ECE 595, Section 10
Numerical Simulations
Lecture 24: Electronic Bandstructure Simulation Tools

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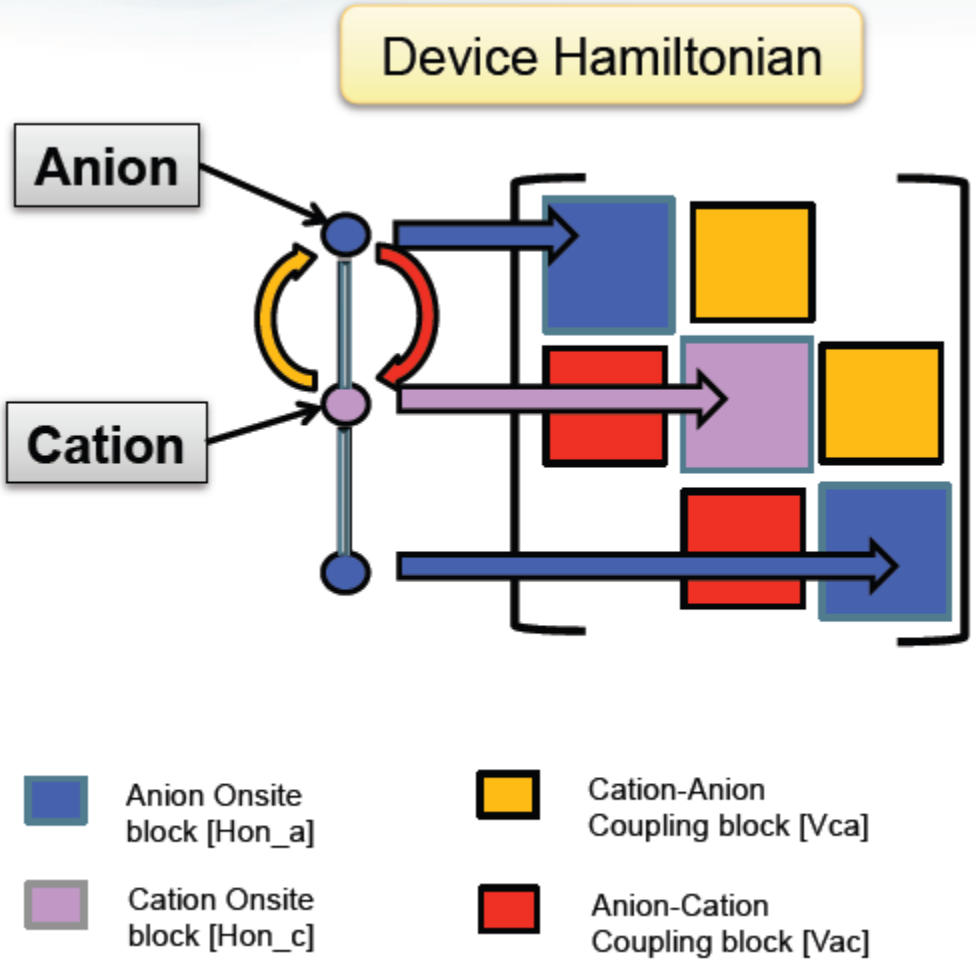
Recap from Monday

- Electronic bandstructure overview
- Calculational methods:
  - Nearly-free electron model
  - Wigner-Seitz method
  - Tight-binding
  - Pseudopotentials

Outline

- Electronic bandstructure lab
  - Basic principles
  - Input Interface
  - Exemplary Outputs
- Density functional theory (DFT)
- DFT in Quantum ESPRESSO

Bandstructure Lab

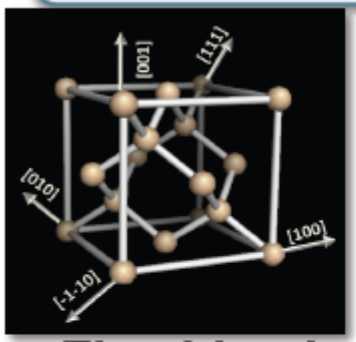


- Device Hamiltonian is assembled using **semi-empirical tight-binding [TB]**
- Each atom is represented using an onsite block [Hon_a or Hon_c].
- Coupling with nearest neighbor is taken in coupling blocks [Vac, Vca]
- Size of these blocks depends on the basis set and spin-orbit coupling
- Basis sets are made of orthogonal atomic orbitals like s,p,d,etc.
- **The Band Structure Lab uses sp3d5s* basis set with 10 basis functions**

