

# 591V Multiscale Materials Modeling

## Computational Lab-3

# Outline: Today's class

## **Outline:**

Using atomic scale modeling kit (PWSCF)

# nanoHUB.org->Tools->MIT Atomistic Scale Modeling Toolkit

**MIT Atomic Scale Modeling Toolkit**  
By Daniel Richards<sup>1</sup>, Elif Ertekin<sup>1</sup>, Jeffrey C Grossman<sup>2</sup>, David Strubbe<sup>1</sup>, Justin Riley<sup>3</sup>  
*1. University of California, Berkeley 2. Massachusetts Institute of Technology 3. Massachusetts Institute of Technology (MIT)*

Launch Tool

Version 4.3w - published on 17 Mar 2015  
doi:10.4231/D3JM23H1H [cite this](#)  
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CategoryToolsPublished on17 Mar 2015

**Abstract**

This set of simulation tools has been developed for use with a course originally developed at UC Berkeley, taught by Jeffrey Grossman, which provides students with the fundamentals of computational problem-solving techniques that are used to understand and predict properties of nanoscale systems. Emphasis is placed on how to use simulations effectively, intelligently, and predict properties that occur at the nanoscale for real systems. The course is designed to present a broad overview of computational nanoscience and is therefore suitable for both experimental and theoretical researchers.

These tools have been updated throughout spring term of 2011. The following simulations are run by the tool:



Atomic Scale Modeling  
Toolkit  
Massachusetts Institute of Technology

Application:  
About this Toolkit

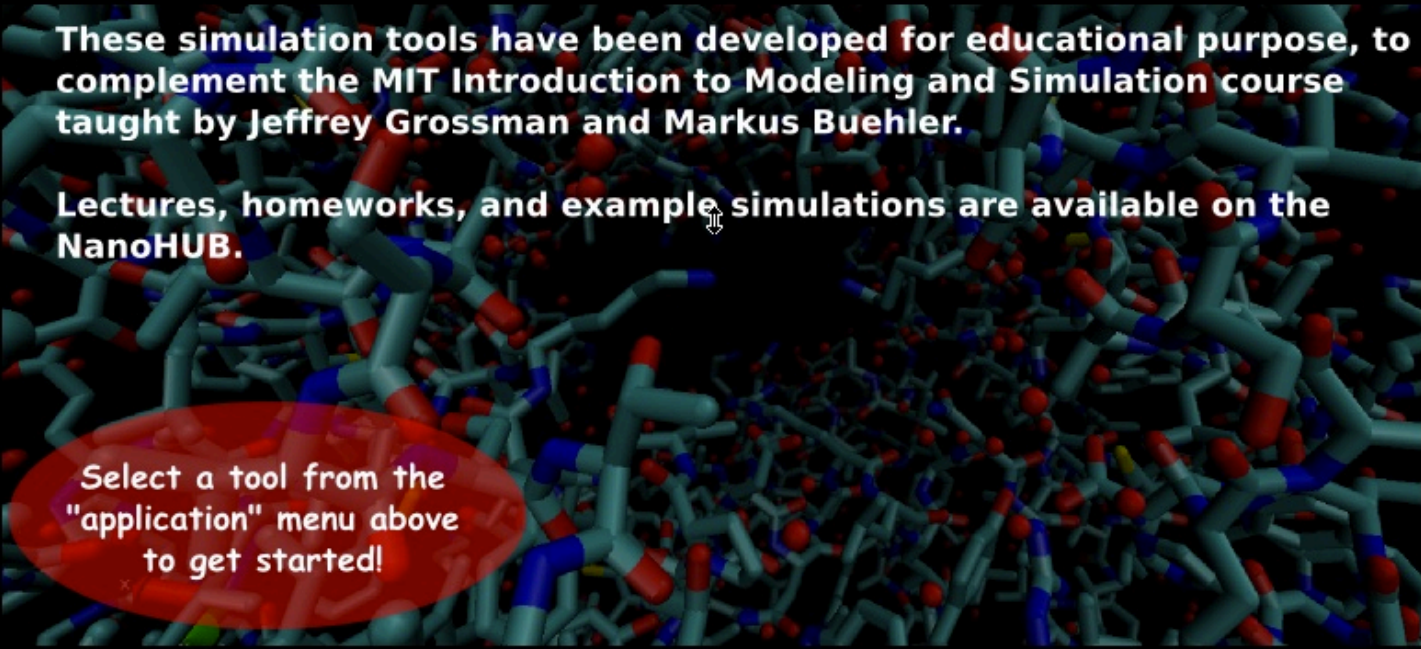
## MIT Atomic Scale Modeling Toolkit

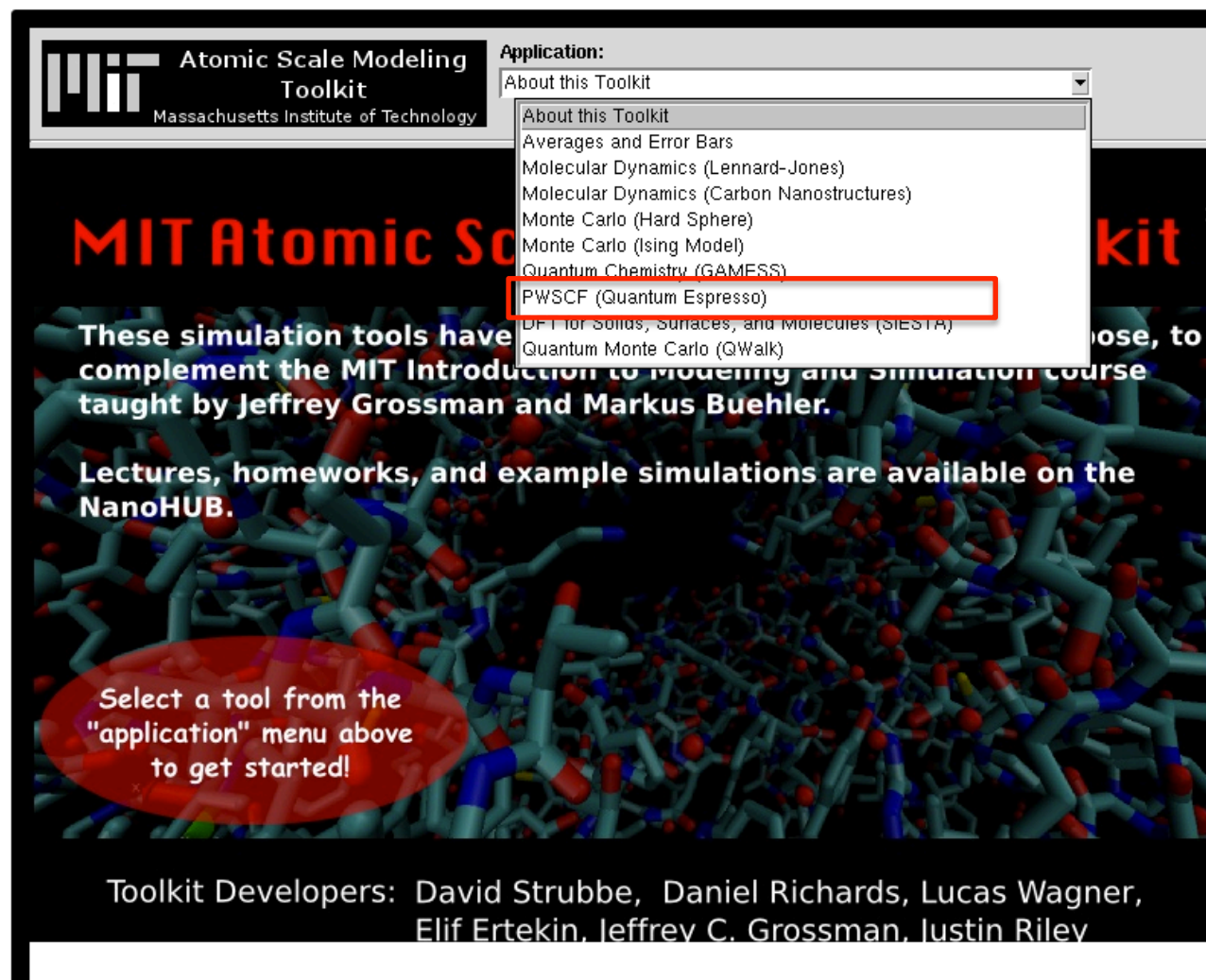
These simulation tools have been developed for educational purpose, to complement the MIT Introduction to Modeling and Simulation course taught by Jeffrey Grossman and Markus Buehler.

Lectures, homeworks, and example simulations are available on the NanoHUB.

Select a tool from the "application" menu above to get started!

