SAND2010-6413P

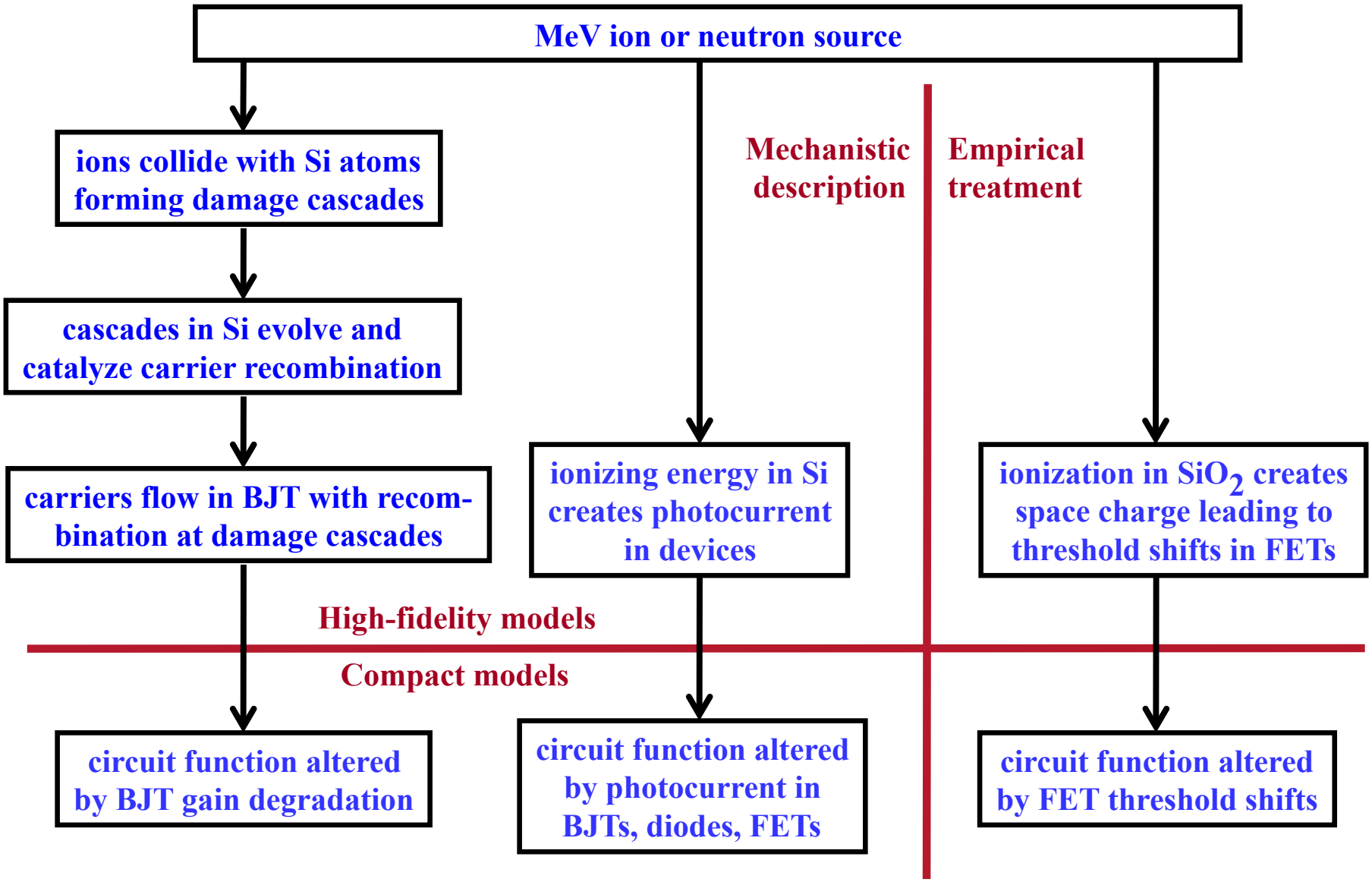
DFT Calculations Pursuant to Modeling Atomic Displacement Damage in Circuits

Wake Forest University
September 13, 2010

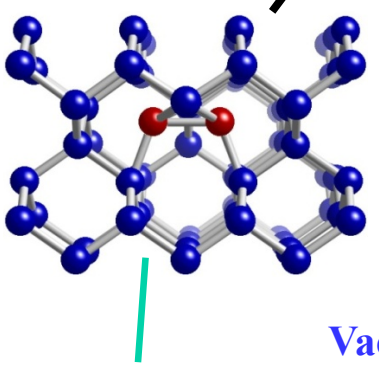
A. F. Wright and N. A. Modine
Sandia National Laboratories

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Relevant phenomena for Si devices



Defect and carrier reactions in atomistic model



Not observed experimentally

Primal species in recoil cascade

Si interstitial (Si_I) (+2,+1,0,–1,–2)

Annihilation

Annihilation

Vacancy (V) (+2,+1,0,–1,–2)