"First Time User Guide" by Abhijeet Paul and Gerhard Klimeck

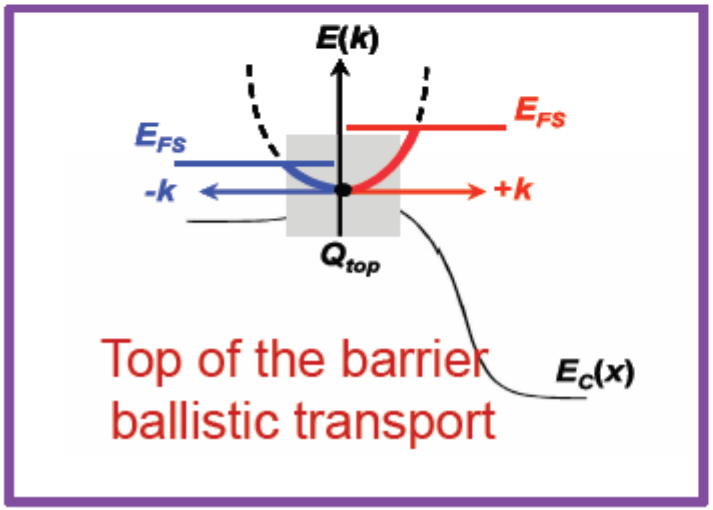
Bandstructure Lab

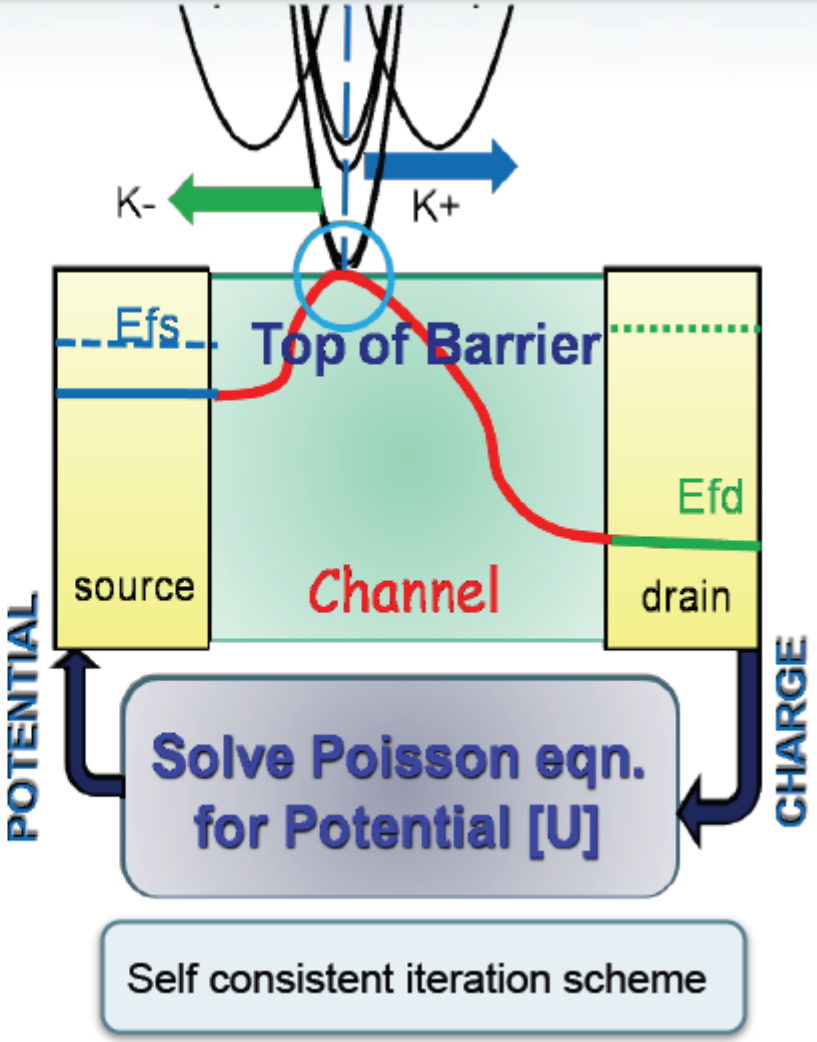
Electronic structure
20 band $sp^3d^5s^*$ model with spin orbit coupling



