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Sandia National Laboratories

The Defect Band Gap

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Is it possible to predict accurate defect levels with a "band gap problem"? …

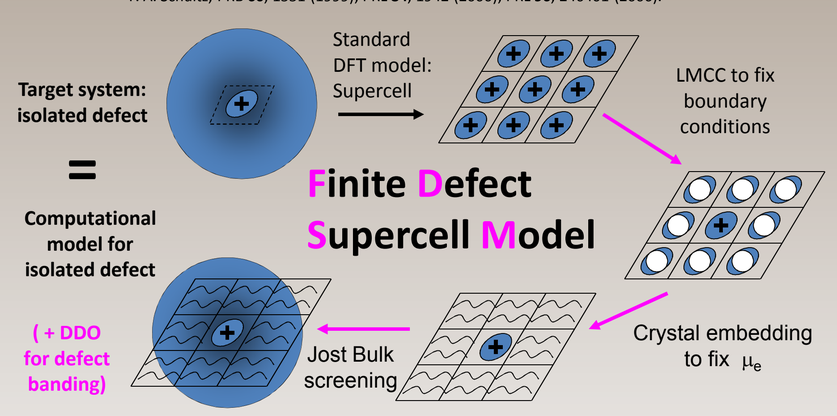
Methods:
SeqQuest DFT Code
LMCC Poisson Solver
FDSM total energy defect levels

LDA and PBE functionals
High-quality norm-conserving PP

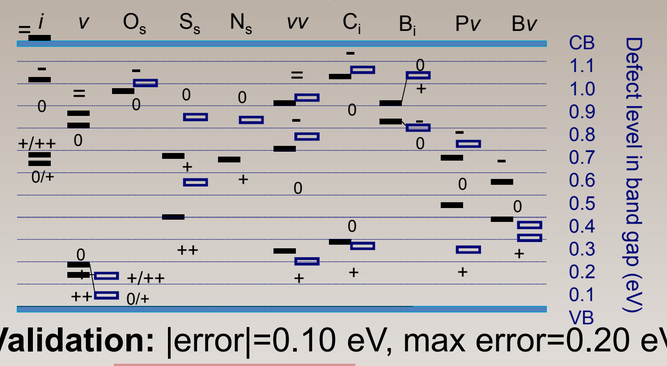
Fully optimized atomic positions
Converged k-sampling, supercells
Calibrated polarization model

Moreover …

P. A. Schultz, PRB **60**, 1551 (1999); PRL **84**, 1942 (2000); PRL **96**, 246401 (2006).



Si: DFT/PBE vs. Experimental Levels

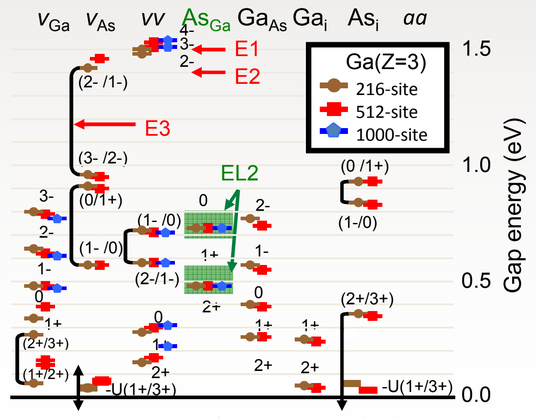


Validation: |error|=0.10 eV, max error=0.20 eV

… Yes!

