2011 NCN Summer School

Ab initio and Molecular Dynamics and simulations of materials

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PURDUE UNIVERSITY

Multiscale Materials Modeling

Electrons → Atoms → Meso → Elements → Certification

Time

lifetime

second

microsec

nanosec.

picosec.

femtosec.

Goal: predictive, validated models can help design and certify new materials

Components

Mesoscale

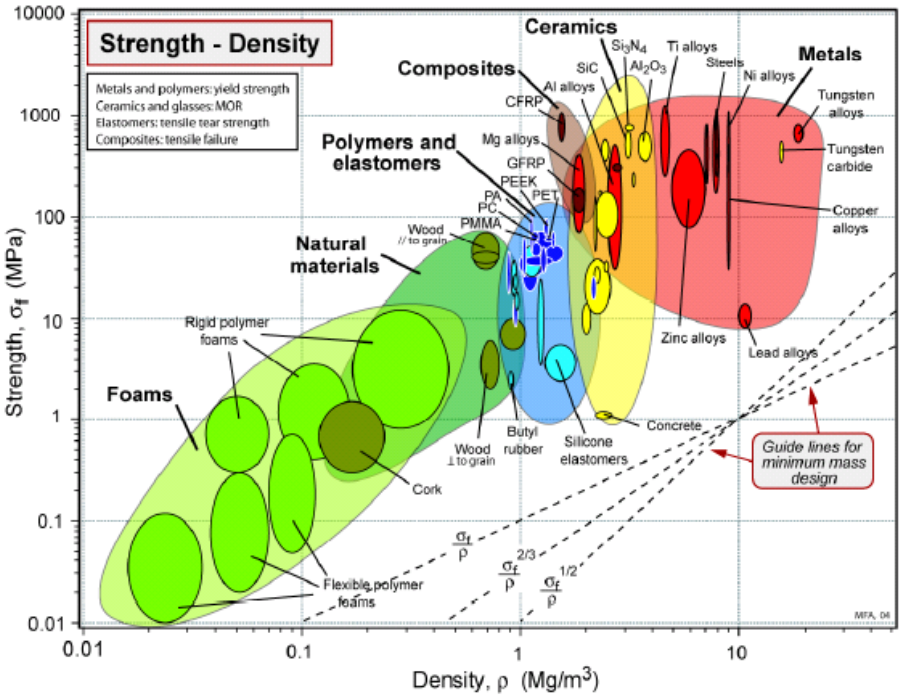
Molecular dynamics

Quantum Mechanics

Length

nanometer micron mm meters

Why multiscale materials modeling?



Materials Selection in Mechanical Design (3rd edition)
by MF Ashby, Butterworth Heinemann, 2005

- Difference in bonding alone can not explain the enormous range in observed values for materials properties
- Atomic structure and microstructure (defects, interfaces, etc.) play a key role

Ab initio and MD simulations

$$H\psi = E\psi$$

Wavefunction of electrons for a give set of atomic positions

- Optical and electronic properties
- Atomic interactions
- Chemical reactions

- H: Hamiltonian operator
- Ψ: Wavefunction of electrons (in the field created by the ions)
- E: Total energy (atoms are not moving)

Eigenvalue problem: you get WF and energy

$$F_i = m_i a_i$$

Motion of atoms

- Thermo-mechanical properties
- Mass and heat transport
- Chemistry

- F: Total force on atom i (surrounding atoms and external fields)
- m_i: Mass of atom i
- a_i: Acceleration of atom i

Initial condition problem: you get atomic positions, velocities and forces

Ab initio and MD simulations

Electrons coordinates

$$H\left(\{\rho_i\};\{r_i\}\right)\psi\left(\{\rho_i\}\right)= E\left(\{r_i\}\right)\psi\left(\{\rho_i\}\right)$$

Ionic positions

Energy (eigenvalue) is a function of ionic positions

If I have energy as a function of atomic positions I can calculate force and perform MD:

$$\vec{F}_i = -\vec{\nabla}_{r_i} E\left(\{r_j\}\right)$$

$$\vec{F}_i = m_i \vec{a}_i$$

- This is called ab initio MD simulations (forces come from first principles)
- Accurate but computationally very intensive

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Part I: ab initio simulations of materials

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Quantum mechanics 101: electronic structure

1. The state of electrons is determined by their wave function

$$\Psi(\rho, t)$$

2. Physical observables ↔ linear operators

Position ↔ Multiply by ρ

Momentum ↔ $\hat{p} = \frac{\hbar}{i}\vec{\nabla}$

Linear:

$$O(a\Psi) = aO\Psi$$

$$O(\Psi_1 + \Psi_2) = O\Psi_1 + O\Psi_2$$

Quantum mechanics 101: electronic structure

3. Average results of measurements is given by

$$\langle O \rangle = \int \Psi^*(\rho) O \Psi(\rho) d^3\rho = \langle \Psi | O | \Psi \rangle$$

Example:

$$\langle \rho \rangle = \int \Psi^*(\rho) \rho \Psi(\rho) d^3\rho = \int \rho |\Psi(\rho)|^2 d^3\rho$$

$|\Psi(\rho)|^2$ Probability density of electron being in volume $d^3\rho$ around ρ

Quantum mechanics 101: electronic structure

4. Time evolution of ψ is given by Schrödinger equation:

$$i\hbar\frac{d}{dt}\Psi(\rho,t) = H\Psi(\rho,t)$$

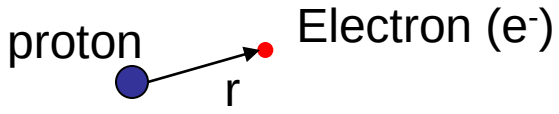
If Hamiltonian does depend on time: time-independent Schrödinger equation

$$H\psi(\rho) = E\psi(\rho)$$

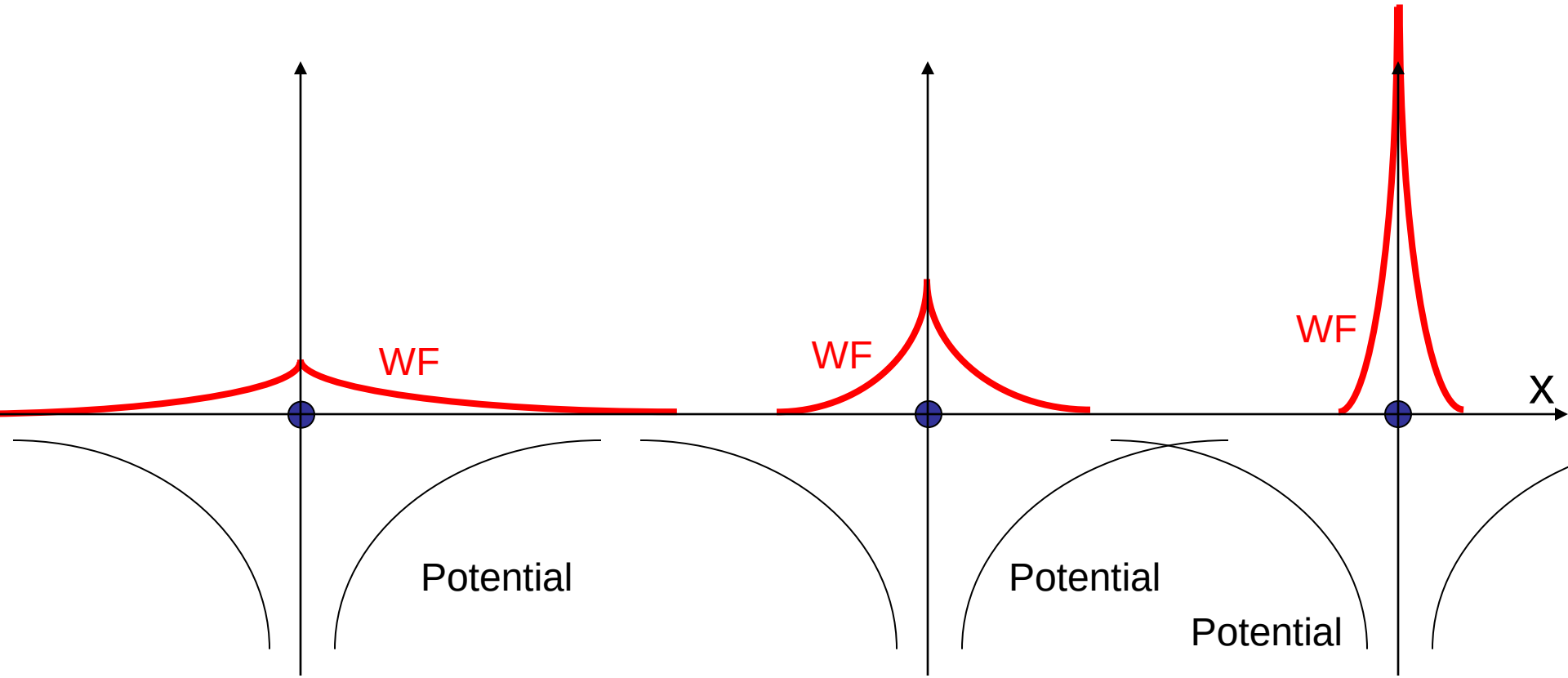
5. Pauli's exclusion principle

- Two electrons maximum per orbital
- Electrons in one orbital must have different spin