Toolkit Developers: David Strubbe, Daniel Richards, Lucas Wagner, Elif Ertekin, Jeffrey C. Grossman, Justin Riley





**MIT** Atomic Scale Modeling Toolkit  
Massachusetts Institute of Technology

**Application:**  
About this Toolkit

- About this Toolkit
- Averages and Error Bars
- Molecular Dynamics (Lennard-Jones)
- Molecular Dynamics (Carbon Nanostructures)
- Monte Carlo (Hard Sphere)
- Monte Carlo (Ising Model)
- Quantum Chemistry (GAMESS)
- PWSCF (Quantum Espresso)**
- DFT for Solids, Surfaces, and Molecules (SIESTA)
- Quantum Monte Carlo (QWalk)

**MIT Atomic Scale Modeling Toolkit**

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# <http://www.quantum-espresso.org/>



QUANTUM ESPRESSO

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## NEWS

24.09.15

### QUANTUM ESPRESSO V.5.2.1

Version 5.2.1 of Quantum ESPRESSO is available for download.

20.06.15

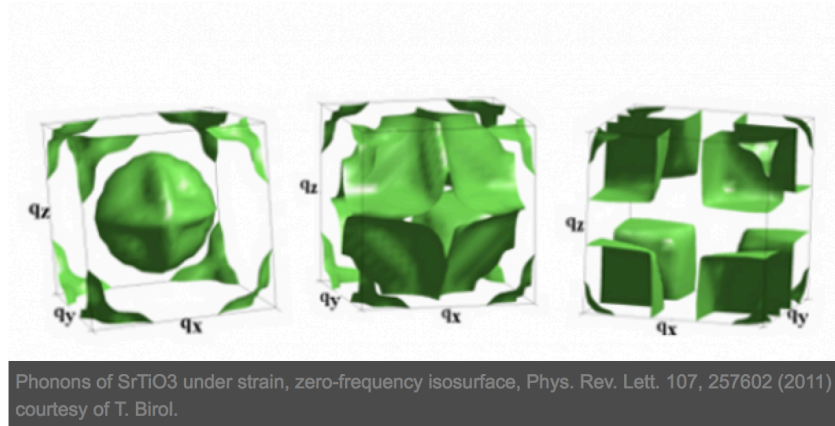
### QUANTUM ESPRESSO V.5.2.0

Version 5.2.0 of Quantum ESPRESSO is available for download.

09.03.15

### QUANTUM ESPRESSO V.5.1.2

Version 5.1.2 of Quantum ESPRESSO is available for download.