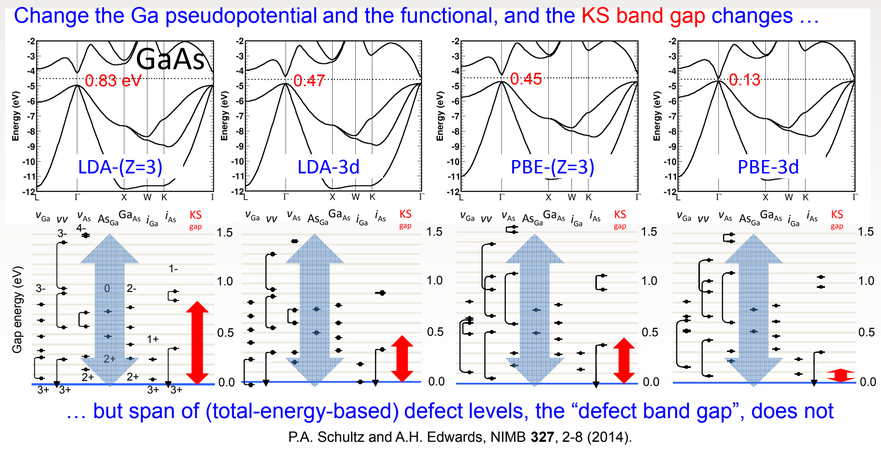
Verification: converged with supercell size
Predictive: reassign E1-E2, E3 defect centers

GaAs defect levels: LDA



P.A. Schultz and O.A. von Lilienfeld, MSMSE **17**, 084007 (2009).
P.A. Schultz, JPCM **27**, 075801 (2014).

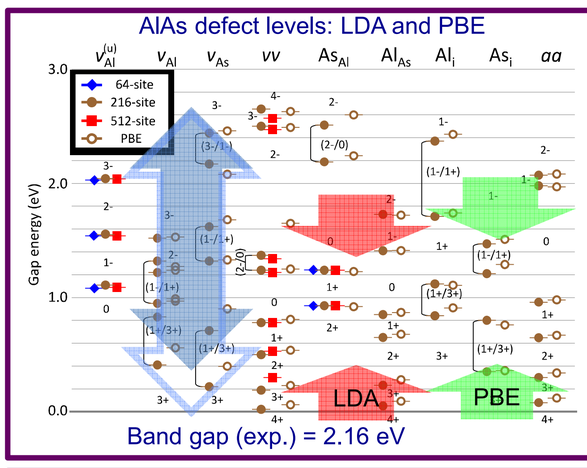
Computed defect levels insensitive to KS gap



… but span of (total-energy-based) defect levels, the "defect band gap", does not

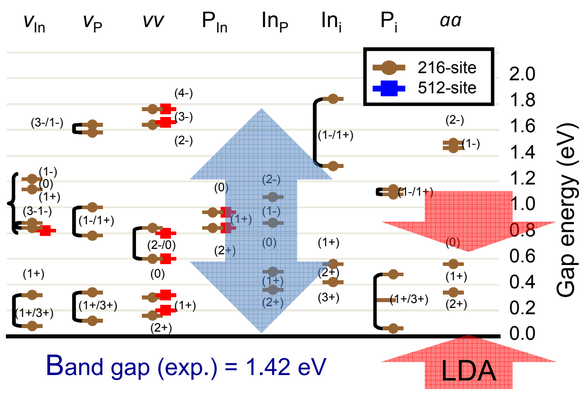
P.A. Schultz and A.H. Edwards, NIMB **327**, 2-8 (2014).