Divacancy (VV) (+1,0,–1,–2)

Carriers e^- & h^+

Reacted species

B_I (+,0,–)

C_I (+,0,-)

VP (+,0,–)

VO (0,–)

VB (+,0)

Secondary reacted species

B_IB (+,0)

B_IO (0,–)

Si_I displaces dopant/impurity

V binds to dopant/impurity

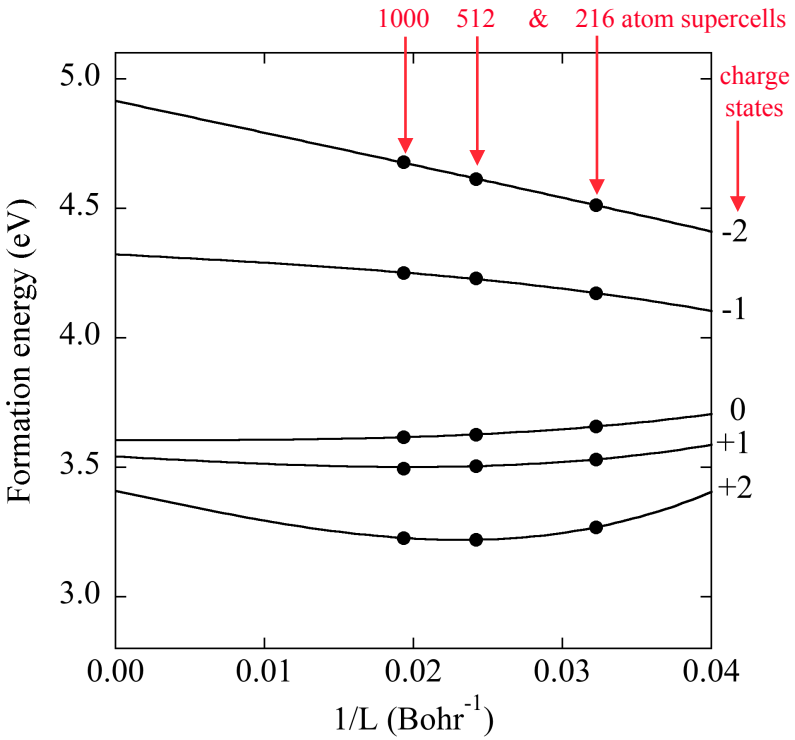
- Assessment of relevant defects and associated physical parameters based on literature.
- Knowledge gaps addressed using density-functional-theory (DFT).
- Final parameter refinement using model-development irradiation experiments.

DFT results for the Si vacancy

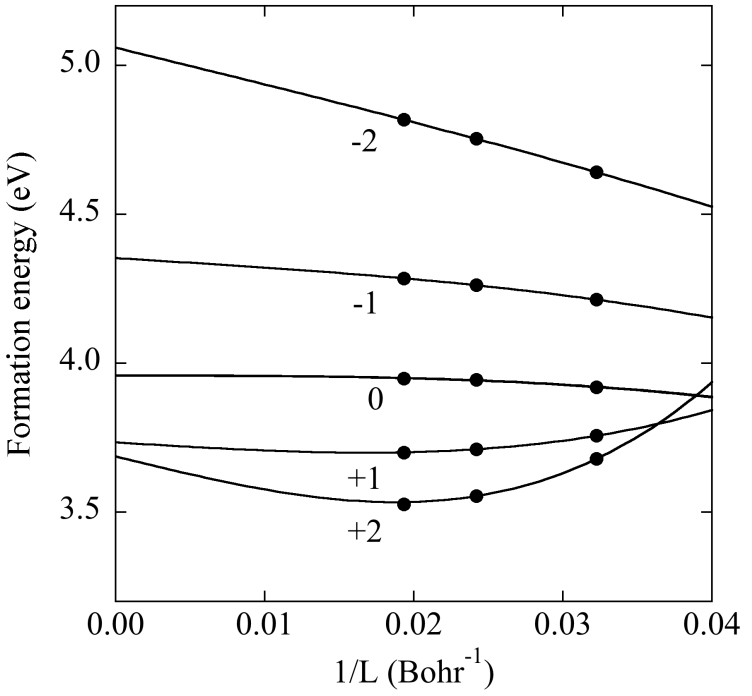
Supercell-size effects addressed by computing formation energies in 216-, 512-, and 1000-atom supercells and fitting to the Makov-Payne expression:

$$E^f\left[\mathrm{V}_{\mathrm{Si}}^q;L\right] = E^f\left[\mathrm{V}_{\mathrm{Si}}^q;L\to\infty\right] - \frac{2.8373q^2}{\varepsilon L} + \frac{A_3}{L^3}$$

