From Atoms to Materials: Predictive Theory and Simulations

Week 1: Quantum Mechanics and Electronic Structure
Lecture 1.1: Course Overview

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Materials are everywhere

Structural materials
http://www.boeing.com/commercial/787family/

Pharmaceuticals
Kwong, Kauffman, Hurter & Mueller
Nature Biotechnology, 29, 993 (2011)

Nanoelectronics “The High-k Solution”, Bohr, Chau, Ghani, and Mistry
http://www.spectrum.ieee.org/oct07/5553
Learning objectives

In *Atoms to Materials* you will:

- Learn the basics physics that govern materials at atomic scales
- Relate these processes to the macroscopic world
- Use online simulations to enhance learning
  - Density functional theory
  - Molecular dynamics
Molecular materials

Ceramics & semiconductors

Metals
Materials properties

Materials Selection in Mechanical Design (3rd edition) by MF Ashby, Butterworth Heinemann, 2005
"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved."

Quantum mechanics:
• A group of atoms can be fully described by their wavefunction
• The time evolution of this wavefunction is given by the Schrödinger equation

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

Too complex to be solved even with supercomputers

Electrons:
Time independent Schrödinger Eq.

$$H \psi = E \psi$$

Ions:
Classical (Newton’s) mechanics

$$F = ma$$
Electronic and atomic processes

Initial condition
\[
\{R_i\} \quad \{V_i\}
\]

Time evolution
\[
\dot{R}_i = V_i \\
\dot{V}_i = \frac{F_i}{M_i}
\]

Energy & forces
\[
H \psi = E \psi \\
F_i = -\nabla_{R_i} E(\{R_i\})
\]
Molecular dynamics

Initial conditions
\[ \{ R_i \} \quad \{ V_i \} \]

Compute energy & forces
\[ H \psi = E \psi \]
\[ F_i = -\nabla_{R_i} E(\{ R_i \}) \]

Integrate Eqs. of Motion
\[ R_i(t) \rightarrow R_i(t + \Delta t) \]
\[ V_i(t) \rightarrow V_i(t + \Delta t) \]
Microscopic and macroscopic worlds
Course outline

• Week 1: Quantum mechanics & electronic structure
  • How QM explains atomic structure
  • Predict color of dye molecules

• Week 2: Electronic structure & bonding of molecules and crystals
  • Structure of simple molecules and crystals
  • Bonding, band structure & elastic constants

• Week 3: Dynamics of atoms
  • Classical mechanics applied to atoms
  • Perform MD simulations on various materials

• Week 4: Connecting atomic processes to the macroscopic world
  • Vibrations, optical and dielectric response
  • Predicting thermo-mechanical properties from MD

• Week 5: Case studies
  • Applying the topics learned to problems of current interest