CLASSICAL OR QUANTUM?
Reading Material (Bonding)


Further readings for the first half of the course (bonding); from less to more advanced (Hayden reserve, or instructor):

- Atkins and de Paula *Physical Chemistry (7th ed)*, Freeman & Co (2002)
Goal

To provide a direct, rational connection between microscopic understanding and macroscopic properties, reinforced ‘just-in-time’ with real-life examples in lectures and labs.

Understand what holds materials together, why they organize themselves in simple or very complex structures, and how we characterize (measure !) and describe these structures.

Such understanding is central to engineering
Advanced Materials

Photos of various research removed for copyright reasons.
Bottom-up Approach: Bonding, then Structure (4 sections, 2 weeks each)

1. Atoms (quantum)
   (3.014: Light emission in CdSe nanocrystals…)

2. Molecules (bonding)
   (3.014: XPS core electron shifts…)

   (3.014: Phase transitions in piezoelectric actuators…)

4. Liquids, glasses, polymers (disorder)
   (3.014: Glass transition in acrylate polymers…)

3.012 Fundamentals of Materials Science: Bonding - Nicola Marzari (MIT, Fall 2005)
The Master Plan for Bonding (first 2 sections):

- Discrete energy states
- The nature of the periodic table
- The scanning tunneling microscope
- The chemistry of small molecules
- The structure of carbon compounds
- Hybridization and bonding
- Exclusion principle and compressibility
- The quantization of vibrations
Homework for Fri 9

• Read: 12.1, 12.2, 12.4
• Study: 12.5, 13.2, 13.3,
• Refresh: A.1 (complex numbers)
• Problem P12.10
Round Up the Usual Suspects

• Particles and electromagnetic fields

• Forces

• Dynamics
Particles and EM Fields

① NUCLEI (PROTIONS + NEUTRONS)
② ELECTRONS
③ PHOTON

INTERACTIONS
① ELECTROMAGNETIC
② GRAVITATIONAL
③ STRONG
④ WEAK
Particles and EM Fields

Electromagnetic Waves / Photons

\[ E = h\nu = h\frac{c}{\lambda} = kT \]

- \( h \) is Planck’s constant = \( 6.626 \times 10^{-34} \) J s
- \( k \) is Boltzmann’s constant = \( 1.381 \times 10^{-23} \) J/K
THE ELECTROMAGNETIC SPECTRUM

Penetrates Earth Atmosphere?

Wavelength (meters)

Radio 10^3  Microwave 10^{-2}  Infrared 10^{-5}  Visible .5 x 10^{-6}  Ultraviolet 10^{-8}  X-ray 10^{-10}  Gamma Ray 10^{-12}

About the size of...

Buildings  Humans  Honey Bee  Pinpoint  Protozoans  Molecules  Atoms  Atomic Nuclei

Frequency (Hz)

10^4  10^8  10^{12}  10^{15}  10^{16}  10^{18}  10^{20}

Temperature of bodies emitting the wavelength (K)

1 K  100 K  10,000 K  10 Million K

Examples: http:// imagers.gsfc.nasa.gov/ems/ems.html

3.012 Fundamentals of Materials Science: Bonding - Nicola Marzari (MIT, Fall 2005)
Forces

1. \( F \cdot R \)
2. GRAVITY
3. STRONG
4. WEAK
Dynamics

1. \[ F = ma \]

2. Schrödinger equation.
Standard Model of Matter

- Atoms are made by massive, point-like nuclei (protons+neutrons)
- Surrounded by tightly bound, rigid shells of core electrons
- Bound together by a glue of valence electrons (gas vs. atomic orbitals)
Material Properties From First-Principles

- Energy at our living conditions (300 K): 0.04 eV (kinetic energy of an atom in an ideal gas).

- Differences in bonding energies are within one order of magnitude of 0.29 eV (hydrogen bond).

- Binding energy of an electron to a proton (hydrogen): 13.6058 eV = 0.5 atomic units (a.u)

- Everything, from the muscles in our hands to the minerals in our bones, is made of atomic nuclei and core electrons bonded together by valence electrons (standard model of matter)
Why do we need quantum mechanics?

Structural properties (fracture in silicon)

Image of a propagating fracture in silicon, removed for copyright reasons.
Electronic, optical, magnetic properties

Courtesy of Felice Frankel. Used with permission.
It’s for real…

Cu-O bond (experiment !)

Experimental image of a Copper-Oxygen Bond in Cuprite, removed for copyright reasons.

... and it makes it to the NYTimes

Scanned image of a New York Times article removed for copyright reasons.

Mechanics of a Particle

\[ m \frac{d^2 \vec{r}}{dt^2} = F(\vec{r}) \quad \rightarrow \quad \vec{r}(t), \vec{v}(t) \]

The sum of the kinetic and potential energy (E=T+V) is conserved

Photo of two circular waves overlapping. Image removed for copyright reasons.
Description of a Wave

The wave is an excitation (a vibration): We need to know the amplitude of the excitation at every point and at every instant

\[ \Psi = \Psi(\vec{r}, t) \]
Principle of Linear Superposition

Photo courtesy of Spiralz.
Interference patterns

Wave Interactions

Constructive Interference

Destructive Interference

Resultant $A_1 + A_2$

Resultant $A_1 - A_2$

Figure by MIT OCW.
Interference in Action

Figure by MIT OCW.
Interference in Action

Photo of Irving Langmuir and Katherine Blodgett, removed for copyright reasons.

Photo of a Contax camera, with anti-reflective coating first developed by Carl Zeiss.
Photo removed for copyright reasons.

Figure by MIT OCW.
Wave-particle Duality

• *Waves have particle-like properties:*
  – *Photoelectric effect: quanta (photons) are exchanged discretely*
  – *Energy spectrum of an incandescent body looks like a gas of very hot particles*

Diagrams of the photoelectric effect and of a P-N solar cell, removed for copyright reasons.
Wave-particle Duality

- Particles have wave-like properties:
  - Quantum mechanics: Electrons in atoms are standing waves – just like the harmonics of an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926…)
When is a particle like a wave?

Wavelength \cdot momentum = \text{Planck}

\[ \lambda \cdot p = h \]

(\ h = 6.626 \times 10^{-34} \text{ J s} = 2\pi \text{ a.u.})