Ground states



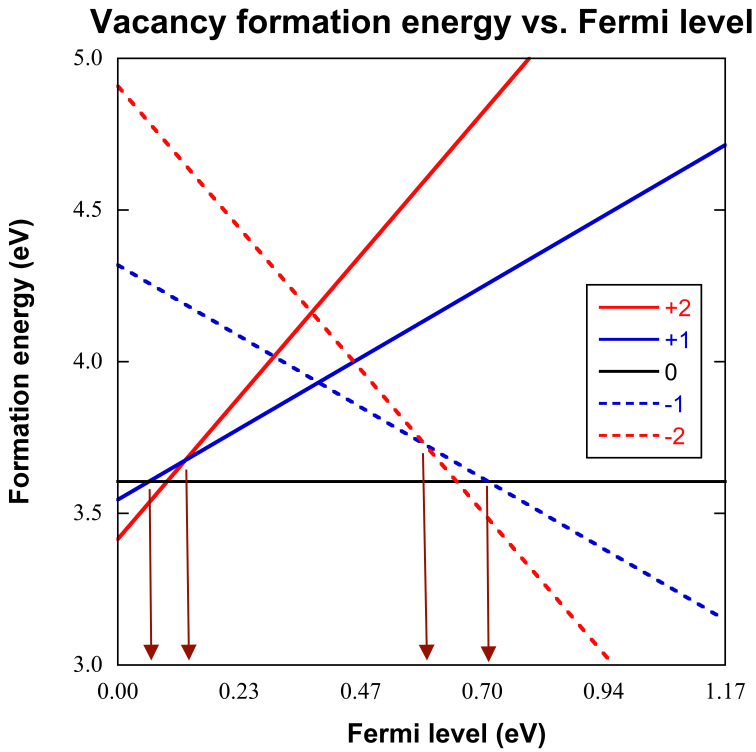
Saddle points



Extracting energy levels and diffusion activation energies

Energy levels are the crossing points in plots of the ground-state formation energies versus Fermi level for charge states differing by 1

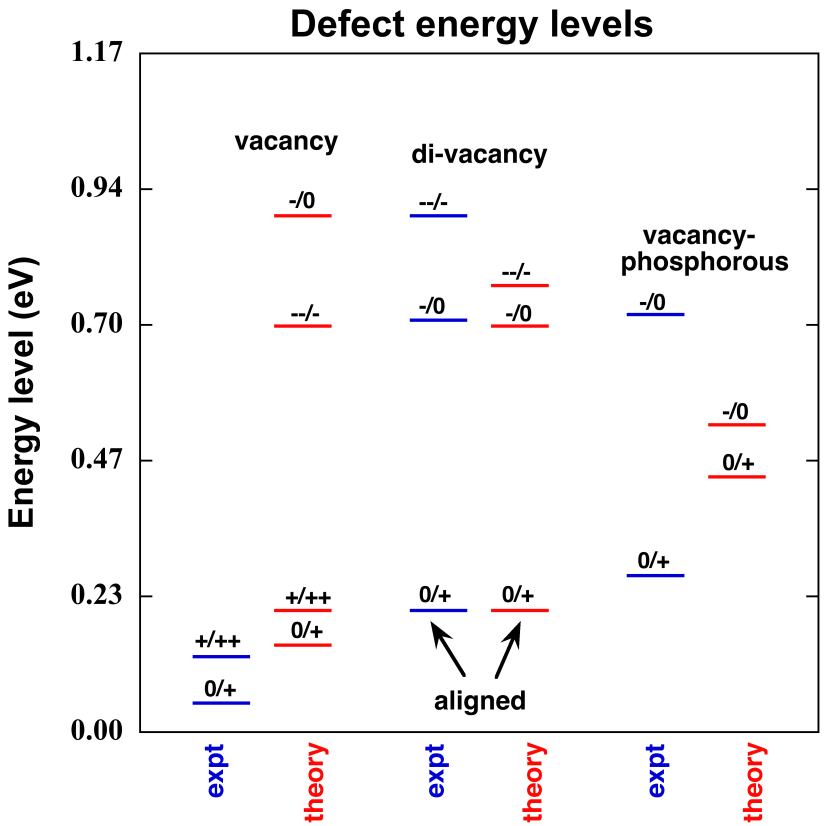
$$E^f\left[\mathrm{V}_{\mathrm{Si}}^q;\mathrm{E}_\mathrm{F}\right] = E^f\left[\mathrm{V}_{\mathrm{Si}}^q;L\to\infty\right] + q\mathrm{E}_\mathrm{F}$$

