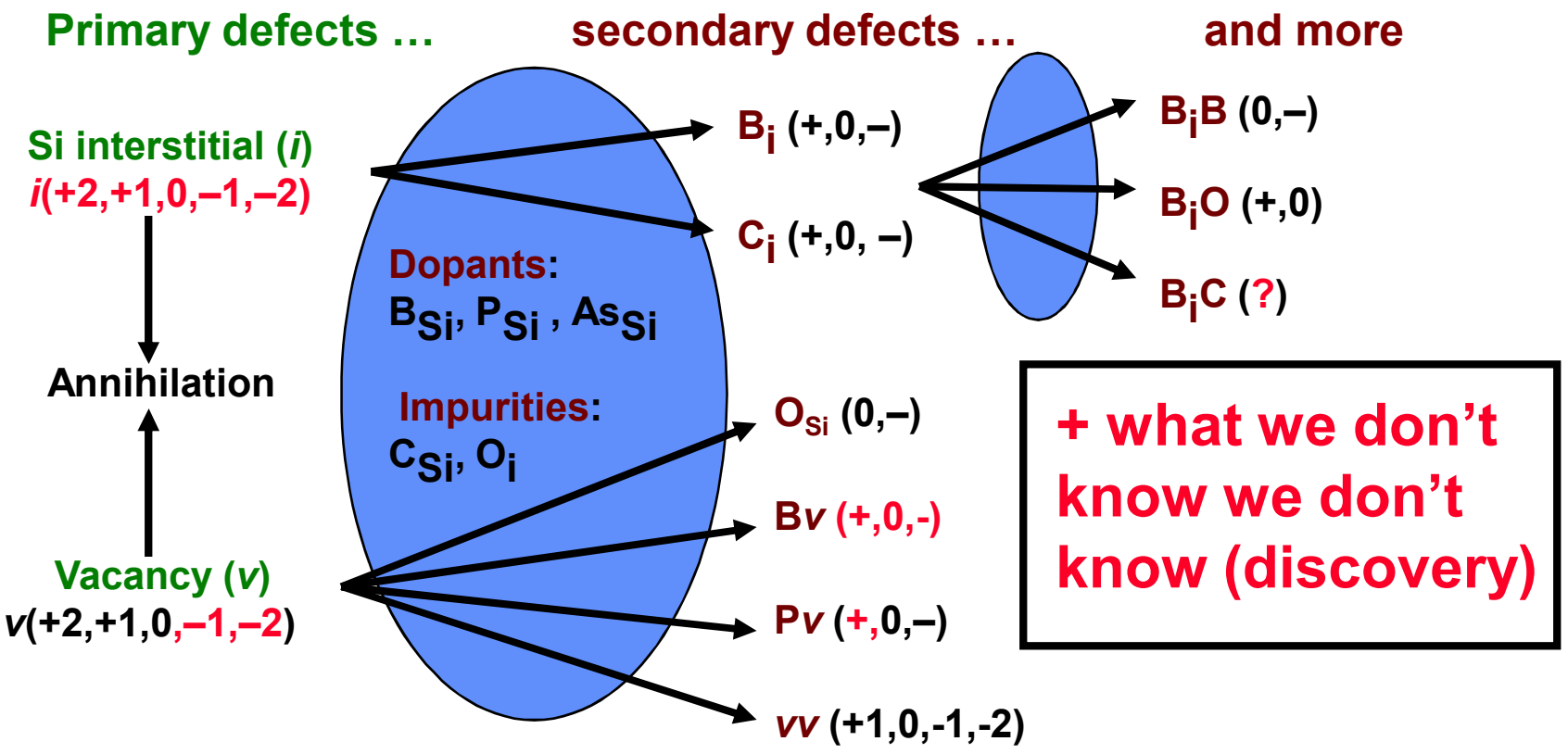
Radiation defects chemistry - Si



Need to know defects species, levels, chemical evolution …
DFT most accurate (sometimes only) probe of defect behavior
This chemistry map almost entirely blank in GaAs - unknown

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