1.021, 3.021, 10.333, 22.00 : Introduction to Modeling and Simulation : Spring 2011

Part II – Quantum Mechanical Methods : Lecture 6

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

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Part II Outline

theory & practice

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. From Atoms to Solids
5. Quantum Modeling of Solids: Basic Properties
6. Advanced Prop. of Materials: What else can we do?

example applications

7. Nanotechnology
8. Solar Photovoltaics: Converting Photons into Electrons
9. Thermoelectrics: Converting Heat into Electricity
10. Solar Fuels: Pushing Electrons up a Hill
11. Hydrogen Storage: the Strength of Weak Interactions
12. Review

Lesson outline

- Review some stuff
- Optical properties
- Magnetic properties
- Transport properties
- Vibrational properties

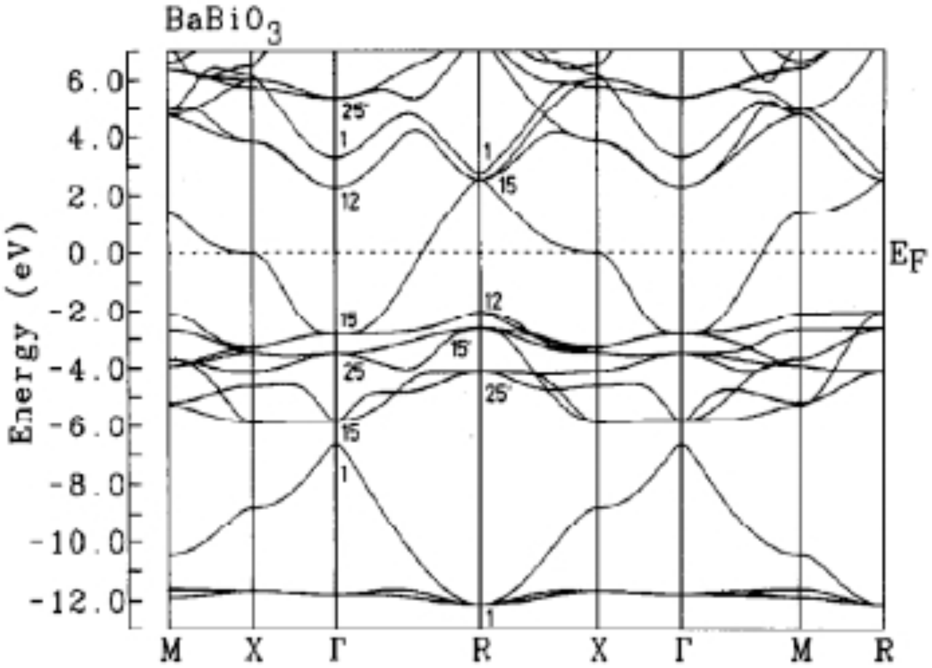
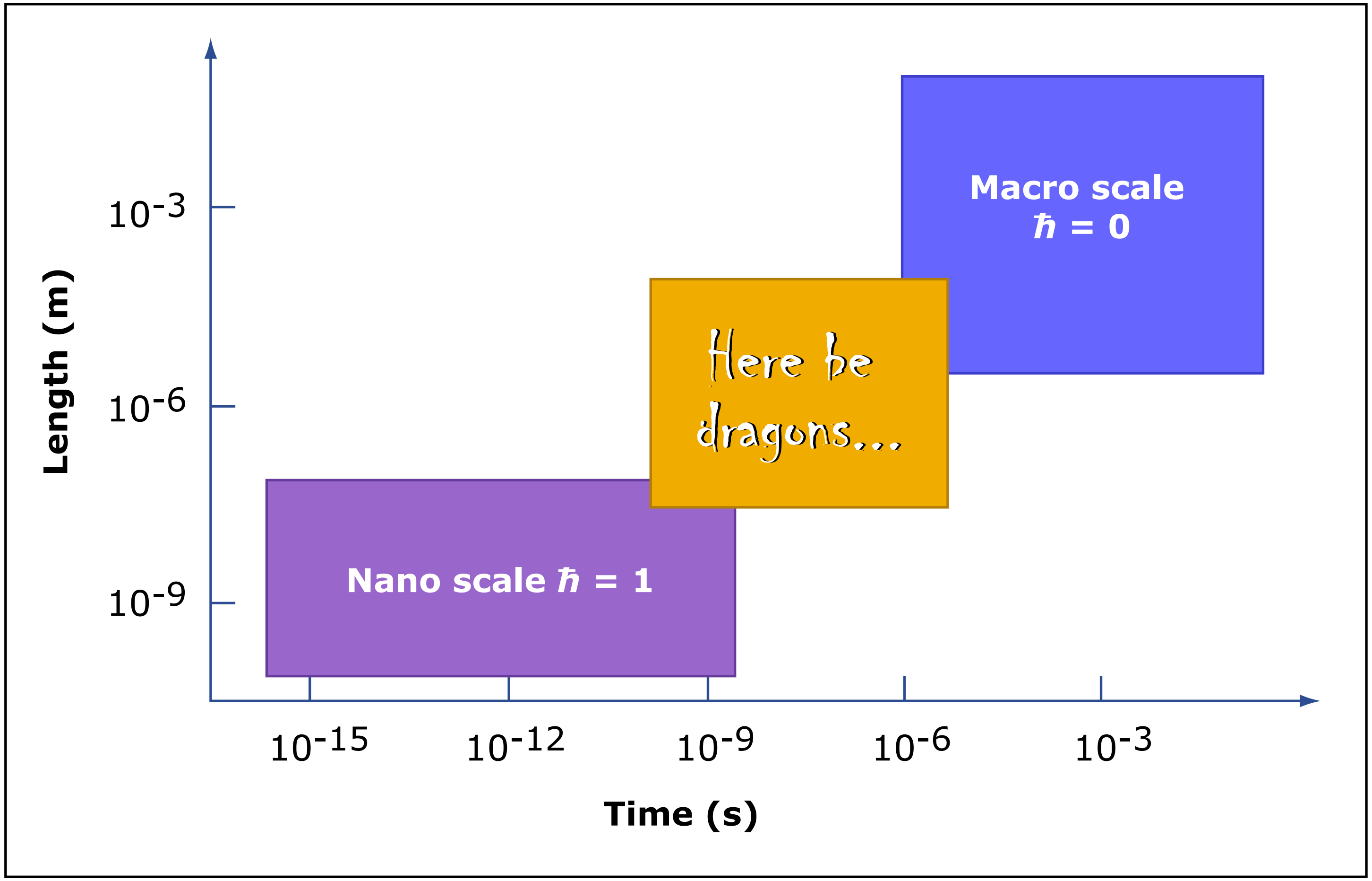