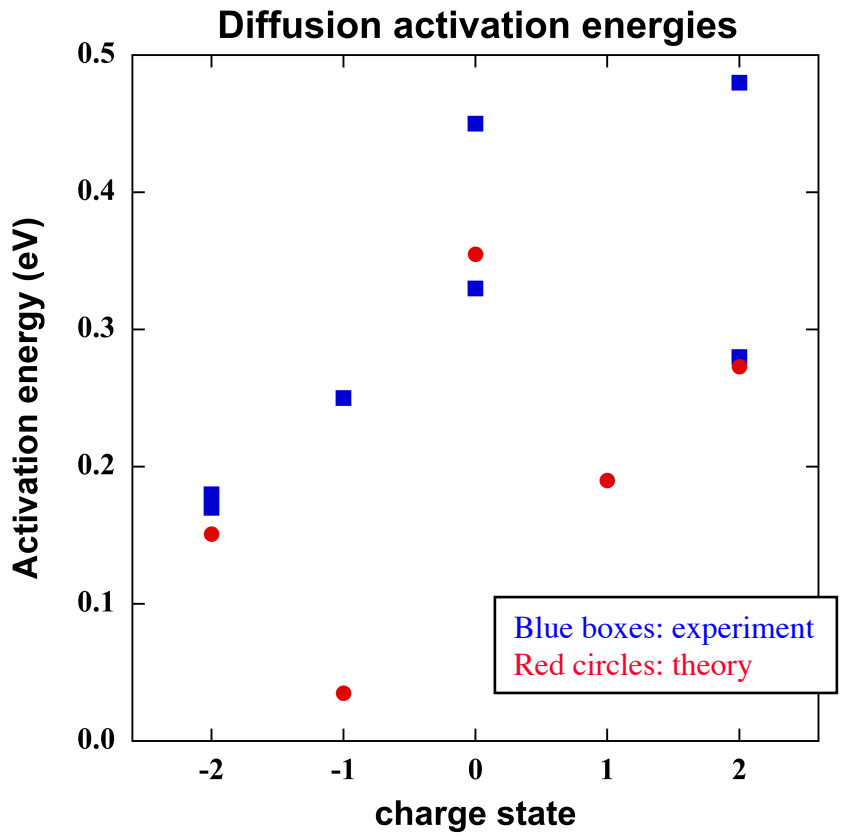


Diffusion activation energies are the differences in the extrapolated saddle-point (SP) and ground state (GS) formation energies

$$E^A\left[\mathrm{V}_{\mathrm{Si}}^q\right] = E^f\left[\mathrm{V}_{\mathrm{Si}}^q;\mathrm{SP};L\to\infty\right] - E^f\left[\mathrm{V}_{\mathrm{Si}}^q;\mathrm{GS};L\to\infty\right]$$

Comparison with experiments



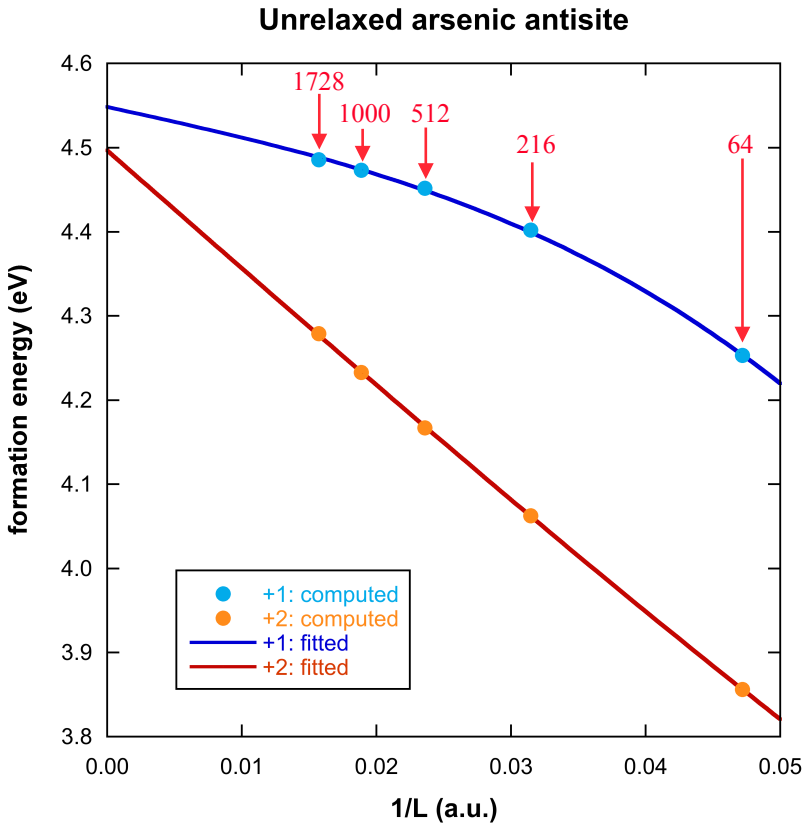


[Phys. Rev. B 74, 165116 (2006)] for vacancy results
[Phys. Rev. B 74, 205208 (2006)] for divacancy results
[J. Appl. Phys. 103, 083517 (2008)] for vacancy diffusion results

Atomic displacement damage in GaAs

- Current work is focusing on defects in GaAs
- The need for DFT results for GaAs is more urgent because less is known about defects in GaAs than defects in Si
- Also, DLTS is unlikely to shed light on the energy levels or populations of individual defects following MeV ion irradiation