Zinc blend

- Appropriate for treating atomic level disorder
- Strain treatment at atomic level
- Structural, material & potential variations treated easily





"First Time User Guide" by Abhijeet Paul and Gerhard Klimeck

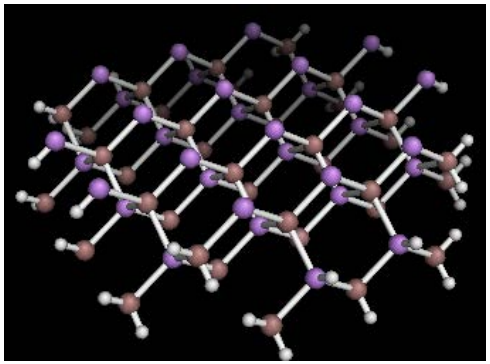
Bandstructure Lab: Input

- Step 1A: Choose basic geometry:
  - Nanowire (cylindrical 1D) – also choose device cross-section
  - Ultra-thin body (2D-periodic) – also choose body thickness
  - Bulk silicon (3D periodic)
- Step 1B: Choose material: Si, Ge, GaAs, or InAs

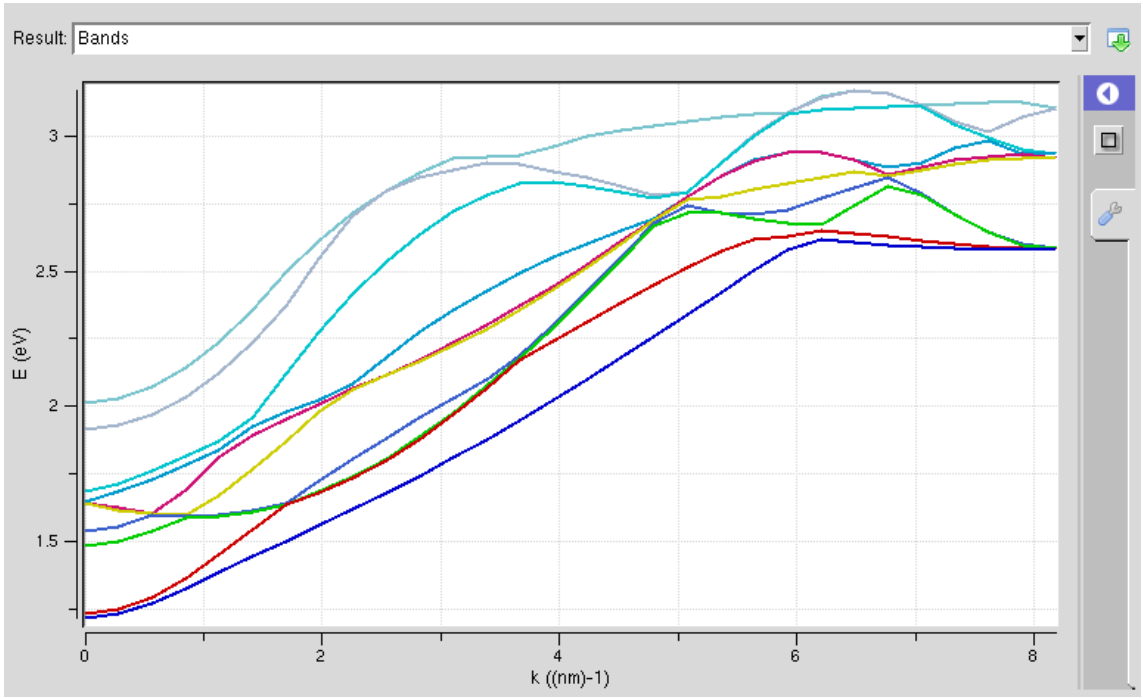
Bandstructure Lab: Input

- Step 2: Choose Device Physics:
  - Tight bonding model
  - Spin-orbit coupling
  - Dangling bond energy
  - Strain
- Step 3: Choose k-space of bandstructure
- Step 4: Choose k-interpolation, number of bands, and simulation venue