Fig. 3. Self-consistent APW energy band structure for $BaBiO_3$.

The Saga of Length and Time Scales



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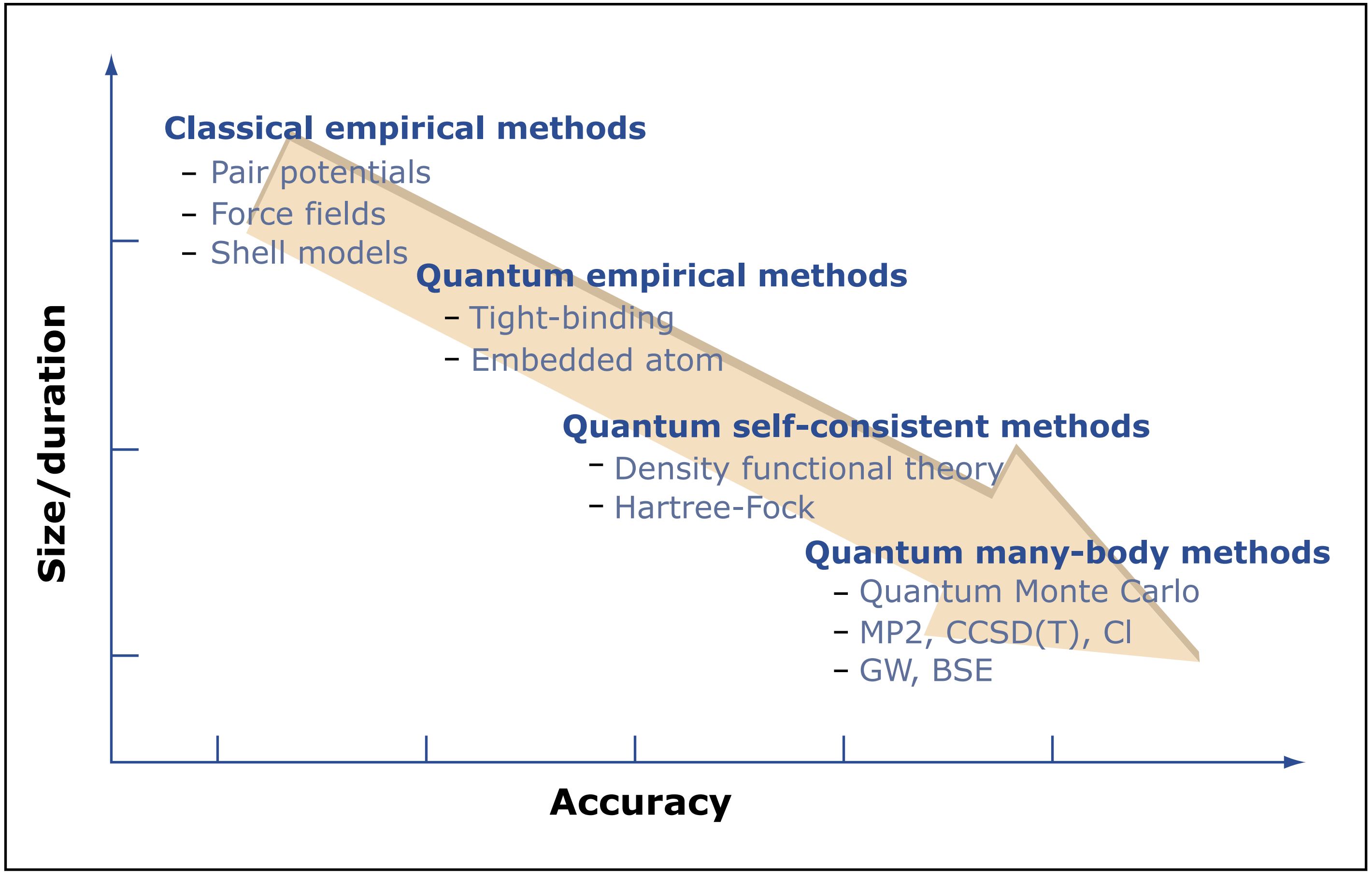
Size vs. Accuracy