The hydrogen atom



$$\langle H \rangle = \int \Psi(\rho) \left[-\frac{h\nabla^2}{2m} \right] \Psi(\rho) d^3\rho - \int \Psi(\rho) \left[\frac{e^2}{\rho} \right] \Psi(\rho) d^3\rho$$



Ab initio simulations

$$H\psi = E\psi$$

Hamiltonian operator of a group of electrons and ions is:

$$H = K_{elec} + K_{ions} + V_{ei} + V_{ii} + V_{ee}$$

Born-Oppenheimer approximation: take massive ions as stationary and solve for the electrons

$$H_{BO}\left(\rho_1, \rho_2, ..., \rho_n; \{r_i\}\right) = -\sum_{i=1}^{n} \frac{\hbar^2 \left|\vec{\nabla}_{\rho_i}\right|^2}{2m_e} - \sum_{i,j}^{n,N} \frac{Z_i e^2}{\left|\rho_i - r_j\right|} + \sum_{i<j}^{n} \frac{e^2}{\left|\rho_i - \rho_j\right|}$$

The challenge:

Solve: $H_{BO}\psi = E\psi$

$$H_{BO}\left(\rho_1, \rho_2, ..., \rho_n; \{r_i\}\right) = -\sum_{i=1}^{n} \frac{\left|\vec{\nabla}_{\rho_i}\right|^2}{2m_e} - \sum_{i,j}^{n,N} \frac{Z_i e^2}{\left|\rho_i - r_j\right|} + \sum_{i<j}^{n} \frac{e^2}{\left|\rho_i - \rho_j\right|}$$

Wavefunction lives in 3n-dimensional space

$$\psi\left(\{\rho_i\}\right)$$

Silicon unit cell: 28-dimensional space!

GaAs unit cell: 64-dimensional space!

The challenge:

Let's say you have a TeraFLOP machine on your desk

10^6 floating point operations per second

- Integral in 3D space (assume you discretize space in 10 bins)
- 10^3 operations
- Your integral comes back in 10^{-3} s=1 ms

- Integral in 28-D space (Si unit cell)
- 10^{28} operations
- Your integral comes back in 10^{22} s (age of the earth is ~1.4^{19} s)

Need an approximate solution

Solve: $H_{BO}\psi = E\psi$

$$H_{BO}\left(\rho_1, \rho_2, ..., \rho_n; \{r_i\}\right) = -\sum_{i=1}^{n} \frac{\left|\vec{\nabla}_{\rho_i}\right|^2}{2m_e} - \sum_{i,j}^{n,N} \frac{Z_i e^2}{\left|\rho_i - r_j\right|} + \sum_{i<j}^{n} \frac{e^2}{\left|\rho_i - \rho_j\right|}$$

Mean field approximation:

$$\psi\left(\{\rho_i\}\right) = \phi_1(\rho_1)\phi_2(\rho_2)...\phi_n(\rho_n)$$

Wavefunction is a product of single-electron wave functions (no correlations)

Need an approximate solution

Plug: $$\psi\left(\{\rho_i\}\right) = \phi_1(\rho_1)\phi_2(\rho_2)\ldots\phi_n(\rho_n)$$

Into Schrodinger equation:

$$\left(-\sum_{i=1}^{n}\frac{\left|\vec{\nabla}_{\rho_i}\right|^2}{2m_e} - \sum_{i,j}^{n,N}\frac{Z_i e^2}{\left|\rho_i - r_j\right|} + \sum_{i<j}^{n}\frac{e^2}{\left|\rho_i - \rho_j\right|}\right)\psi\left(\{\rho_i\}\right) = E\psi\left(\{\rho_i\}\right)$$

Leads to the Hartree equation (Hartree, 1927):

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \sum_{i}^{N}\frac{Z_i e^2}{\left|r_i - \rho\right|} + \sum_{i\neq j}^{n} e^2\int\frac{\left|\phi_i(\rho')\right|^2}{\left|\rho - \rho'\right|}d^3\rho'\right]\phi_j(\rho) = E'\phi_j(\rho)$$

Hartree

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \sum_i^N \frac{Z_i e^2}{|r_i-\rho|} + \sum_{i\neq j}^n e^2 \int \frac{|\phi_i(\rho')|^2}{|\rho-\rho'|} d^3\rho'\right]\phi_j(\rho) = E'\phi_j(\rho)$$

Now I need to find n 3-dimensional functions (instead of 1 3n dimensional one) – Much better!

But… No free lunch

- The Hamiltonian depends on the orbitals I want to find
- Self-consistent field calculation
- Iterative solution

Total energy is the expectation value of the Hamiltonian:

$$\langle H\rangle = \sum_{i=1}^n \int d^3\rho \phi_1^*(\rho)\left[-\frac{\left|\vec{\nabla}\right|^2}{2m_e} - \sum_j^N \frac{Z_i e^2}{|\rho - r_j|}\right]\phi_i(\rho) + \sum_{i<j}^n \int d^3\rho_i d^3\rho_j \frac{e^2|\phi_i(\rho_i)|^2|\phi_j(\rho_j)|^2}{|\rho_i-\rho_j|}$$

The problems with the Hartree theory

$$\psi\left(\{\rho_i\}\right) = \phi(\rho_1)\phi(\rho_2)\ldots\phi(\rho_n)$$

- No correlations
- Electrons are distinguishable (swapping two electrons changes the function)

Symmetry of WF's:

$$\psi(\rho_1,\rho_2,\ldots,\rho_i,\ldots,\rho_j,\ldots,\rho_n) = c\psi(\rho_1,\rho_2,\ldots,\rho_j,\ldots,\rho_i,\ldots,\rho_n)$$

$$c = \begin{cases} 1 & \text{Bosons} \\ -1 & \text{Fermions} \end{cases}$$

The problems with the Hartree theory

$$\psi(\rho_1,\rho_2,\ldots,\rho_i,\ldots,\rho_j,\ldots,\rho_n)=-\psi(\rho_1,\rho_2,\ldots,\rho_j,\ldots,\rho_i,\ldots,\rho_n)$$

$$\psi(\rho_1,\rho_2)=\phi_1(\rho_1)\phi_2(\rho_2)$$ Not possible

$$\psi(\rho_1,\rho_2)=\frac{1}{\sqrt{2}}\left(\phi_1(\rho_1)\phi_2(\rho_2)-\phi_2(\rho_1)\phi_1(\rho_2)\right)$$ OK

General solution: Slater determinants

$$\Psi(\rho_1,\ldots,\rho_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\rho_1) & \phi_2(\rho_1) & \ldots & \phi_N(\rho_1)\\ \phi_1(\rho_2) & \phi_2(\rho_2) & \ldots & \phi_N(\rho_2)\\ \text{M} & \text{M} & & \\ \phi_1(\rho_N) & \phi_2(\rho_N) & \ldots & \phi_N(\rho_N)\end{vmatrix}$$

Hartree-Fock

Plug: $$\Psi(\rho_1,\ldots,\rho_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\rho_1) & \phi_2(\rho_1) & \ldots & \phi_N(\rho_1)\\ \phi_1(\rho_2) & \phi_2(\rho_2) & \ldots & \phi_N(\rho_2)\\ \text{M} & \text{M} & & \\ \phi_1(\rho_N) & \phi_2(\rho_N) & \ldots & \phi_N(\rho_N)\end{vmatrix}$$