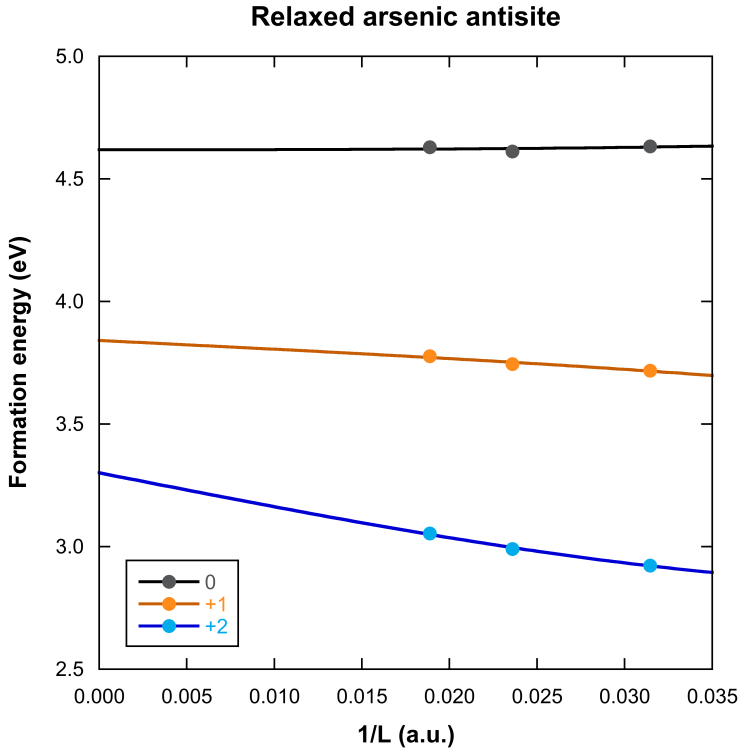
An aside: estimating a value for ε of GaAs

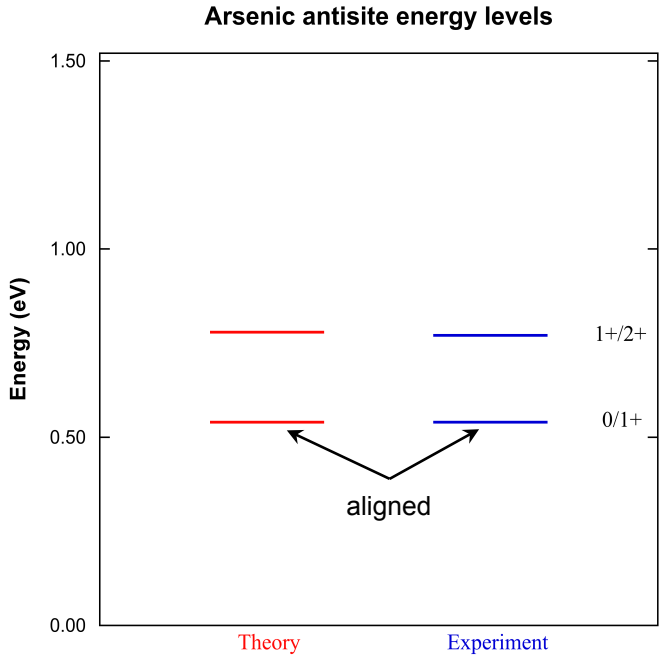


The fits were constrained to use the same value of ε yielding 11.0.

Published values are:
DFT: 10.9 – 14.4
Experiment: 10.6, 10.9

Results for the relaxed arsenic antisite

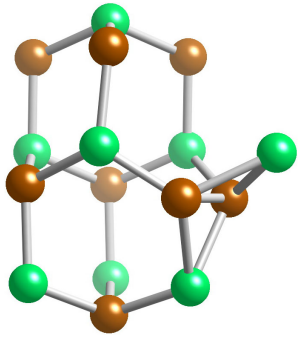




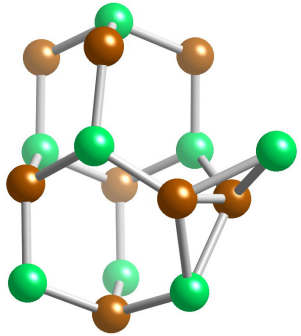
A shift was computed by aligning the computed 0/1+ level with the measured 0/1+ value. The computed 1+/2+ level then differs from the measured 1+/2+ level by 10 meV.