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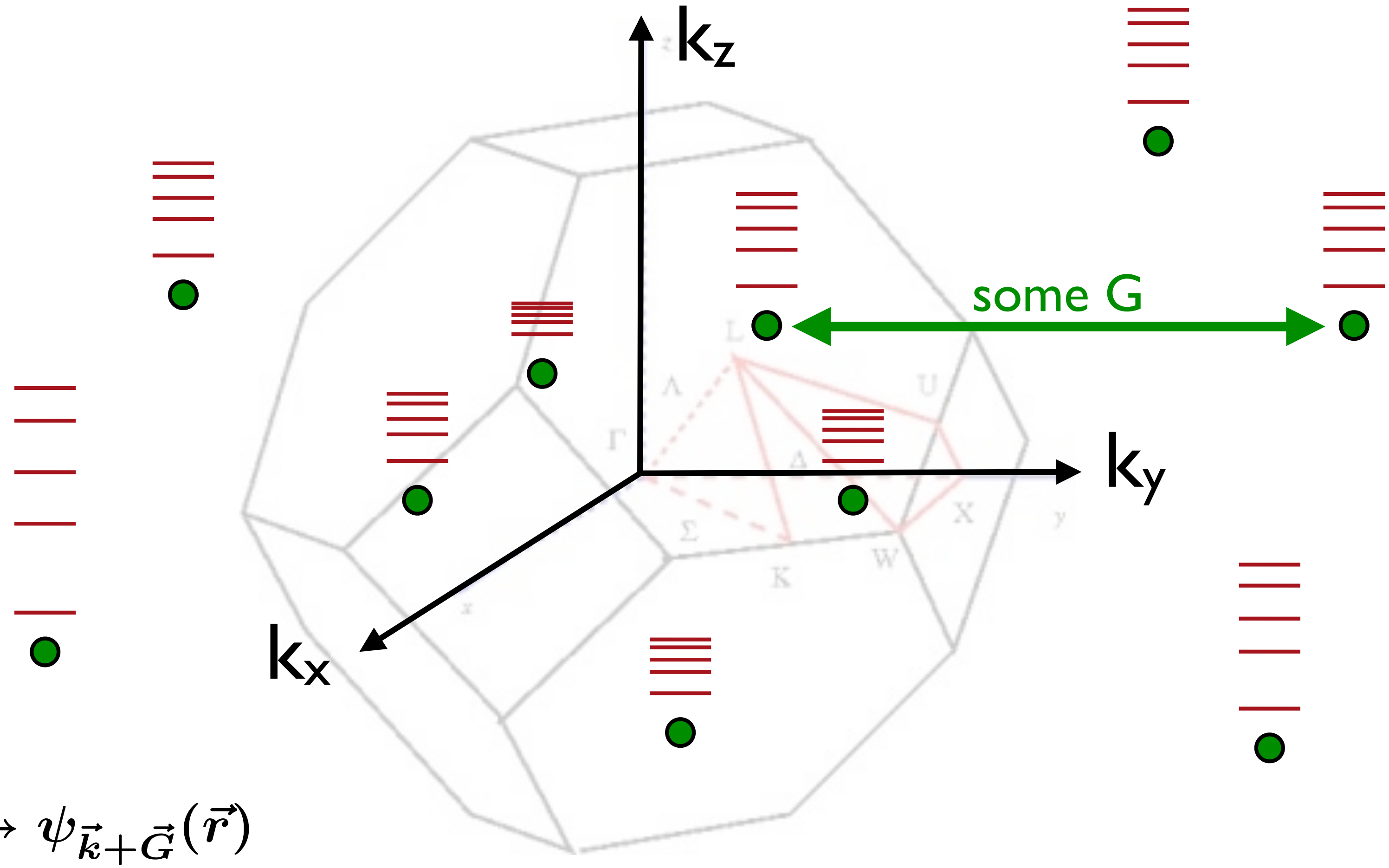
Review: inverse lattice