Into Schrodinger equation:

$$\left(\sum_{i=1}^{n}-\frac{\left|\vec{\nabla}_{\rho_i}\right|^2}{2m_e}-\sum_{i,j}^{n,N}\frac{Z_i e^2}{\left|\rho_i-r_j\right|}+\sum_{i<j}^{n}\frac{e^2}{\left|\rho_i-\rho_j\right|}\right)\psi\left(\{\rho_i\}\right)=E\psi\left(\{\rho_i\}\right)$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2-\sum_{i}^{N}\frac{Z_i e^2}{\left|r_i-\rho\right|}\right]\phi_j(\rho)+\sum_{i}^{n}e^2\int\frac{\left|\phi_i(\rho')\right|^2\phi_j(\rho)}{\left|\rho-\rho'\right|}d^3\rho'-\sum_{i}^{N}e^2\int\frac{\phi_i^*(\rho')\phi_j(\rho')\phi_i(\rho)}{\left|\rho-\rho'\right|}d^3\rho'=E_j\phi_j(\rho)$$

Hartree-Fock vs. Hartree

Hartree

Kinetic energy

Electron-electron interactions

$$\langle H \rangle = \sum_{i=1}^{n} \int d^3\rho \phi_1^*(\rho) \left[\frac{\vec{\nabla}}{2m_e} - \sum_j^N \frac{Z_i e^2}{|\rho - r_j|} \right] \phi_i(\rho) + \sum_{i<j}^{n} \int d^3\rho_i d^3\rho_j \frac{e^2 |\phi_i(\rho_i)|^2 |\phi_j(\rho_j)|^2}{|\rho_i - \rho_j|}$$

Electron ion-interactions

Hartree-Fock

$$\langle H \rangle = \sum_{i=1}^{n} \int d^3 r \phi_1^*(\rho) \left[\frac{\vec{\nabla}}{2m_e} - \sum_j^N \frac{Z_i e^2}{|\rho - r_j|} \right] \phi_i(\rho) + \sum_{i<j}^{n} \int d^3\rho d^3\rho' \frac{e^2 |\phi_i(\rho)|^2 |\phi_j(\rho')|^2}{|\rho - \rho'|}$$

$$- \sum_{i<j}^{n} \int d^3\rho d^3\rho' \frac{e^2 \phi_i^*(\rho) \phi_j^*(\rho') \phi_i(\rho') \phi_j(\rho)}{|\rho - \rho'|}$$

Exchange energy (no classical counterpart)

Hartree-Fock predictions

Predicted geometries vs. experiments

Table 3.18 SCF equilibrium bond lengths (a.u.) of H_2

Basis set	Bond length
STO-3G	1.346
4-31G	1.380
6-31G**	1.385
Experiment	1.401

Table 3.19 SCF equilibrium bond lengths (a.u.) of N_2 and CO

Basis set	N_2	CO
STO-3G	2.143	2.166
4-31G	2.050	2.132
6-31G*	2.039	2.105
Near-HF-limit	2.013[a]	2.081[b]
Experiment	2.074	2.132

[a] P. E. Cade, K. D. Sales, and A. C. Wahl, *J. Chem. Phys.* **44:** 1973 (1966).
[b] W. M. Huo, *J. Chem. Phys.* **43:** 624 (1965).

Table 3.20 SCF equilibrium bond lengths (a.u.) of the ten-electron series

Basis set	CH_4	NH_3	H_2O	FH
STO-3G	2.047	1.952	1.871	1.807
4-31G	2.043	1.873	1.797	1.742
6-31G*	2.048	1.897	1.791	1.722
6-31G**	2.048	1.897	1.782	1.703
Near-HF-limit	2.048[a]	1.890[b]	1.776[c]	1.696[d]
Experiment	2.050	1.912	1.809	1.733

[a] W. Meyer, *J. Chem. Phys.* **58:** 1017 (1973).
[b] A. Rauk, L. C. Allen, and E. Clementi, *J. Chem. Phys.* **52:** 4133 (1970).
[c] B. J. Rosenberg, W. C. Ermler, and I. Shavitt, *J. Chem. Phys.* **65:** 4072 (1976).
[d] P. E. Cade and W. J. Huo, *J. Chem. Phys.* **47:** 614 (1967).

Modern Quantum Chemistry
Szabo and Ostlund

Density functional theory

Hohenberg and Kohn (1964)

- Ground state (GS) wave function $\Psi_0(r_1, r_2 \ldots r_n)$ is a functional of GS electronic density $n_0(r)$

  - Electronic density: $n(r) = \int d^3 r_2, d^3 r_3, \ldots, d^3 r_n \left| \psi(r, r_2, \ldots, r_n) \right|^2$

  - Ground state energy is also a functional of density:

$$E_0 = \left\langle \Psi_0[n_0] \middle| H \middle| \Psi_0[n_0] \right\rangle = E[n_0]$$

- Variational property: the electron density that minimizes the energy functional is the ground state density

$$E[n_0] \leq E[n]$$

Density functional theory

$$E[n] = T_s[n] + U_H[n] + V_{ext}[n] + E_{xc}[n]$$

Exchange and correlation functional

Kohn-Sham equations (1965):

Exchange and correlation potential

And the solution is: $$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{ext}(r) + v_H(r) + v_{xc}(r) \right] \phi_i = \varepsilon_i \phi_i$$

With: $$n(r) = \sum \left| \phi_i(r) \right|^2$$

Exchange and correlation functional

- Local density approximation (LDA)

  Exchange: can be calculated exactly for a non-interacting homogeneous electron gas:

$$E_x^{Hom}(n) = -\frac{3q^2}{4}\left(\frac{3}{\pi}\right)^{1/3} n^{4/3} \qquad E_x^{LDA}[n(r)] = -\frac{3q^2}{4}\left(\frac{3}{\pi}\right)^{1/3} \int d^3r\, n(r)^{4/3}$$

  Correlation: no analytical solution. Alder and Ceperley (1980) performed Quantum Monte Carlo simulations

  Various fits: Perdew-Zunger (PZ), Perdew-Wang (PW)

- Generalized Gradient Approximation (GGA)

$$E_{xc}^{GGA}[n(r)] = \int d^3r\, e_{xc}^{GGA}(n(r), \nabla n(r))$$

PBE: Perdew, Burke, Ernzerhof (1996)
BLYP: Becke's exchange + Lee, Yang and Parr (1988)
B3LYP: mix 30% of exact exchange (HF) (hyper-GGA)

Numerical issues in DFT calculations

- Basis sets $\phi_i(r) = \sum_j c_{ij} \chi_j(r)$

Two main options:

- **Plane waves**: expand orbitals in plane waves up to a cutoff frequency (given as the corresponding kinetic energy)
  - The kinetic energy cutoff should be increased until convergence is achieved

- **Local basis sets**: functions centered on atoms (LCAO)
  - Usually smaller number of basis functions needed
  - Common choice: double-zeta + polarization
    - Each occupied valence state is described by two functions and one function for the first unoccupied angular orbital

Numerical issues in DFT calculations

- Pseudo-potentials
  - Most physical phenomena depend on valence electrons more strongly than on core electrons
  - Replace core electrons with “pseudopotential” that leads to wave function identical to original one for large *r*

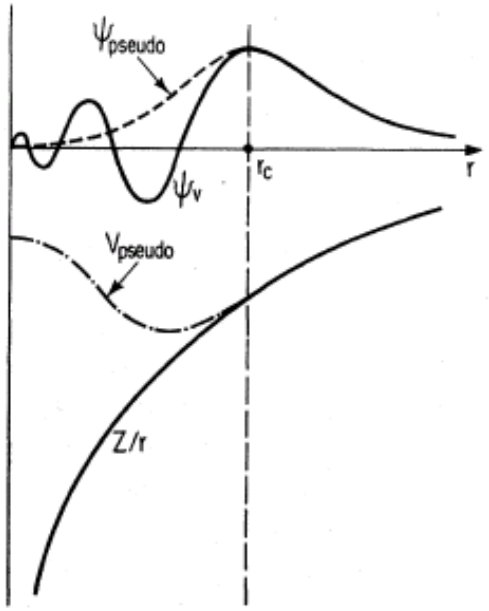


FIG. 5. Schematic illustration of all-electron (solid lines) and pseudoelectron (dashed lines) potentials and their corresponding wave functions. The radius at which all-electron and pseudoelectron values match is designated r_c.

Payne et al.