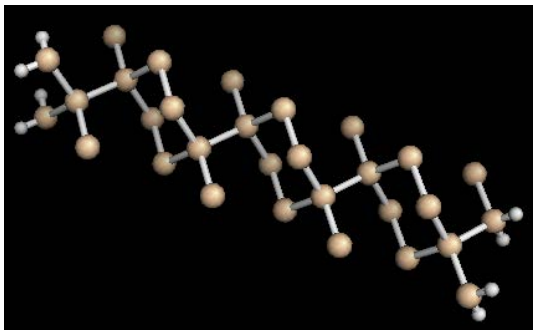
Bandstructure Lab: Output



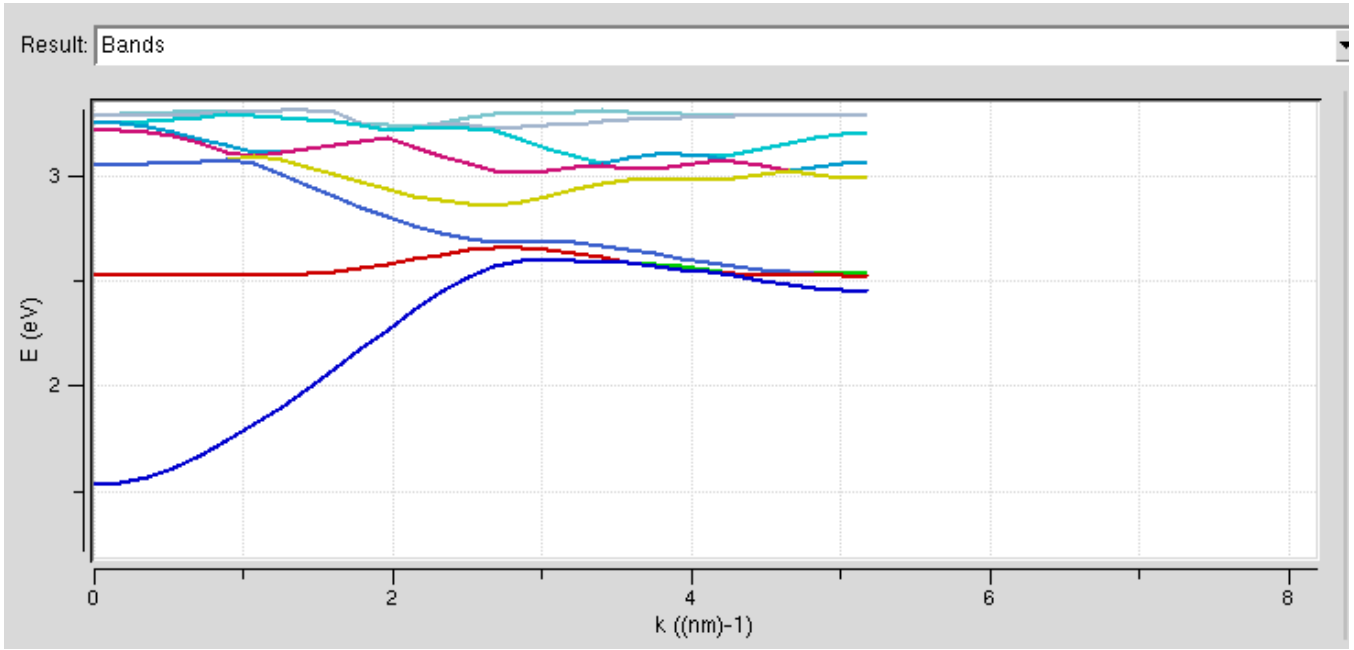
2D ultra-thin body (E_g=1.12 eV)
Height z = 2.1 nm



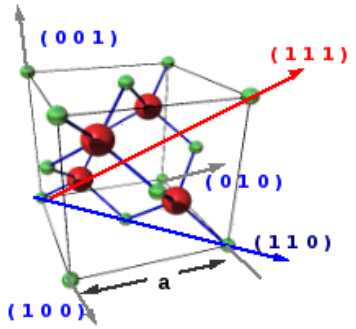
Electronic Bandstructure Lab:



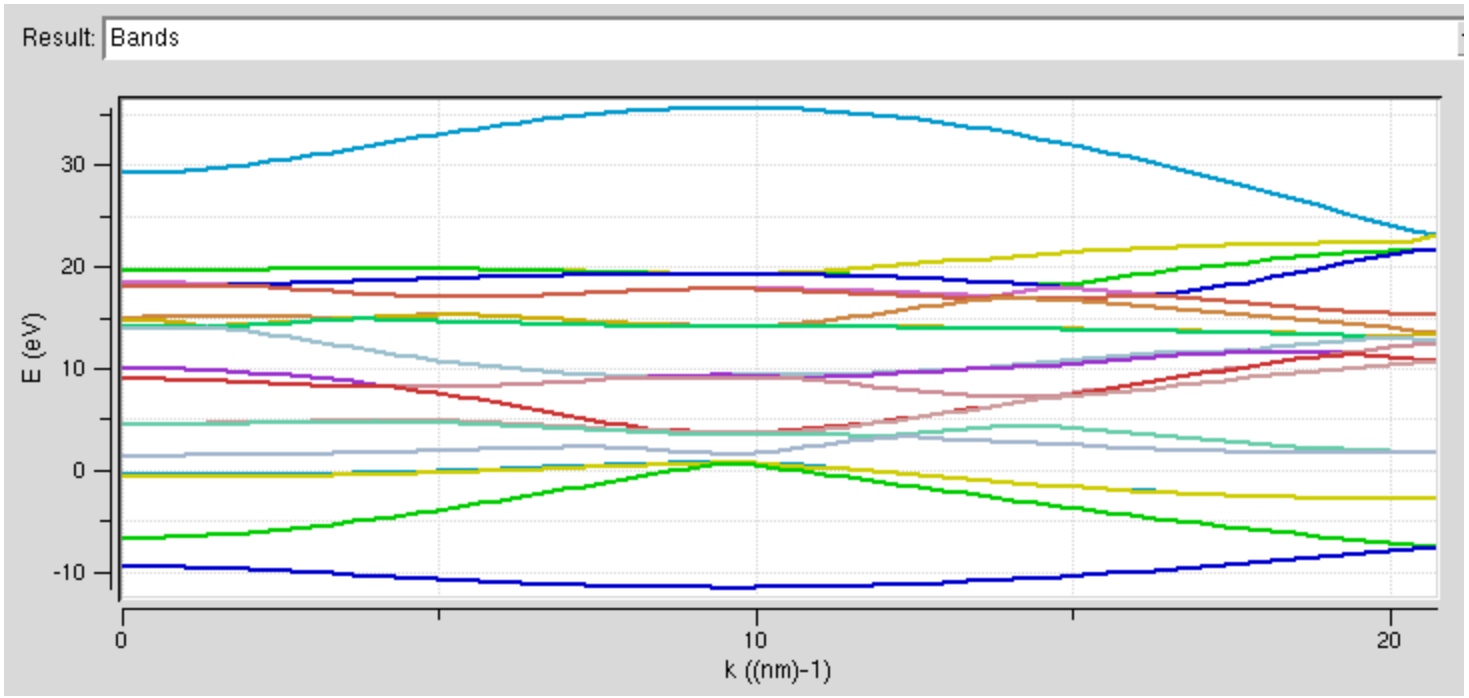
1D NW of InAs (E_g=0.17 eV)
Circular cross-section, r = 2.1 nm



Bandstructure Lab: Output



3D periodic Ge
Diamond lattice (E_g=0.67 eV)



Density Functional Theory

- Consider the *N*-electron Hamiltonian including electron-electron interactions:

$$\sum_i \left[-\frac{\hbar^2}{2m} \boldsymbol{\nabla}_i^2 + V(\boldsymbol{r}_i) + \sum_j U(\boldsymbol{r}_i, \boldsymbol{r}_j) \right] \Psi = E\Psi$$

- Can try to solve using:
  - Hartree-Fock (treating electron-electron interactions as mean field
  - Post-Hartree-Fock (e.g., configuration interaction, coupled cluster, Moller-Plesset)
  - Density functional theory

Density Functional Theory

- Write all functions in terms of particle density:

$$n(r) = N \int d^3 r_2 \int d^3 r_3 \, |\Psi(r, r_2, \cdots, r_N)|^2$$

- Now system energy becomes:

$$E[n] = T[n] + U[n] + \int d^3 r \, V(r) n(r)$$

- Where $T[n]$ and $U[n]$ are universal functionals, and $V[n]$ is a non-universal functional

Density Functional Theory

- Electron correlations mean greatest difficulty is in evaluating $V[n]$. Strategies include:
  - Local density approximation:

$$E_{XC}[n] = \int d^3r\, n(r)\, \epsilon_{XC}(n)$$

  - Localized spin density approximation
  - Generalized gradient approximation:

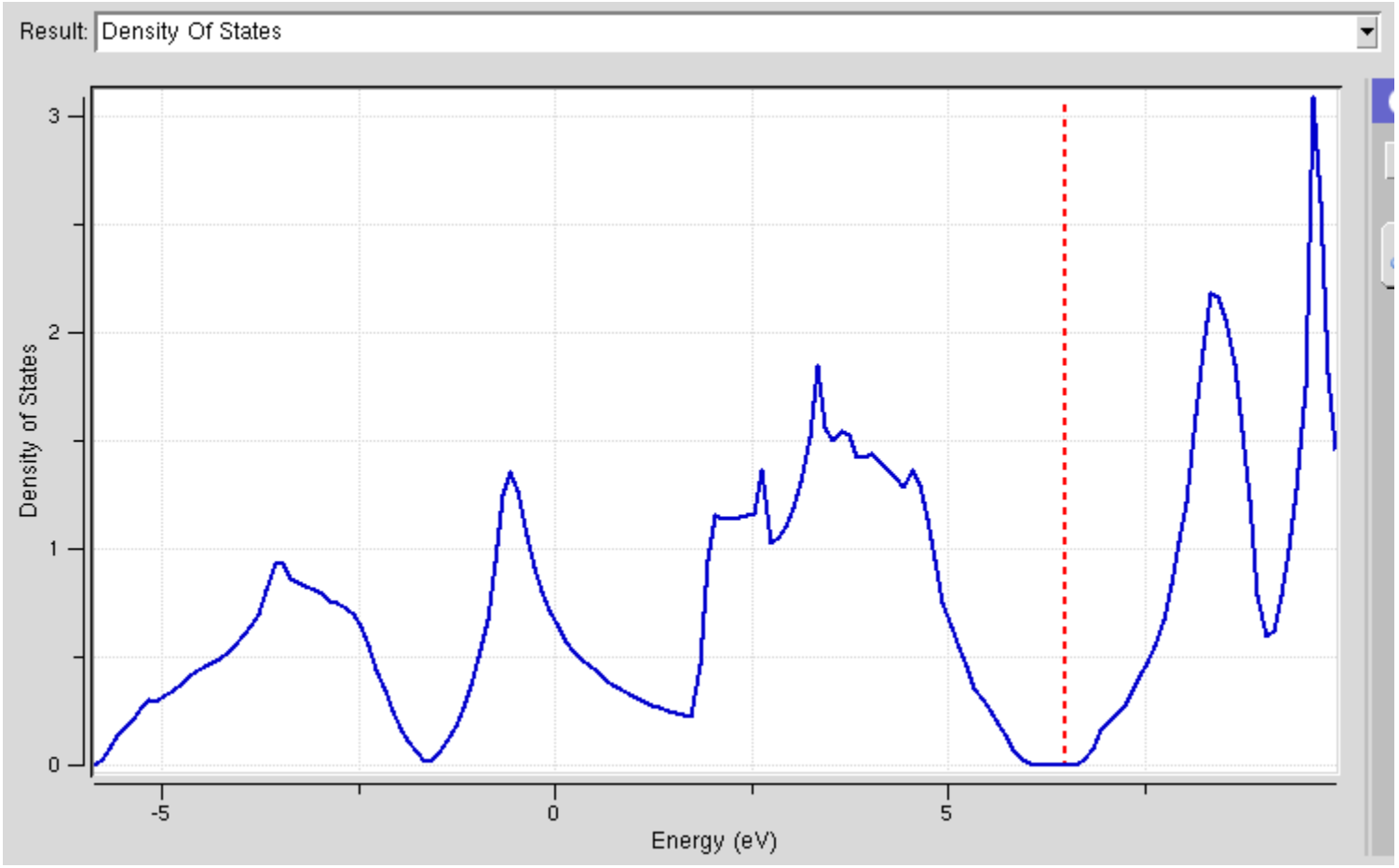
$$E_{XC}[n_\uparrow, n_\downarrow] = \int d^3r\, n(r)\, \epsilon_{XC}(n_\uparrow, n_\downarrow, \nabla n_\uparrow, \nabla n_\downarrow)$$