Schrödinger equation	certain symmetry	quantum number
hydrogen atom	spherical symmetry $[H, L^2] = HL^2 - L^2H = 0$ $[H, L_z] = 0$	$\psi_{n,l,m}(\vec{r})$
periodic solid	translational symmetry $[H, T] = 0$	$\psi_{n,\vec{k}}(\vec{r})$

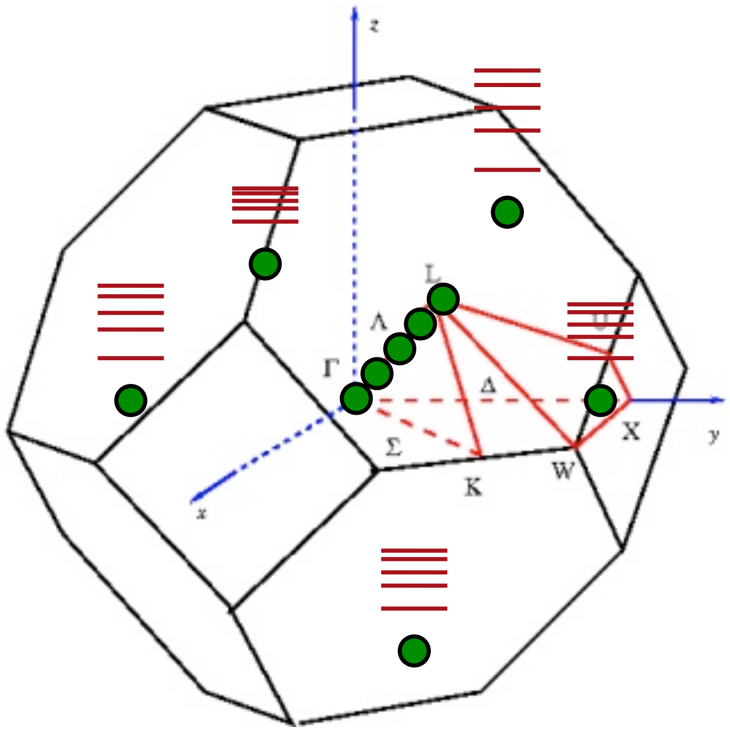
Review: inverse lattice



$$\psi_{\vec{k}}(\vec{r}) \longrightarrow \psi_{\vec{k}+\vec{G}}(\vec{r})$$

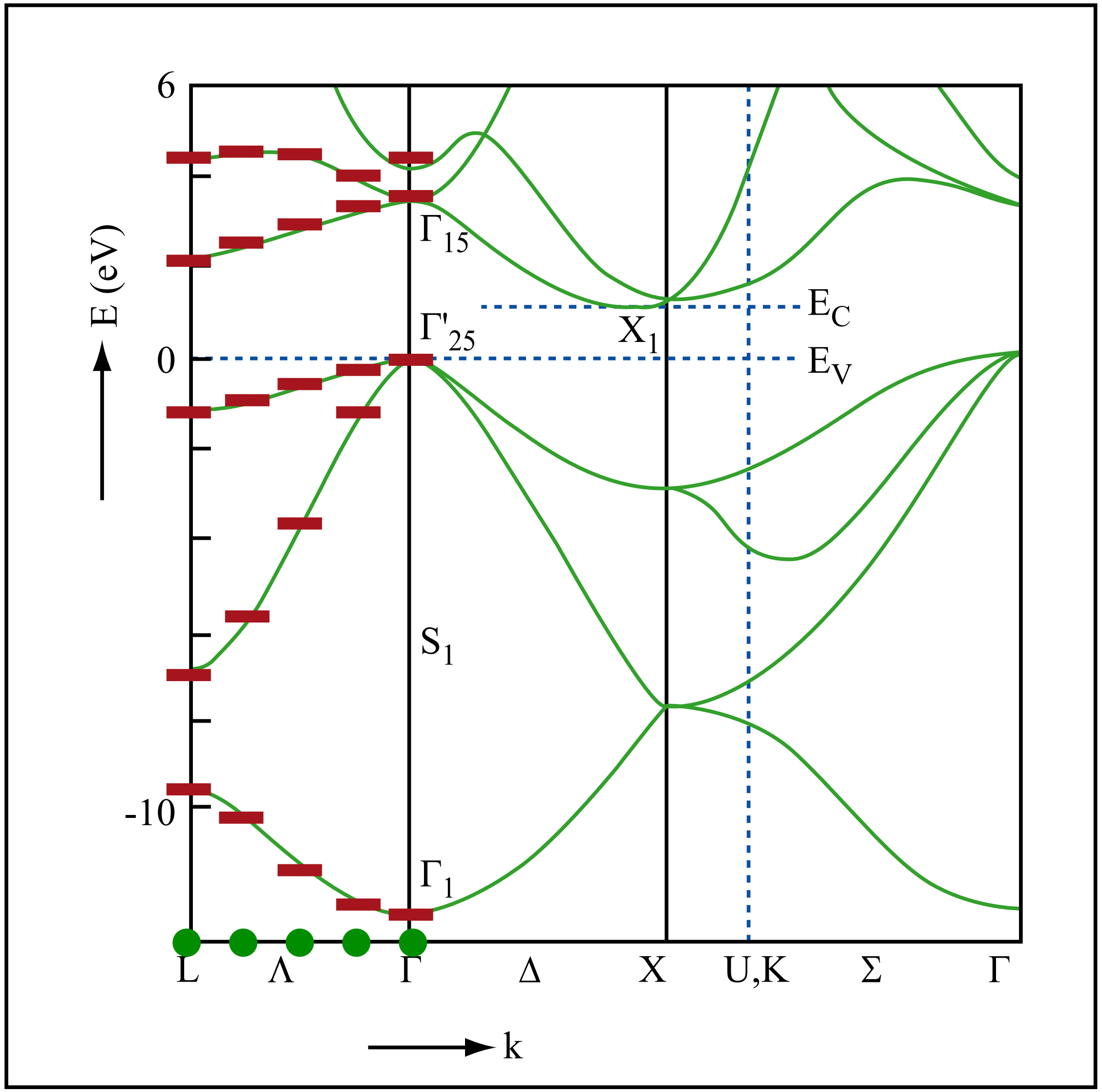
$$E_{\vec{k}} = E_{\vec{k}+\vec{G}}$$

Review: The band structure