Reviews of Modern Physics, Vol. 64, No. 4, October 1992

Reciprocal space

$$P = \left(\frac{1}{V_{BZ}}\right)\int_{BZ} dk \sum_{n} p_n(k)\, f\left[\varepsilon_n(k)\right]$$

$$f\left(\varepsilon_n(k)\right) = \theta\left(\varepsilon_F - \varepsilon_n(k)\right)$$

$$f\left(\varepsilon_n(k)\right) = \frac{1}{1+\exp\left\{\left[\varepsilon_F - \varepsilon_n(k)\right]/kT\right\}}$$

Replace integral over 1st BZ by a sum over k-points

- Special, high-symmetry points are used (HJ MONKHORST, JD PACK, Phys Rev. B 1976 vol. 13 (12) pp. 5188-5192)

- Few k-points OK for insulators and semiconductors

- Metals are more challenging since there are states available infinitesimally near the Fermi energy.

Reciprocal space sampling

INSTITUTE OF PHYSICS PUBLISHING MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING

Modelling Simul. Mater. Sci. Eng. **13** (2005) R1–R31 doi:10.1088/0965-0393/13/1/R01

TOPICAL REVIEW

Designing meaningful density functional theory calculations in materials science—a primer

Ann E Mattsson[1], Peter A Schultz[1], Michael P Desjarlais[2], Thomas R Mattsson[2] and Kevin Leung[3]

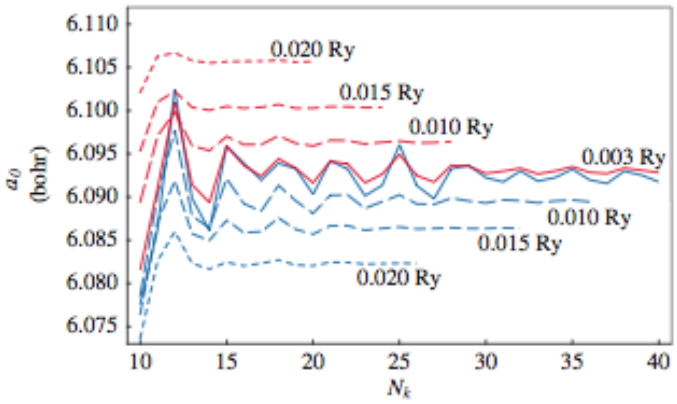


Figure 5. The computed equilibrium lattice constant, a_0, of Ta as a function of Fermi filling temperature and $\boldsymbol{k}$ point sample. The a_0 computed as the point of zero stress is in red, and a_0 at the minimum of the potential energy curve is in blue. Both these methods converge better versus the $\boldsymbol{k}$ sample with higher Fermi occupation temperatures. However, for both methods the lattice constant drifts as the occupation temperature increases, and the drift is in opposite directions.

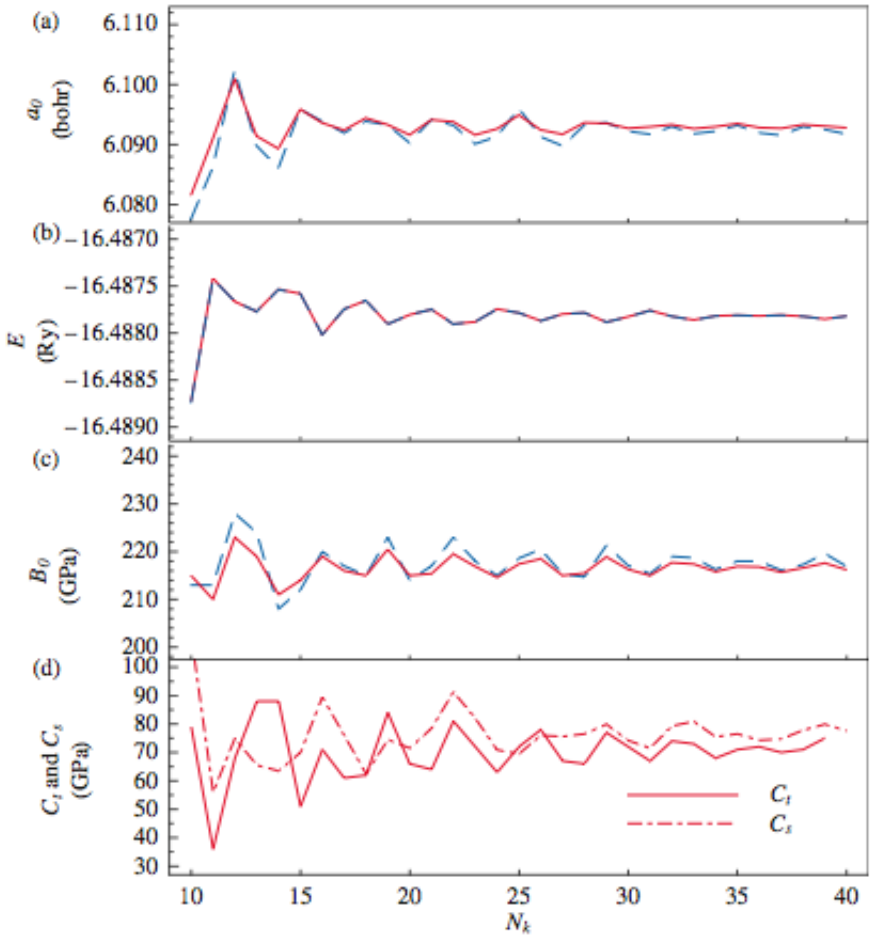
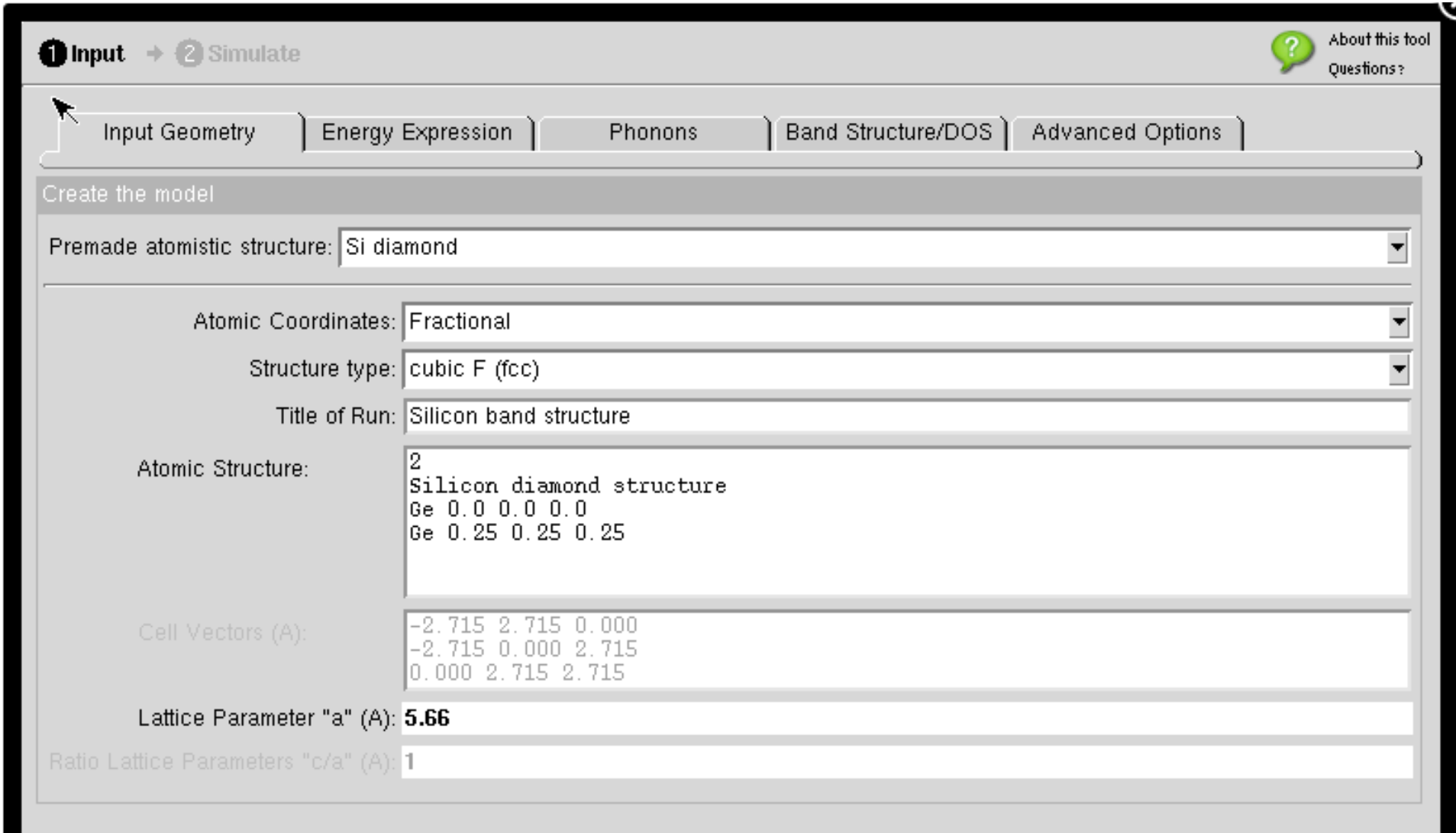


Figure 4. The convergence of computed equilibrium quantities for bcc Ta as a function of the $\boldsymbol{k}$ sample: (*a*) lattice constant; (*b*) total energy; (*c*) bulk modulus; (*d*) shear moduli. The values extracted using the computed stress tensor are given as solid red lines, and the values obtained using fits to the potential energy surface are dashed blue (the shear moduli in (*d*) were both obtained from the stress calculation). While the total energy, lattice parameter and bulk modulus appear to converge, if slowly, the computed shear moduli (*d*) are much more sensitive to the $\boldsymbol{k}$ sample, and are still varying over a range of 5 GPa at a $\boldsymbol{k}$ grid of 40^3.