DFT results for the As interstitial in GaAs

[110] Split Interstitial : C_{2v} symmetry

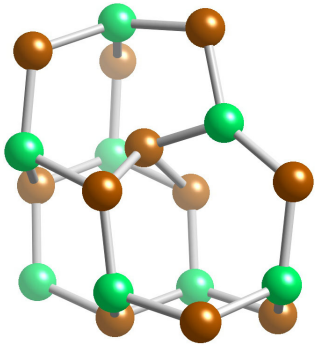


-1 charge state



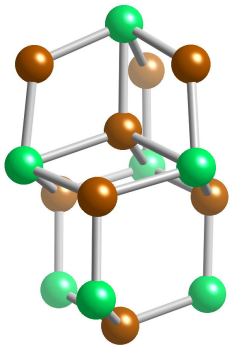
0 charge state

Bridging : C_{1h} symmetry

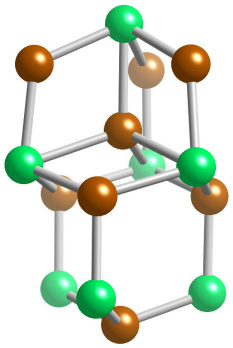


+1 charge state

Tetrahedral : T_d symmetry

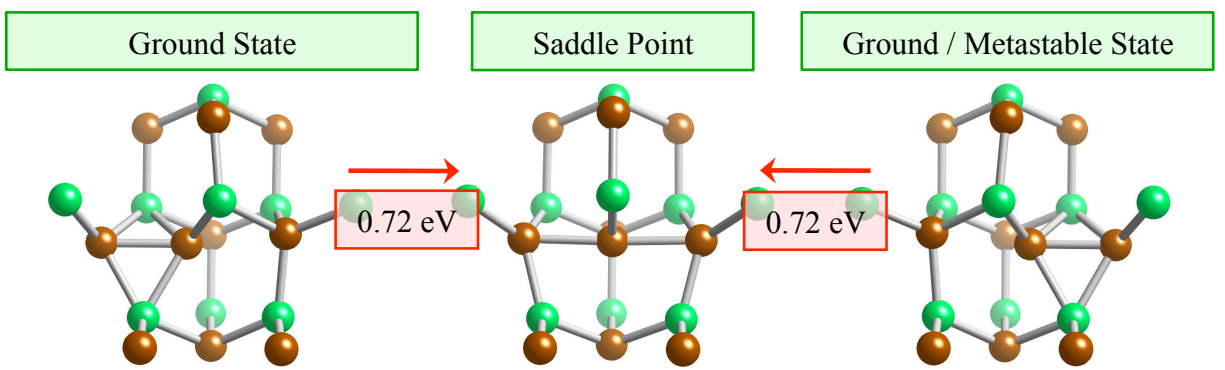


+2 charge state

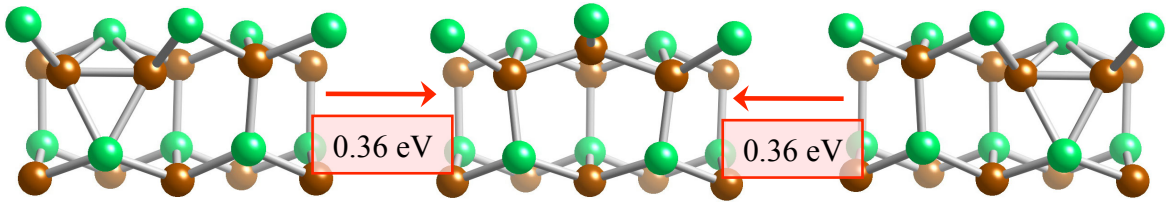


+3 charge state

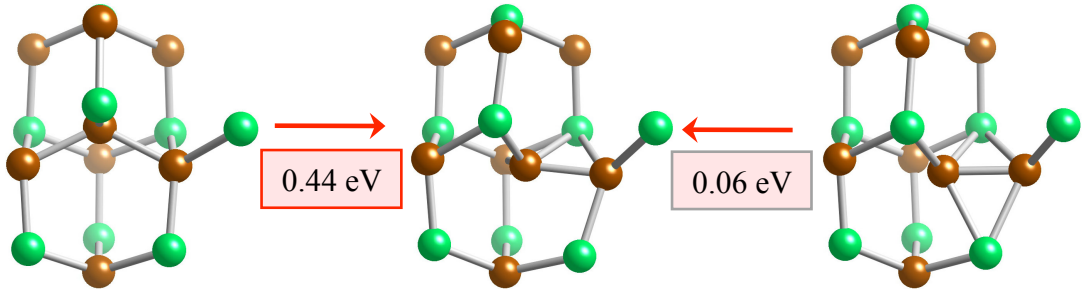
As_I thermal diffusion pathways



-1 charge state: barrier = 0.72 eV

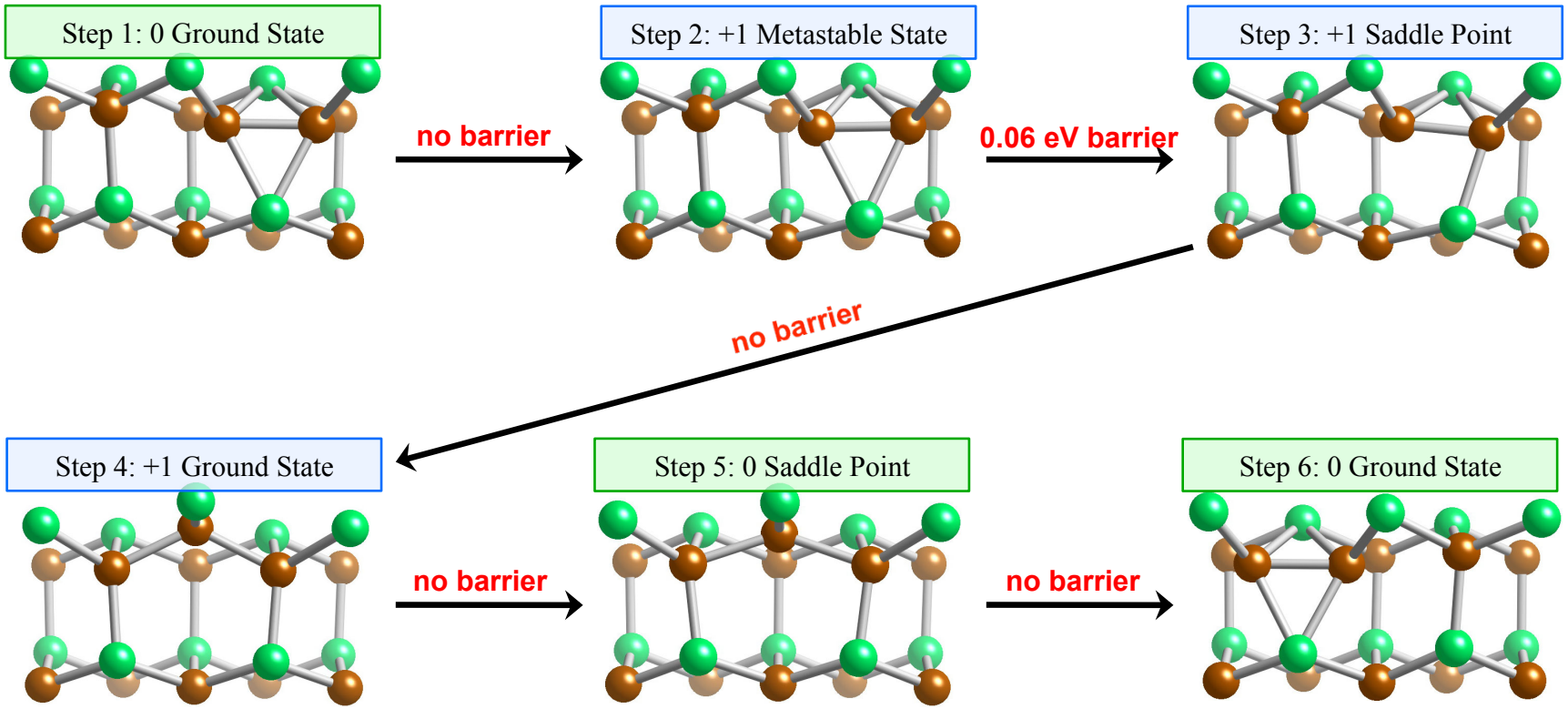


0 charge state: barrier = 0.36 eV



+1 charge state: barrier = 0.44 eV
(metastable state – on the right hand side – is traversed in the diffusion path)

Carrier assisted diffusion