AlAs defect levels: LDA and PBE



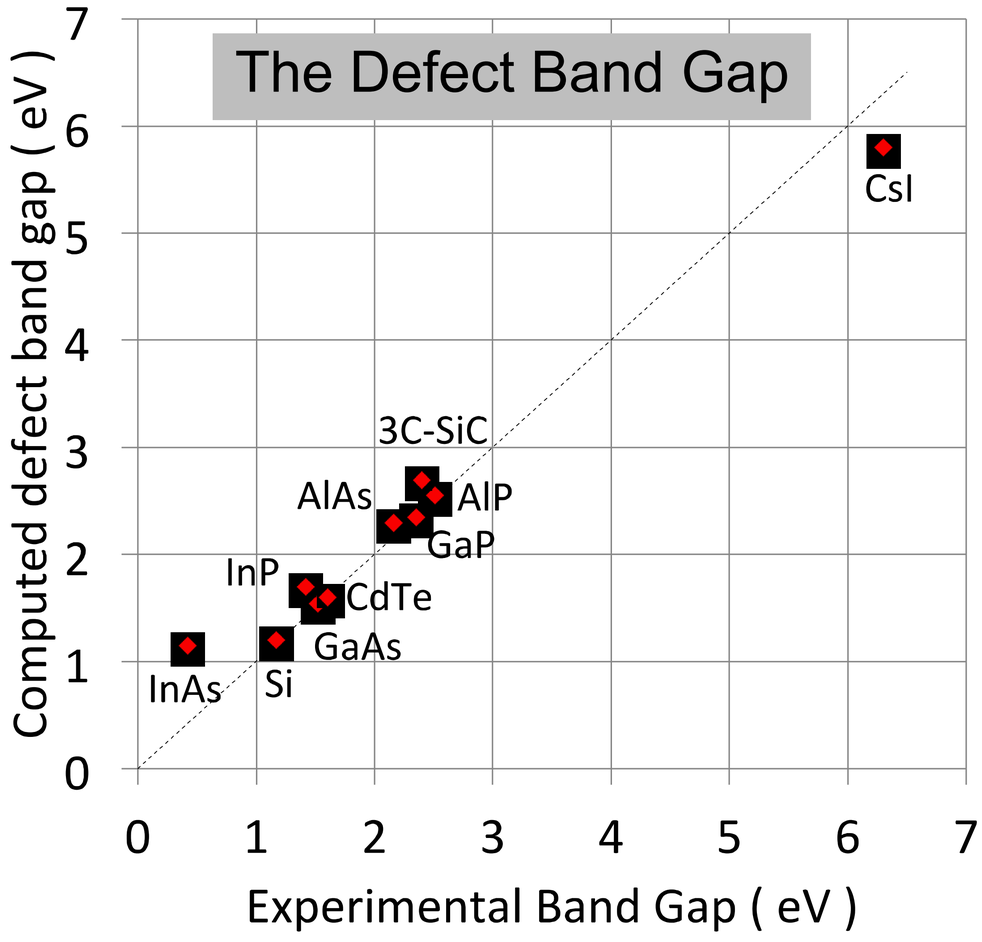
Band gap (exp.) = 2.16 eV

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

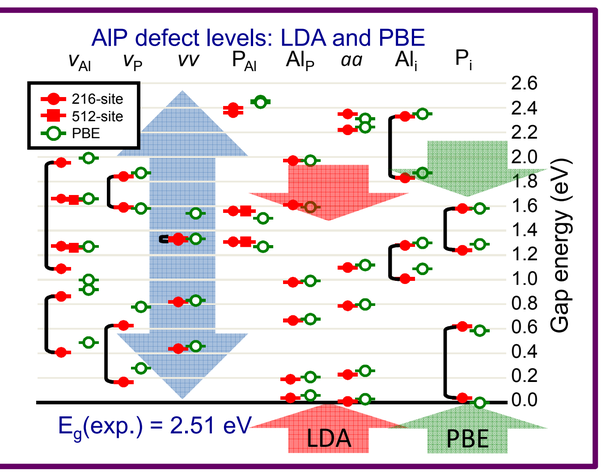


Band gap (exp.) = 1.42 eV

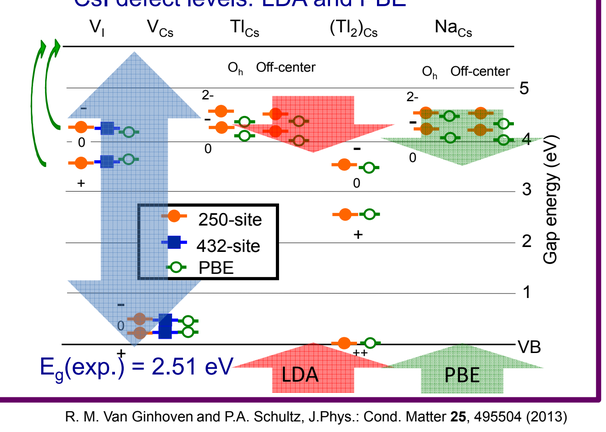
The Defect Band Gap



AlP defect levels: LDA and PBE



CsI defect levels: LDA and PBE



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

The span of computed defect levels is predictive of the band gap.
What defines the band gap problem?

U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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SeqQuest DFT code information: http://dft.sandia.gov/Quest

paschul@sandia.gov http://www.cs.sandia.gov/~paschul