Demos and examples

Simple calculations using Quantum Espresso Tool in nanoHUB



Exchange and correlation functional

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Kohn-Sham equations (1965):

Exchange and correlation potential

And the solution is: $$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{ext}(r) + v_H(r) + v_{xc}(r) \right] \phi_i = \varepsilon_i \phi_i$$

With: $$n(r) = \sum \left| \phi_i(r) \right|^2$$

The "DFT bandstructure" problem

The Kohn-Sham eigenvalues do not represent the band structure of the material

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{ext}(r) + v_H(r) + v_{xc}(r)\right]\phi_i = \varepsilon_i\phi_i$$

As in our examples, the K-S bandgap is significantly smaller than the material's bandgap

The "DFT bandstructure" problem: solution

Perform charge-state calculations where electrons are added or removed for perfect and defective samples.

PRL **96,** 246401 (2006) PHYSICAL REVIEW LETTERS week ending 23 JUNE 2006

Theory of Defect Levels and the "Band Gap Problem" in Silicon

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(Received 10 November 2005; published 19 June 2006)

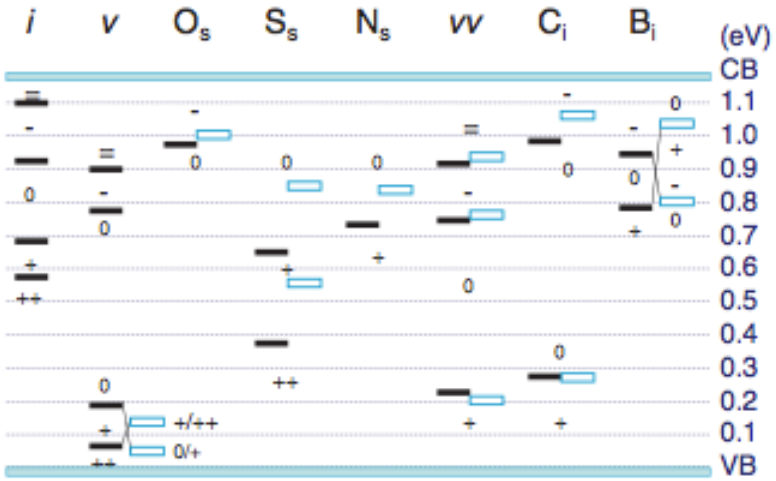
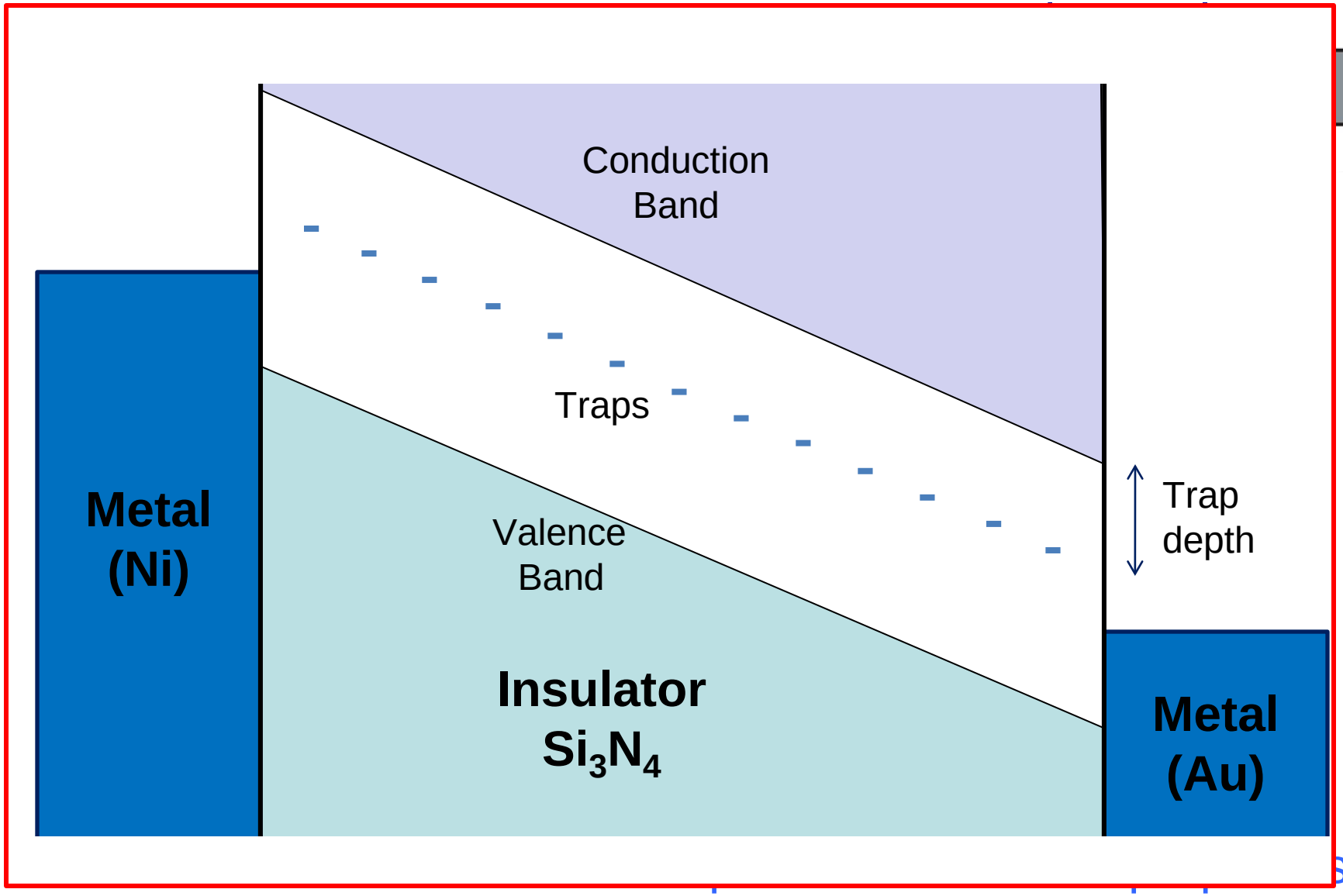


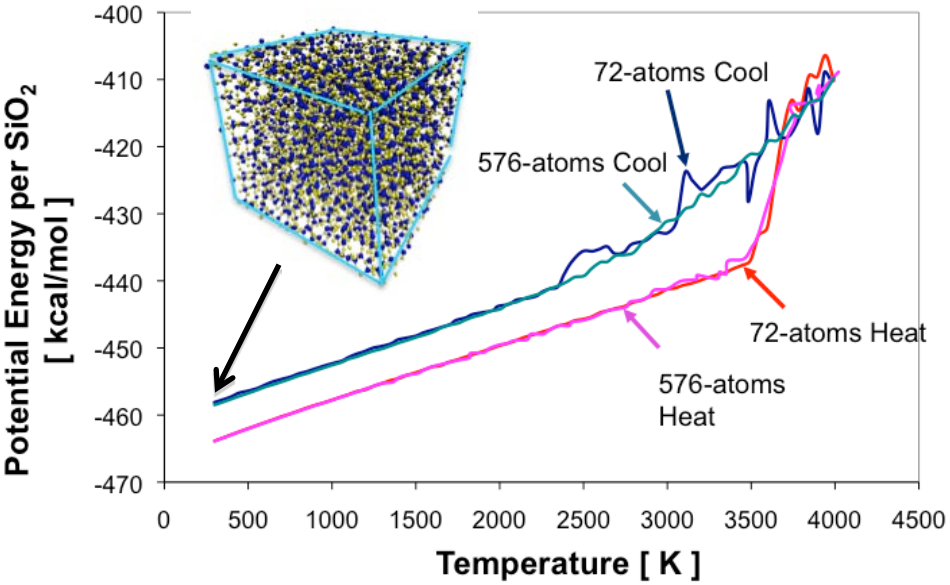
FIG. 3 (color). Computed LDA defect levels (solid blocks) are compared against experimental defect levels (open), aligned within the band gap. Agreement between LDA and experiment is good for all defects, in all parts of the band gap.

