2011 NCN Summer School

Ab initio and Molecular Dynamics and simulations of materials

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Multiscale Materials Modeling

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

**Length**
- nanometer
- micron
- mm
- meters

**Time**
- femtosec.
- picosec.
- nanosec.
- second
- lifetime

**Components**
- Electrons
- Atoms
- Meso
- Elements
- Certification

**Molecular dynamics**

**Quantum Mechanics**

**Mesoscale**
Why multiscale materials modeling?

- Difference in bonding alone cannot 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**

\[ H\psi = E\psi \quad \text{and} \quad F_i = m_i a_i \]

Wavefunction of electrons for a give set of atomic positions
- Optical and electronic properties
- Atomic interactions
- Chemical reactions

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

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 \( i \)

Eigenvalue problem: you get WF and energy

Initial condition problem: you get atomic positions, velocities and forces
Ab initio and MD simulations

\[ H(\{\rho_i\}, \{r_i\})\psi(\{\rho_i\}) = E(\{r_i\})\psi(\{\rho_i\}) \]

Electrons coordinates

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:

\[ \vec{F}_i = -\nabla_{r_i} E(\{r_j\}) \]

\[ \vec{F}_i = m_i \ddot{a}_i \]

• 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 \( \rho \)

Momentum ↔ \( \hat{p} = \frac{\hbar}{i} \nabla \)

Linear:

\[ O(a\Psi) = aO\Psi \]
\[ O(\Psi_1 + \Psi_2) = O\Psi_1 + O\Psi_2 \]
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 \( \rho \)
Quantum mechanics 101: electronic structure

4. Time evolution of $\psi$ 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

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

\[ H\psi = E\psi \]

Hamiltonian operator of a group of electrons and ions is:

\[ H = K_{\text{elec}} + K_{\text{ions}} + V_{\text{ei}} + V_{\text{ii}} + V_{\text{ee}} \]

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

\[
H_{BO}(\rho_1, \rho_2, \ldots, \rho_n; \{r_i\}) = -\sum_{i=1}^{n} \frac{\hbar^2}{2m_e} \left| \nabla \rho_i \right|^2 - \sum_{i,j}^{n,N} \frac{Z_i e^2}{|\rho_i - r_j|} + \sum_{i<j}^{n} \frac{e^2}{|\rho_i - \rho_j|}
\]
The challenge:

Solve:

\[ H_{BO} \psi = E\psi \]

\[
H_{BO} (\rho_1, \rho_2, \ldots, \rho_n; \{r_i\}) = -\sum_{i=1}^{n} \frac{|\nabla \rho_i|^2}{2m_e} - \sum_{i,j}^{n,N} \frac{Z_i e^2}{|\rho_i - r_j|} + \sum_{i<j}^{n} \frac{e^2}{|\rho_i - \rho_j|}
\]

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 $\sim 1.4^{19}$ s)
Need an approximate solution

Solve: \[ H_{BO} \psi = E \psi \]

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

Mean field approximation:

\[
\psi(\{\rho_i\}) = \phi_1(\rho_1)\phi_2(\rho_2)\ldots\phi_n(\rho_n)
\]

Wavefunction is a product of single-electron wave functions (no correlations)
Need an approximate solution

Plug: \[ \psi (\{ \rho_i \}) = \phi_1 (\rho_1) \phi_2 (\rho_2) \ldots \phi_n (\rho_n) \]

Into Schrödinger equation:

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

Leads to the Hartree equation (Hartree, 1927):

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

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

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:

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

\[ \psi(\{\rho_i\}) = \phi(\rho_1)\phi(\rho_2)\ldots\phi(\rho_n) \]

- 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

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

\[ \psi(\rho_1, \rho_2) = \phi_1(\rho_1)\phi_2(\rho_2) \quad \text{Not possible} \]

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

General solution: Slater determinants

\[ \Psi(\rho_1, \ldots, \rho_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\rho_1) & \phi_2(\rho_1) & \ldots & \phi_N(\rho_1) \\ \phi_1(\rho_2) & \phi_2(\rho_2) & \ldots & \phi_N(\rho_2) \\ \phi_1(\rho_N) & \phi_2(\rho_N) & \ldots & \phi_N(\rho_N) \end{vmatrix} \]
Plugging into the Hartree-Fock equation:

\[
\Psi(\rho_1, ..., \rho_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\phi_1(\rho_1) & \phi_2(\rho_1) & \cdots & \phi_N(\rho_1) \\
\phi_1(\rho_2) & \phi_2(\rho_2) & \cdots & \phi_N(\rho_2) \\
\phi_1(\rho_N) & \phi_2(\rho_N) & \cdots & \phi_N(\rho_N)
\end{vmatrix}
\]

Into the Schrödinger equation:

\[
\left( \sum_{i=1}^{n} -\frac{\hbar^2}{2m_e} \nabla_{\rho_i} \right)^2 - \sum_{i,j}^1 \frac{Z_i e^2}{|\rho_i - r_j|} + \sum_{i<j}^n \frac{e^2}{|\rho_i - \rho_j|} \right) \psi(\{\rho_i\}) = E \psi(\{\rho_i\})
\]

And

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 - \sum_{i=1}^{N} \frac{Z_i e^2}{r_i - \rho} \right] \phi_j(\rho) + \sum_i^n e^2 \int \frac{\phi_i(\rho')}{|\rho - \rho'|} d\rho' - \sum_i^n e^2 \int \frac{\phi_i^*(\rho') \phi_j(\rho') \phi_j(\rho)}{|\rho - \rho'|} d\rho' = E_j \phi_j(\rho)
\]
Hartree-Fock vs. Hartree