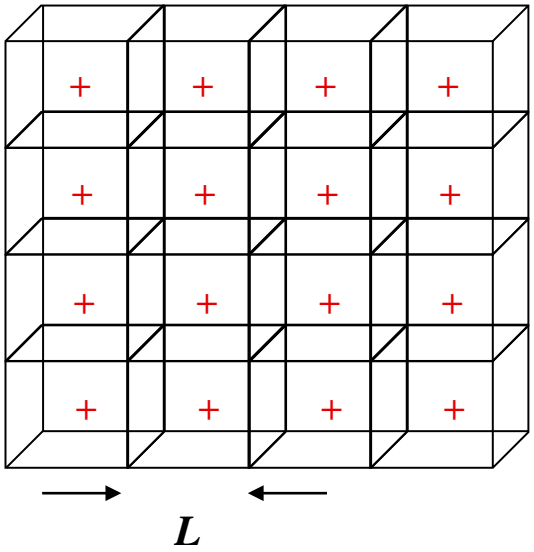


Summary

- Sandia is undertaking to develop a multiscale model of atomic displacement damage in Si and GaAs-based circuits
- DFT is being used to provide information about defect properties when these are not available from experiments
- Current state-of-the-art DFT energy levels appear to differ from measured values by 0.1 – 0.2 eV
- Additional activities:
  - The same protocals are being applied to the Ga vacancy in GaN
  - We are exploring the use of exact exchange via an optimized effective potential

Supplementary material: Treating charged defects in DFT calculations

A significant challenge is treating the long-ranged electrostatic potentials arising from charged defects when using supercells and periodic boundary conditions