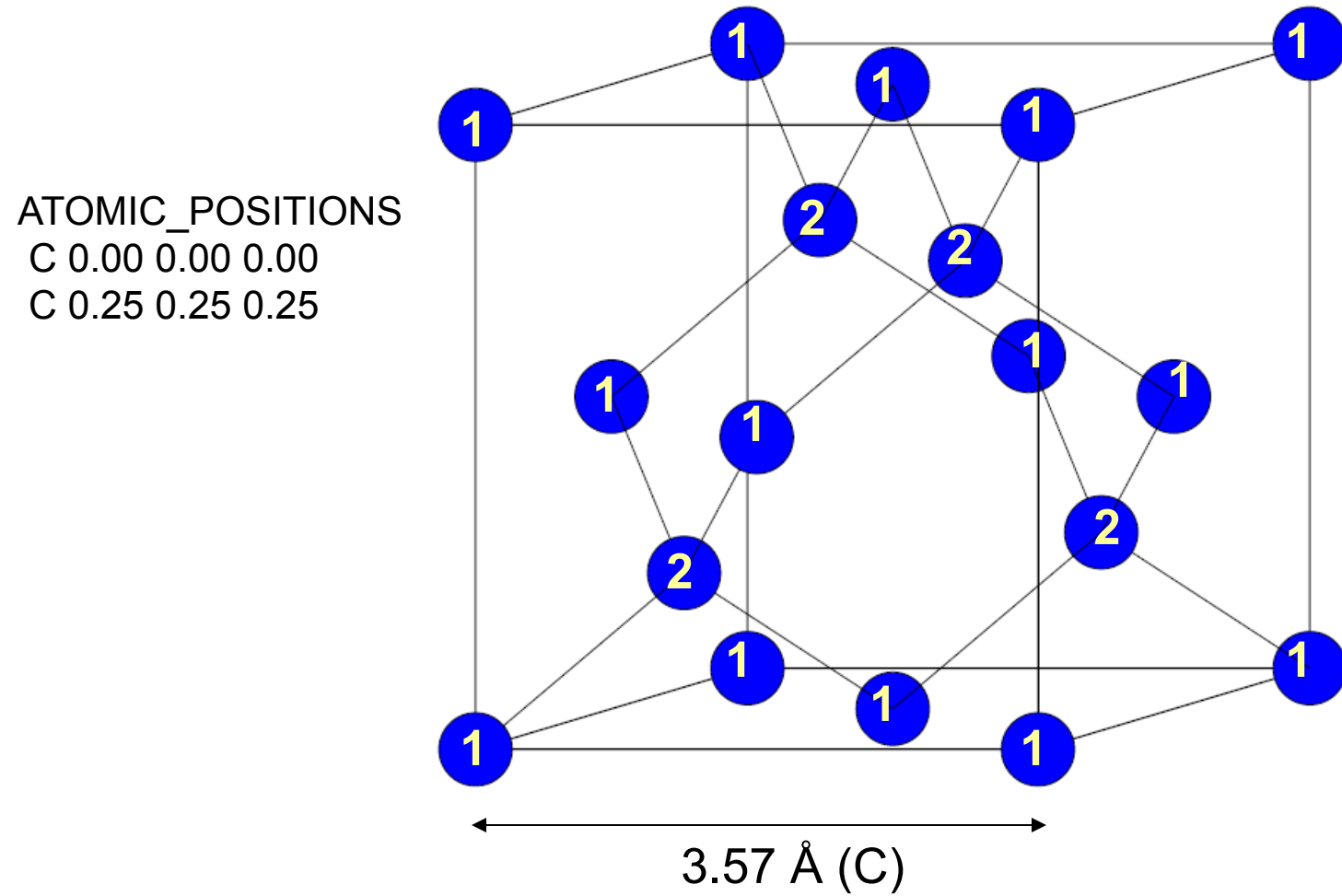


## QUANTUM ESPRESSO

is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

[READ MORE >](#)

# Diamond structure in PWSCF



1 Bohr = 0.529177249 Å



# Atomic Scale Modeling Toolkit

Massachusetts Institute of Technology

Application:

PWSCF (Quantum Espresso)

1 Input → 2 Simulate



About this tool  
Questions?

System

Atomic Coordinates

K Points

Looping

DOS

BANDS

Calculation: scf

**SCF: self-consistent field calculation for converged charge density**

Bravais lattice: cubic F (face centered cubic)

Lattice constant: 7.5

**Units (in Bohr=0.529177249 Å)**

**Discussed later**

Occupations: smearing

Smearing: gaussian

Degauss value: 0.07

**To do a spin-polarized calculation**

Perform spin-polarized calculation?: ☐ no

Starting spin polarization: 0.0

Specify number of bands?: ☒ yes

Number of bands to calculate: 8

Wavefunction kinetic energy cutoff: 30.0

**Energy cut-off for plane waves (in Ry, 1 Ry = 13.6 eV)**

Specify charge density cutoff?: ☒ yes

Charge density kinetic energy cutoff: 300.0

**Energy cut-off for charge density calculation**

Specify FFT mesh for charge density?: ☒ yes

**Convergence threshold: definition of convergence  
for charge density**

Simulate >





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Coordinate units: alat

Atomic positions:  
C 0.0 0.0 0.0  
C 0.25 0.25 0.25

**Atom type and atomic coordinates:  
Currently the toolkit has H, C, Al, Fe  
and Cu.**

Simulate >



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K points: automatic

K Points: 8 8 8 0 0 0

**( $k_x$ ,  $k_y$ ,  $k_z$ , shift\_x, shift\_y, shift\_z)**

**8 points in every direction in Brillouin zone**

**no shift (0) in unit of reciprocal lattice vector**

**The computation time is linearly dependent on  $k_x$ ,  $k_y$ ,  $k_z$   
should check for total energy convergence!**

Simulate >



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Enabling looping?: ☒ yes

Loop settings

Loop variable (x-axis): celldm(1)

