Advanced Prop. of Materials: What else can we do?

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Part II Topics

1. It’s a Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. From Many-Body to Single-Particle; Quantum Modeling of Molecules
4. Application of Quantum Modeling of Molecules: Solar Thermal Fuels
5. Application of Quantum Modeling of Molecules: Hydrogen Storage
6. From Atoms to Solids
7. Quantum Modeling of Solids: Basic Properties
8. Advanced Prop. of Materials: What else can we do?
10. Application of Quantum Modeling of Solids: Solar Cells Part II
11. Application of Quantum Modeling of Solids: Nanotechnology
Lesson outline

- Brief Review
- Optical properties
- Magnetic properties
- Transport properties
- Vibrational properties

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“At some point his theory becomes so abstract it can only be conveyed using interpretive dance.”

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Review: inverse lattice

Schrödinger equation  
certain symmetry  
quantum number

hydrogen atom  
spherical symmetry  
$\psi_{n,l,m}(\vec{r})$

periodic solid  
translational symmetry  
$\psi_{n,\vec{k}}(\vec{r})$

$[H, L^2] = HL^2 - L^2 H = 0$
$[H, L_z] = 0$

$[H, T] = 0$
Review: inverse lattice

\[ \psi_{\mathbf{k}}(\mathbf{r}) \longrightarrow \psi_{\mathbf{k} + \mathbf{G}}(\mathbf{r}) \]
\[ E_{\mathbf{k}} = E_{\mathbf{k} + \mathbf{G}} \]
Review: The band structure

$k$ is a continuous variable

Image by MIT OpenCourseWare.
The Fermi energy

Each band can hold:

- 2N electrons and you have \((\text{electrons per unit cell}) \times N\)
- or
- two electrons and you have \((\text{electrons per unit cell})\)
Electrical properties

Are any bands crossing the Fermi energy?
- YES: METAL
- NO: INSULATOR

Number of electrons in unit cell:
- EVEN: MAYBE INSULATOR
- ODD: FOR SURE METAL

Image by MIT OpenCourseWare.
Electrical properties

diamond: insulator
Electron Transport

\[ \frac{dv}{dt} = \frac{eE}{m} - \frac{1}{\tau} v = 0 \]

At equilibrium

\[ v = \frac{e\tau E}{m} \]

Electric current

\[ j = nev = \frac{ne^2\tau}{m} E \equiv \sigma E \]

Electrical conductivity

\[ \sigma = \frac{ne^2\tau}{m} \]
Electron Transport

Calculating $\sigma$ from band structure

$$\sigma = e^2 \tau \int \frac{dk}{4\pi^3} \left(-\frac{\partial f}{\partial E}\right) v(k)v(k)$$

Fermi function

$$v(k) = \frac{1}{\hbar} \nabla_k E(k)$$

Curvature of band structure

Image by MIT OpenCourseWare.
Simple optical properties

$E = h \nu$

Photon has almost no momentum: only vertical transitions possible. Energy conversation and momentum conversation apply.

Image by MIT OpenCourseWare.
Silicon Solar Cells Have to Be Thick ($$$)

It’s all in the band-structure!
Simple optical properties

Image in the public domain.
Magnetism

Origin of magnetism: electron spin
An electron has a magnetic moment of $\mu_B$, Bohr magneton.

$$\mu = \mu_B (n_\uparrow - n_\downarrow)$$

Spin up
$n_\uparrow$

Spin down
$n_\downarrow$
Magnetization

spin-polarized calculation:
separate density for electrons with spin

Integrated difference between up and down density gives the magnetization.
Magnetism

In real systems, the density of states needs to be considered.

\[ \mu = \mu_B \int_{E_F} dE [g_{\uparrow}(E) - g_{\downarrow}(E)] \]
Quantum Molecular Dynamics

…and let us, as nature directs, begin first with first principles. Aristotle (Poetics, I)

Use Hellmann-Feynman!

\[
\frac{\partial E_n}{\partial \lambda} = \int \psi^* \frac{\partial \hat{H}}{\partial \lambda} \psi_n d\tau
\]
Carbon Nanotube Growth
Silicon Nanocluster Growth

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Water

Henry Cavendish was the first to describe correctly the composition of water \((2 \text{ H} + 1 \text{ O})\), in 1781.

He reported his findings in terms of phlogiston (later the gas he made was proven to be hydrogen) and dephlogisticated air (later this was proven to be oxygen).

Cavendish was a pretty neat guy.

A University dropout, he also compared the conductivities of electrolytes and expressed a version of Ohm's law.

His last major work was the first measurement of Newton's gravitational constant, with the mass and density of the Earth. The accuracy of this experiment was not improved for a century.
Water

Which of the following is the correct picture for H₂O?

Cool water site: [http://www.lsbu.ac.uk/water/](http://www.lsbu.ac.uk/water/)
Classical or Quantum?

More than 50 classical potentials in use today for water.

Which one is best?

<table>
<thead>
<tr>
<th>Model</th>
<th>Dipole moment</th>
<th>Dielectric constant</th>
<th>Self diffusion, $10^{-5}$ cm$^2$/s</th>
<th>Average configurational energy, kJ mol$^{-1}$</th>
<th>Density maximum, °C</th>
<th>Expansion coefficient, $10^{-4}$ °C$^{-1}$</th>
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<tr>
<td>SSD</td>
<td>2.35 [511]</td>
<td>72 [511]</td>
<td>2.13 [511]</td>
<td>-13 [511]</td>
<td>-</td>
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<td>TIP4P-FQ</td>
<td>2.64 [197]</td>
<td>79 [197]</td>
<td>1.93 [197]</td>
<td>-41.4 [201]</td>
<td>+7 [197]</td>
<td>-</td>
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<tr>
<td>SWFLEX-AI</td>
<td>2.69 [201]</td>
<td>118 [201]</td>
<td>3.66 [201]</td>
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<td>GCPM</td>
<td>2.723 [859]</td>
<td>84.3 [859]</td>
<td>2.26 [859]</td>
<td>-44.8 [859]</td>
<td>-13 [859]</td>
<td>-</td>
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<td>SVM4-NDP</td>
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<td>-</td>
<td>-</td>
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<tr>
<td>Six-site*</td>
<td>1.89 [491]</td>
<td>33 [491]</td>
<td>-</td>
<td>-14 [491]</td>
<td>2.4 [491]</td>
<td>-</td>
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<tr>
<td>Expt</td>
<td>2.95</td>
<td>78.4</td>
<td>2.30</td>
<td>+3.984</td>
<td>2.53</td>
<td>-</td>
</tr>
</tbody>
</table>

All the data is at 25°C and 1 atm, except * at 20°C and ** at 27°C.

Courtesy of Martin Chaplin, London South Bank University. Used with permission.
Mg++ in Water

Important Differences!

Courtesy of Martin Chaplin, London South Bank University. Used with permission.
Vibrational properties

lattice vibrations are called: phonons

What is the frequency of this vibration?
Vibrational properties

animated phonons on the web

http://dept.kent.edu/projects/ksuviz/leeviz/phonon/phonon.html

• sound in solids determined by acoustical phonons (shock waves)

• some optical properties related to optical phonons

• heat capacity and transport related to phonons
Summary of properties

structural properties

electrical properties

optical properties

magnetic properties

vibrational properties

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Literature

• Charles Kittel, Introduction to Solid State Physics

• Ashcroft and Mermin, Solid State Physics

• wikipedia, “phonons”, “lattice vibrations”, ...

• solar PV: tons of web sites, e.g.: http://pveducation.org/pvcdrom