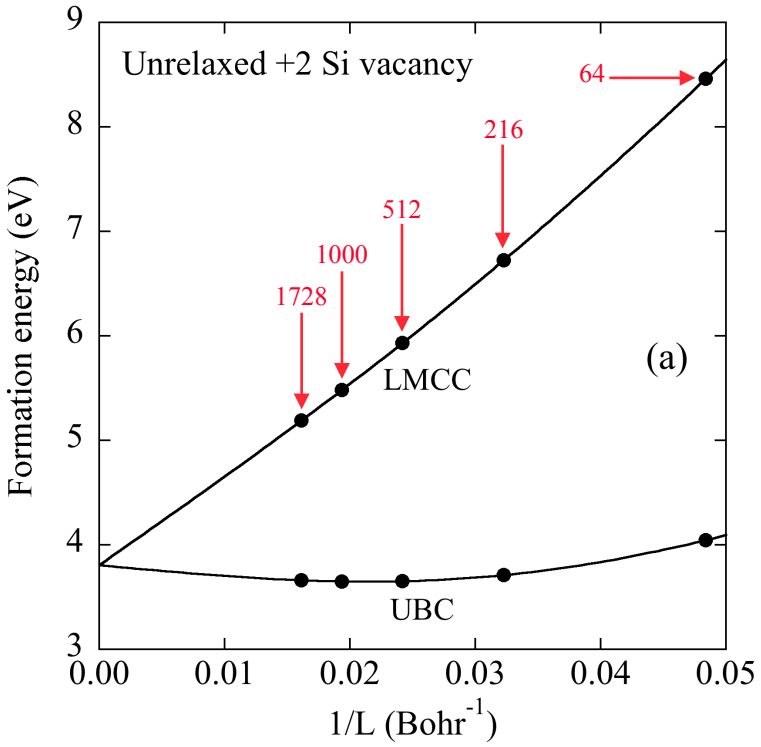
We have considered two methods for doing this:
1) uniform background charge (UBC) method
2) local-moment counter charge (LMCC) method

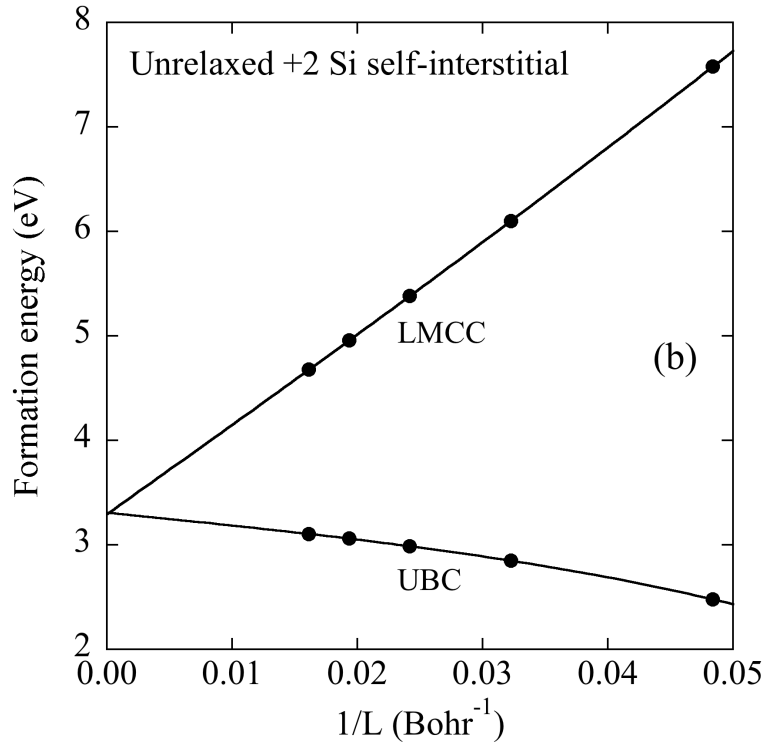
UBC Method: Introduce a uniform charge distribution to nullify the long-ranged electrostatic interactions

LMCC Method: Introduce a gaussian counter charge at the defect site that produces the correct electrostatic potential up to the cell boundary

Supplementary material: Comparison of the UBC and LMCC methods

- It can be shown analytically that both methods give the same formation energy as L goes to infinity [Phys. Rev. B 74, 235209 (2006)]
- This is illustrated below where results obtained in 64-, 216-, 512-, 1000-, and 1728-atom supercells are fit to the expression $E^{f}(L) = E^{f}(L \to \infty) + \frac{A_1}{L} + \frac{A_3}{L^3} + \frac{A_5}{L^5}$





Supplementary material: Are analytic corrections viable?

- In the UBC method, a simple expression is available for the linear

$$E_1 = -\frac{2.8373 q^2}{\varepsilon L}$$

dependence where *q* is the charge and ε is the dielectric constant

- In the LMCC method, an approximate expression for the polarization

$$E_p = -\left(1 - \frac{1}{\varepsilon}\right)\frac{q^2}{\left(R_{Jost} - \beta\right)} \; ; \; R_{Jost} = L \Big/ \left[\frac{4\pi}{3}\right]^{\frac{1}{3}}$$

energy of the surrounding bulk material can be added to the formation where β is an empirical parameter usually taken to be 0.8 a.u.

- Our tests indicate that these corrections are not adequate for our purposes