  - Meta-generalized gradient approximation

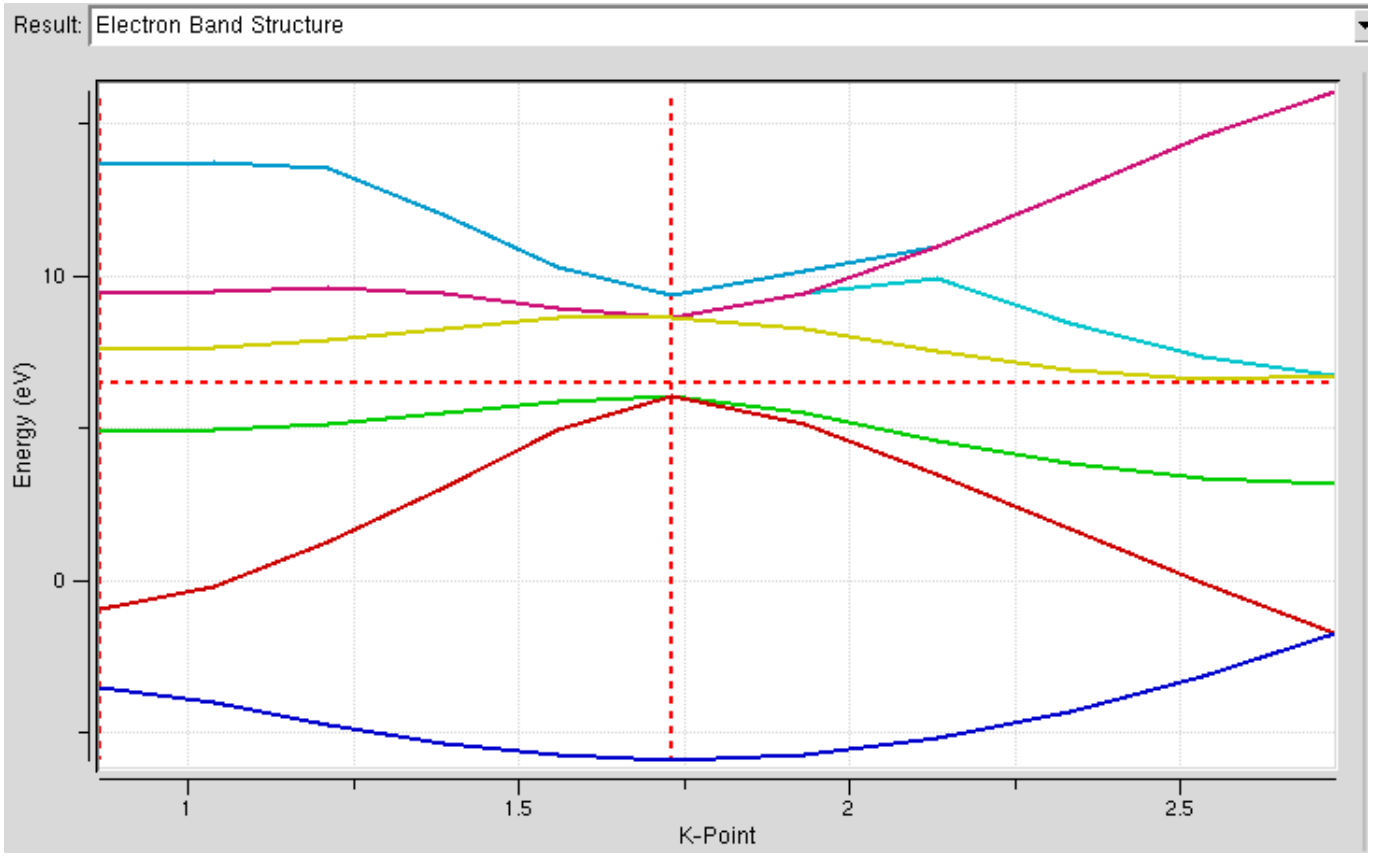
Quantum ESPRESSO: Input

- Step 1: Geometry
  - Atomic basis (e.g., 2 silicon atoms)
  - Lattice (e.g., diamond) and lattice constant *a*
- Step 2: Energy expression:
  - Approximation for E_{XC}
  - Bandstructure k-values
- Step 3: Phonon bands: yes or no
- Step 4: Bandstructure/DOS
  - Choose path for bandstructure
  - Choose energy range for density of states

Quantum ESPRESSO: Output



Quantum ESPRESSO: Output



- Displays bandgap of 0.6 eV, below true value
- GGA + quasi-Newton relaxation improve accuracy

Next Class

- Is on Friday, March 8
- Will conclude discussion of electronic bandstructure simulations