Contacts and dielectric charging



of defects

Ensemble of equilibrated structures



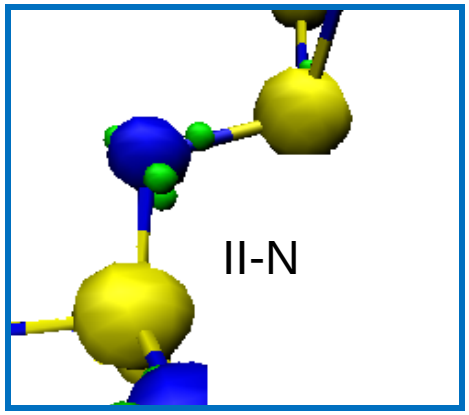
- MD anneal 100's of liquid structures
  - Slow rates to avoid artificially high defect densities
  - Distribution of native defects
- DFT relaxation of MD structures
  - More accurate but more expensive
- Compute electronic properties of defects

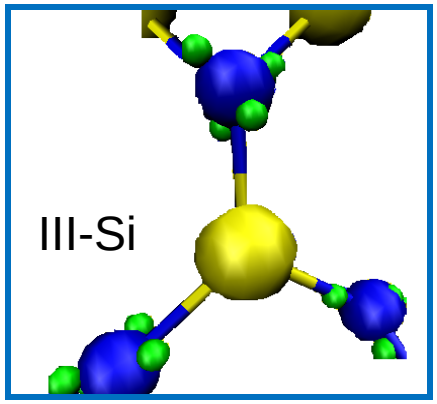
Anderson, Vedula, Schultz, Van Ginhoven, & Strachan, Phys. Rev. Lett. (2011)

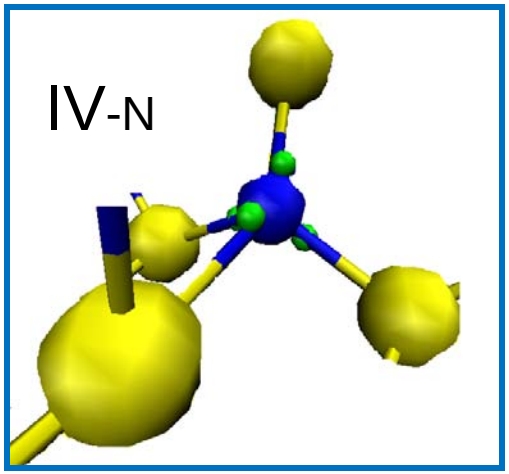
Quantify structural properties & defects

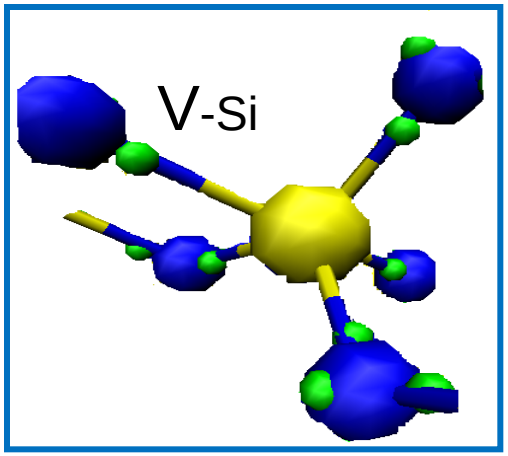
Topological defects in amorphous structures

- Atoms with non-ideal coordination αSi_3N_4
- Distance criterion + Wannier function analysis









Vedula, Anderson, & Strachan, Phys. Rev. B (under review)

Quantify structural properties & defects

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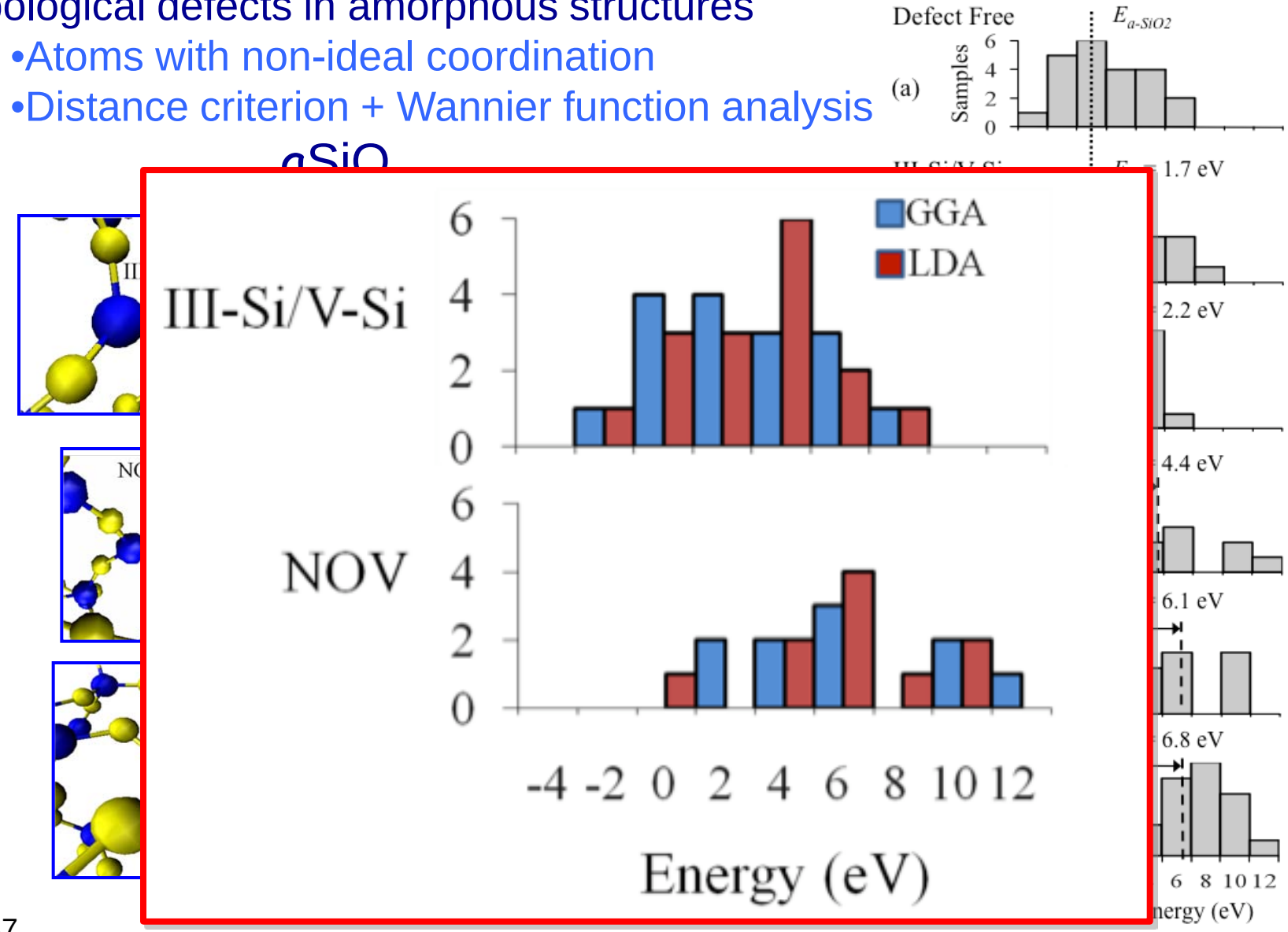
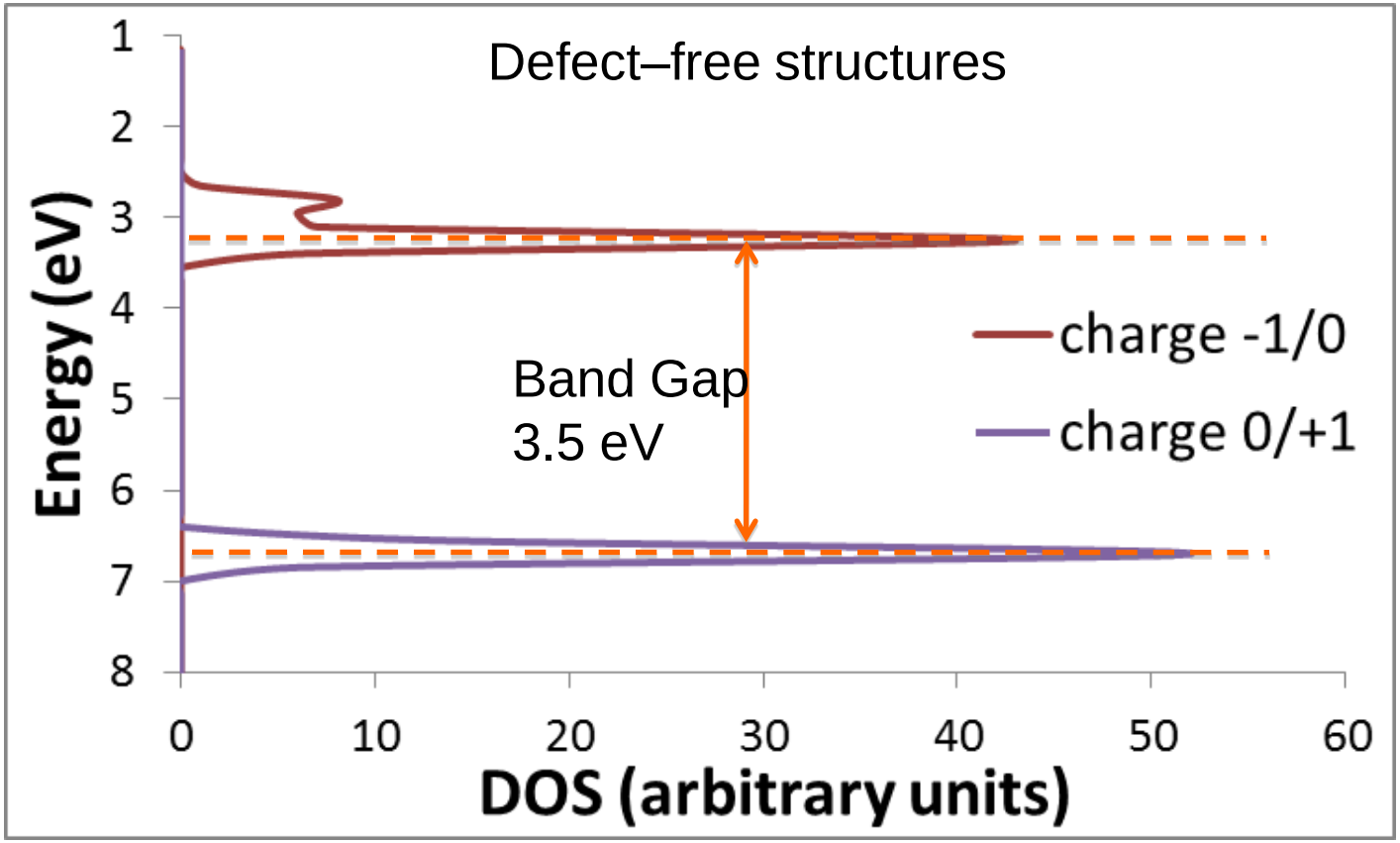