Hartree

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

Kinetic energy

Electron-ion interactions

Electron-electron interactions

Hartree-Fock

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

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

Exchange energy (no classical counterpart)
Hartree-Fock predictions

Predicted geometries vs. experiments

<table>
<thead>
<tr>
<th>Table 3.19 SCF equilibrium bond lengths (a.u.) of N₂ and CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basis set</td>
</tr>
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Modern Quantum Chemistry
Szabo and Ostlund
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: $n(r) = \int d^3 r_2, d^3 r_3, \ldots, d^3 r_n |\psi(r, r_2, \ldots, r_n)|^2$

• Ground state energy is also a functional of density:

\[
E_0 = \langle \Psi_0[n_0] | H | \Psi_0[n_0] \rangle = E[n_0]
\]

• 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):

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

Exchange and correlation potential

And the solution is:

\[ n(r) = \sum |\phi_i(r)|^2 \]

With:
Exchange and correlation functional

• Local density approximation (LDA)

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

\[ E_x^{\text{Hom}}(n) = -\frac{3q^2}{4} \left(\frac{3}{\pi}\right)^{1/3} n^{4/3} \]

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)

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

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 $r$

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Payne et al.

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

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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 $r_c$. 
Reciprocal space

\[ P = \left( \frac{1}{V_{\text{BZ}}} \right) \int_{BZ} d\mathbf{k} \sum_n p_n(k) f[\varepsilon_n(k)] \]

\[ f(\varepsilon_n(k)) = \theta(\varepsilon_F - \varepsilon_n(k)) \]

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

Replace integral over 1\textsuperscript{st} BZ by a sum over k-points

- Special, high-symmetry points are used (HJ MONKHOstärST, 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

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

Ann E Mattsson¹, Peter A Schultz¹, Michael P Desjarlais², Thomas R Mattsson² and Kevin Leung³

Figure 5. The computed equilibrium lattice constant, $a_0$, of Ta as a function of Fermi filling temperature and $k$ 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 $k$ 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 $k$ 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 $k$ sample, and are still varying over a range of 5 GPa at a $k$ grid of 40³.
Demos and examples

Simple calculations using Quantum Espresso Tool in nanoHUB
Exchange and correlation functional

- **Local density approximation (LDA)**

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

  \[
  E_x^{\text{Hom}}(n) = -\frac{3q^2}{4} \left(\frac{3}{\pi}\right)^{1/3} n^{4/3}
  \]

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

  **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)**

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

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

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

Exchange and correlation potential

And the solution is:

\[ n(r) = \sum |\phi_i(r)|^2 \]

With:
The “DFT bandstructure” problem

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

\[
\begin{bmatrix}
-\frac{\hbar^2}{2m} \nabla^2 + v_{\text{ext}}(r) + v_H(r) + v_{\text{xc}}(r)
\end{bmatrix} \phi_i = \varepsilon_i \phi_i
\]

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.

Theory of Defect Levels and the “Band Gap Problem” in Silicon

Peter A. Schultz*

Multiscale Computational Materials Methods, Sandia National Laboratories, Albuquerque, New Mexico 87185-1110, USA
(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

- Charge injection and diffusion into dielectric
- Generate representative structures (including defects)
- Compute the electronic properties of defects

Metal (Ni)

Insulator Si$_3$N$_4$

Metal (Au)

Conduction Band

Valence Band

Traps

Trap depth

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

Quantify structural properties & defects

Topological defects in amorphous structures

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

\[ \text{aSi}_3\text{N}_4 \]

Vedula, Anderson, & Strachan, Phys. Rev. B (under review)
Quantify structural properties & defects

Topological defects in amorphous structures
• Atoms with non-ideal coordination
• Distance criterion + Wannier function analysis

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

![Defect-free structures diagram](image)

Defect–free structures

- Energy (eV)
- Band Gap: 3.5 eV
- DOS (arbitrary units)

- charge -1/0
- charge 0/+1
Step 3: electronic structure of energy levels

Rigorous first principles calculation of trap depths

Trapping an electron

- Conduction Band Edge
- Valence Band Edge

Energy (eV)

DOS (arbitrary units)

Trapping a hole

- Conduction Band Edge
- Valence Band Edge

Energy (eV)

DOS (arbitrary units)
Atomic variability critical to describe experiments

**Trap density:** 4e23 m⁻³

**Capture c-s.:** 1e⁻²² m²

**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

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**Single trap level model**

**Simulation V=10V**

T=300 K

**Simulation V=15V**

T=300 K

**Simulation V=20V**

T=360 K

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**Multiple trap levels model**

**Simulation V=10V**

T=300 K

**Simulation V=15V**

T=300 K

**Simulation V=20V**

T=300 K

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*S. Palit & A. Alam*
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 ...

Learning Module: Bonding and Band Structure in Silicon

by Ravi Pramod Kumar Vedula, Janam Jhaveri, Alejandro Strachan

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.pcf
  - Prelab lecture.pcf
- Hands-on lab involving Density Functional Theory (DFT) simulations via nanoHUB.org
  - Lab handout.pdf

http://nanohub.org/resources/5495

http://nanohub.org/topics/LearningModuleSiliconBandstructureDFT

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

Ann F Mattsson1, Peter A Schultz1, Michael P Desjarlais2, Thomas R Mattsson2 and Kevin Leung3