Start: 5.0

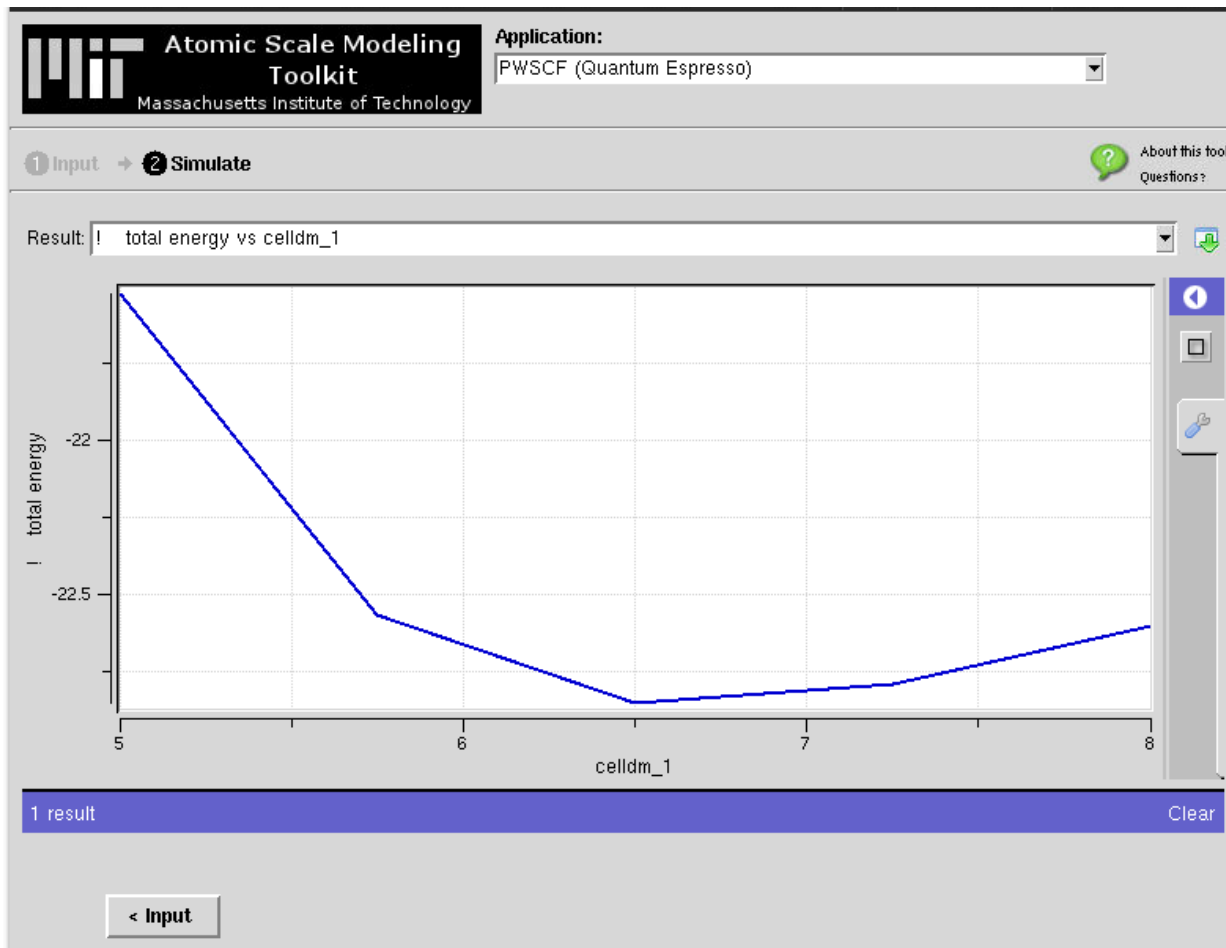
End: 8.0

Steps: 5

Plot variable (y-axis): Total Energy

Used for convergence studies, i.e  
Lattice constant, cut off energy etc.

Simulate >



Can compute:  
Equilibrium lattice  
constant

Units: Total energy (Ry) and celldm\_1 (Bohr)

# Example for metals (Aluminum, Cu)

Occupations: smearing

**define how electrons occupy the energy bands**

Smearing: gaussian

**method for 'smearing'**

Degauss value: 0.07

**Gaussian distribution width for smearing**

The screenshot shows the 'Atomic Scale Modeling Toolkit' interface. The 'Input' tab is active, and the 'BANDS' sub-tab is selected. A red box highlights the 'Occupations: smearing', 'Smearing: gaussian', and 'Degauss value: 0.07' settings. A red arrow points from this box to the corresponding settings in the top summary box. Other visible parameters include 'Calculation: scf', 'Bravais lattice: cubic F (face centered cubic)', 'Lattice constant: 7.5', 'Perform spin-polarized calculation?: no', 'Wavefunction kinetic energy cutoff: 30.0', 'Charge density kinetic energy cutoff: 300.0', 'Specify FFT mesh for charge density?: yes', 'FFT mesh dimension 1: 32', 'FFT mesh dimension 2: 32', 'FFT mesh dimension 3: 32', 'Disable symmetry?: no', and 'Convergence threshold for self-consistency: 1.0e-8'. The 'Simulate' button is at the bottom right.

*For metals (such as Aluminum, copper), in order to determine the position of Fermi surface (maximum energy the electrons can reach, the finite numbers of electrons are filling orbitals from low energy to higher energy), we need some artificial gaussian type smearing function processing, and these three lines specify the method and parameters used.*

Determine the  
equilibrium  
lattice constant