Anderson, Vedula, Schultz, Van Ginhoven, & Strachan, Phys. Rev. Lett. (2011)

Electronic structure of energy levels

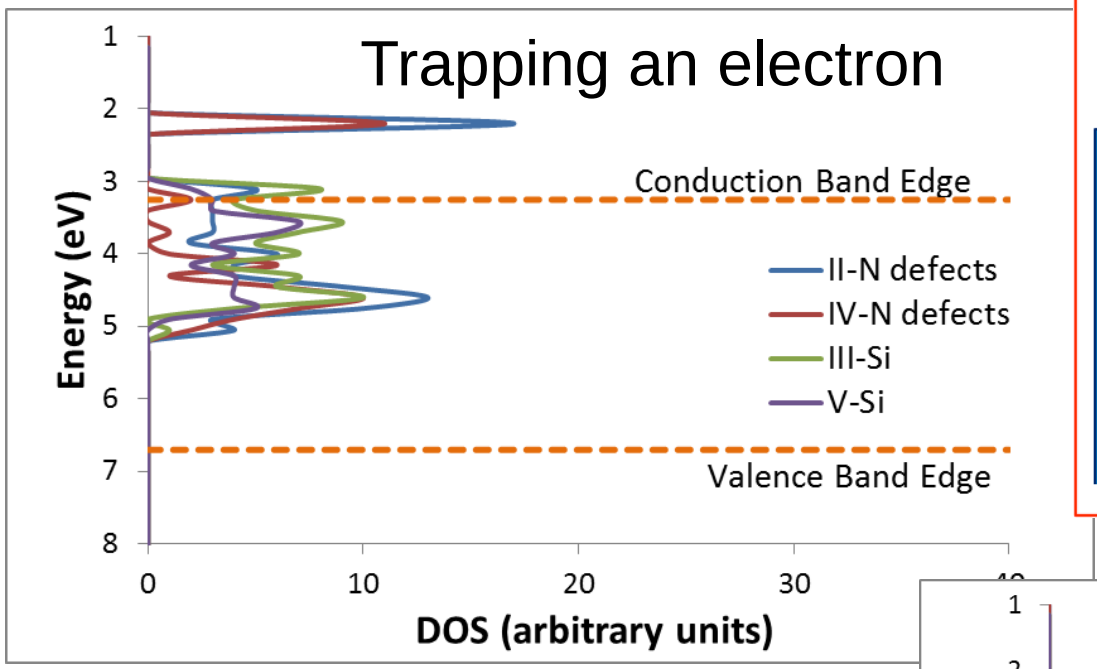
Rigorous calculation of trap depths

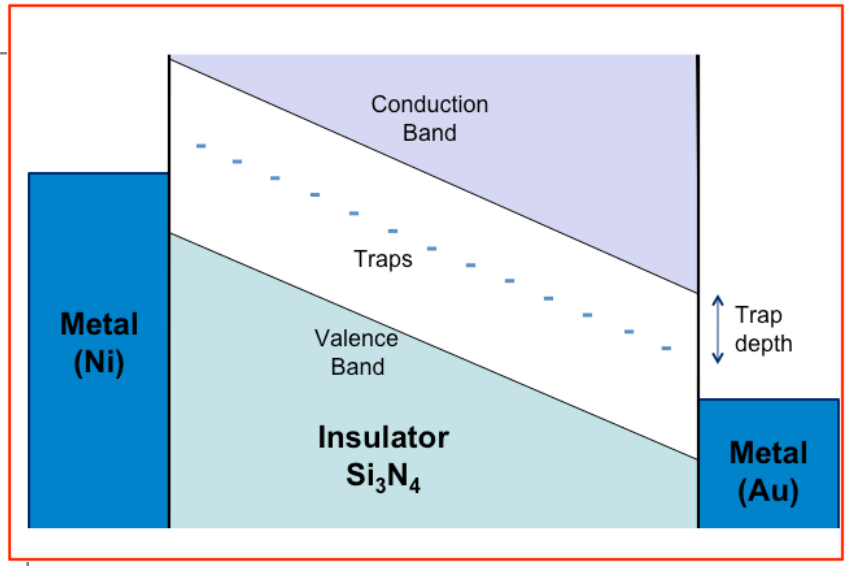
- For every defect perform several charge state calculations (-2, -1, 0, 1, 2)
- The formation energies represent the location of the energy level in the band gap

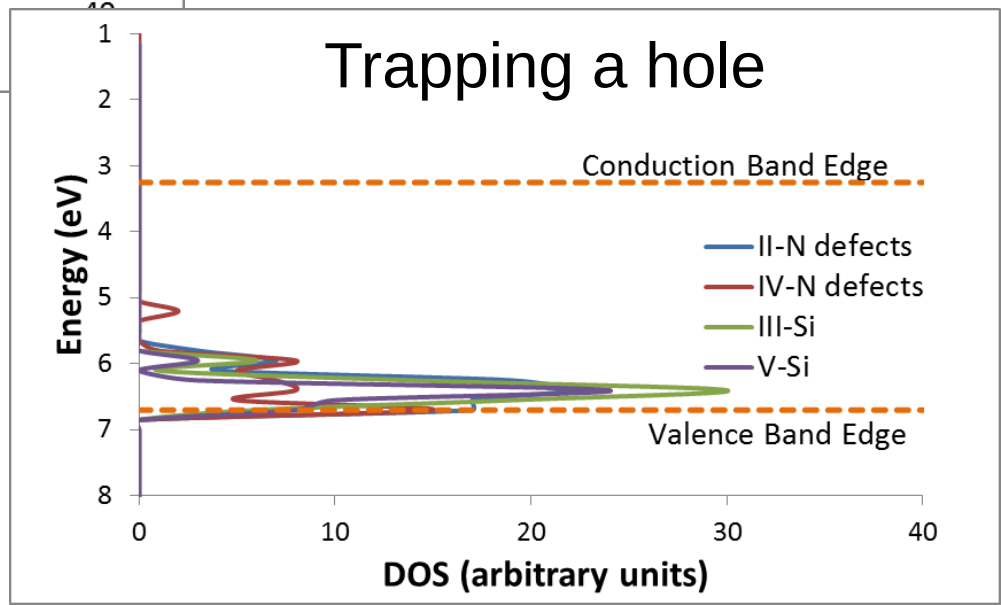


Step 3: electronic structure of energy levels

Rigorous first principles calculation of trap depths



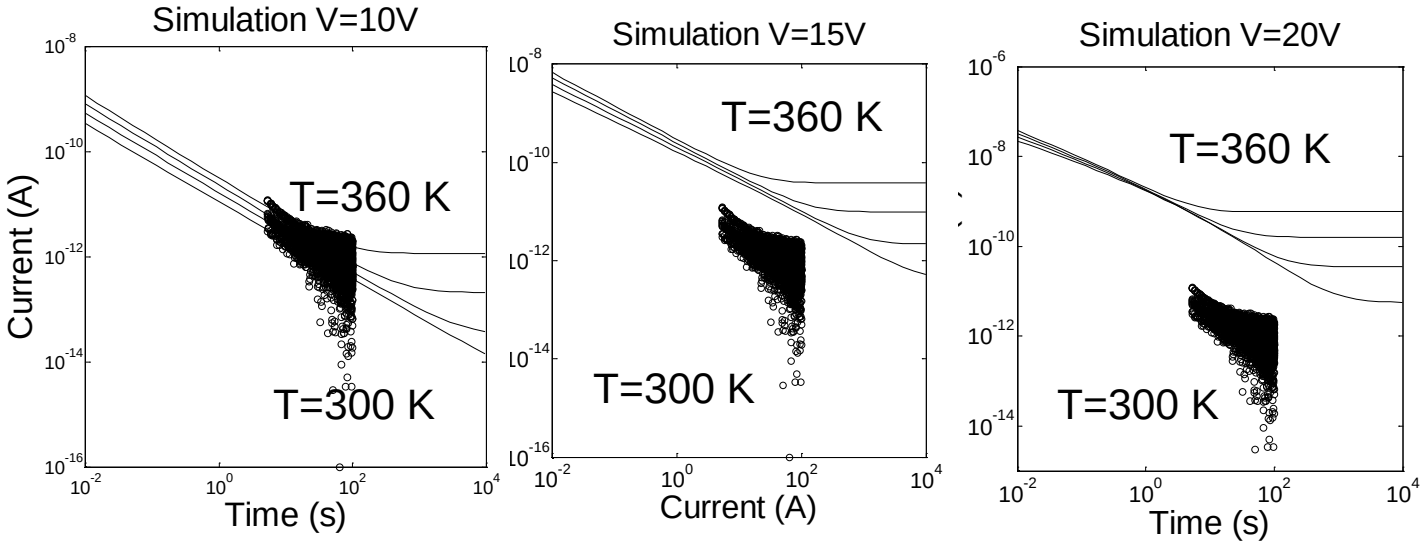




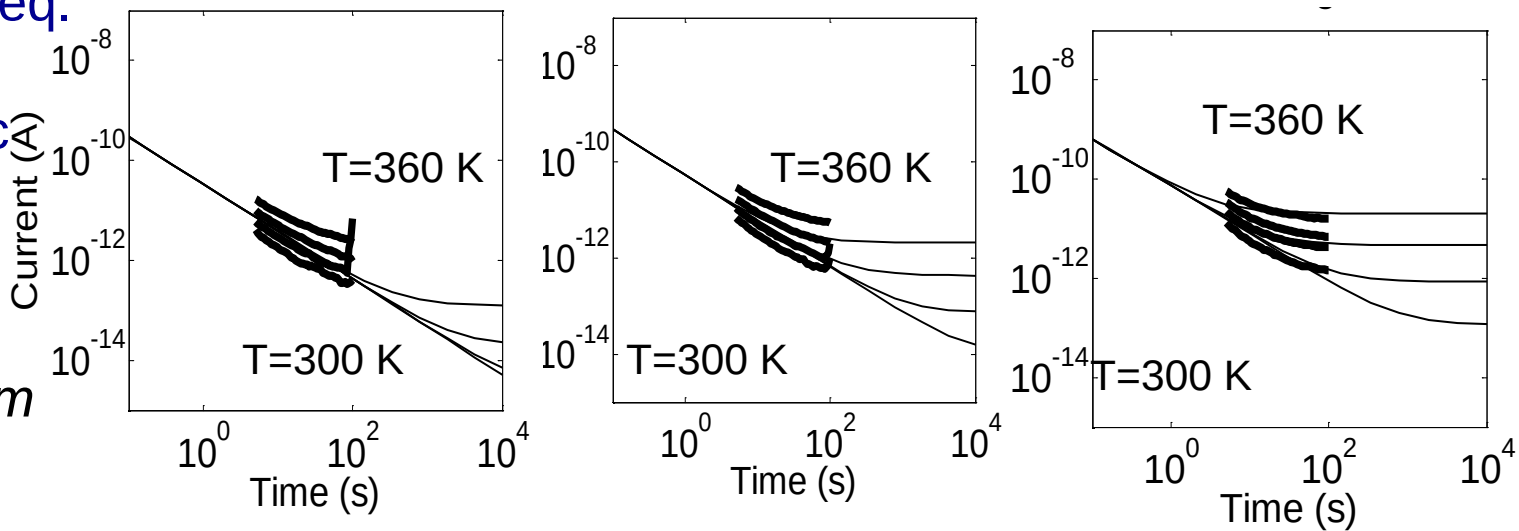
Atomic variability critical to describe experiments

Trap density:
4e23 m^{-3}
Capture c-s.:
1e-22 m^2
Effective mass:
0.5
Barrier height (Φ_B):
1.5 eV
Trap depth (Φ_T):
1.2 – 1.8 eV
Frenkel-Poole freq.
1e12 s-1
Optical dielectric constant: 4

Single trap level model



Multiple trap levels model



S. Palit & A. Alam

Additional online resources @ nanoHUB.org

http://nanohub.org/resources/5495

From density functional theory to defect level in silicon: Does the "band gap problem" matter?

By Peter A. Schultz

Sandia National Laboratories, Albuquerque, NM

Modeling the electrical effects of radiation damage in semiconductor devices requires a detailed description of the properties of point defects generated during and subsequent to irradiation. Such modeling requires physical parameters, such as …

INSTITUTE OF PHYSICS PUBLISHING MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING
Modelling Simul. Mater. Sci. Eng. **13** (2005) R1–R31 doi:10.1088/0965-0393/13/1/R01

TOPICAL REVIEW

Designing meaningful density functional theory calculations in materials science—a primer

Ann E Mattsson[1], Peter A Schultz[1], Michael P Desjarlais[2], Thomas R Mattsson[2] and Kevin Leung[3]

http://nanohub.org/topics/LearningModuleSiliconBandstructureDFT

Learning Module: Bonding and Band Structure in Silicon

by Ravi Pramod Kumar Vedula, Janam Jhaveri, Alejandro Strachan

Article | Edit | History

The main goal of this learning module is to help students learn about the correlation between atomic structure and electronic properties, and help them develop a more intuitive understanding of the origin of electronic bands in a material via hand-on exploration using online electronic structure calculations at nanoHUB.org.

The module consists of:

- Two introductory lecture slides available online as presentations
  - Overview lecture.pdf
  - Prelab lecture.pdf
- Hands-on lab involving Density Functional Theory (DFT) simulations via nanoHUB.org
  - Lab handout.pdf