k is a continuous variable

Silicon



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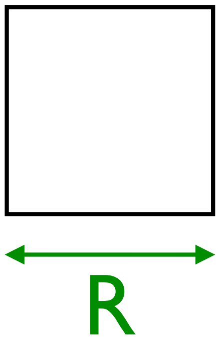
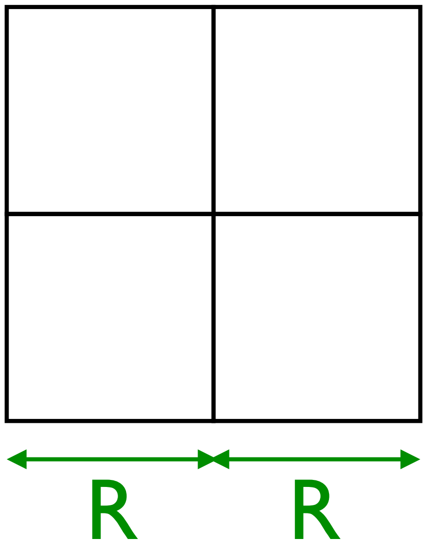
Review: inverse lattice



$$\psi_0(\vec{r} + \vec{R}) = \psi_0(\vec{r})$$

periodic over unit cell

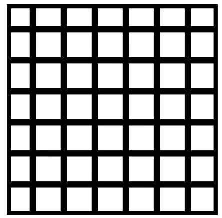


$$\psi_{\vec{G}/2}(\vec{r} + 2\vec{R}) = \psi_{\vec{G}/2}(\vec{r})$$

periodic over larger domain

Review: inverse lattice

choose certain
k-mesh e.g. 8x8x8
N=512



number of
k-points (N)

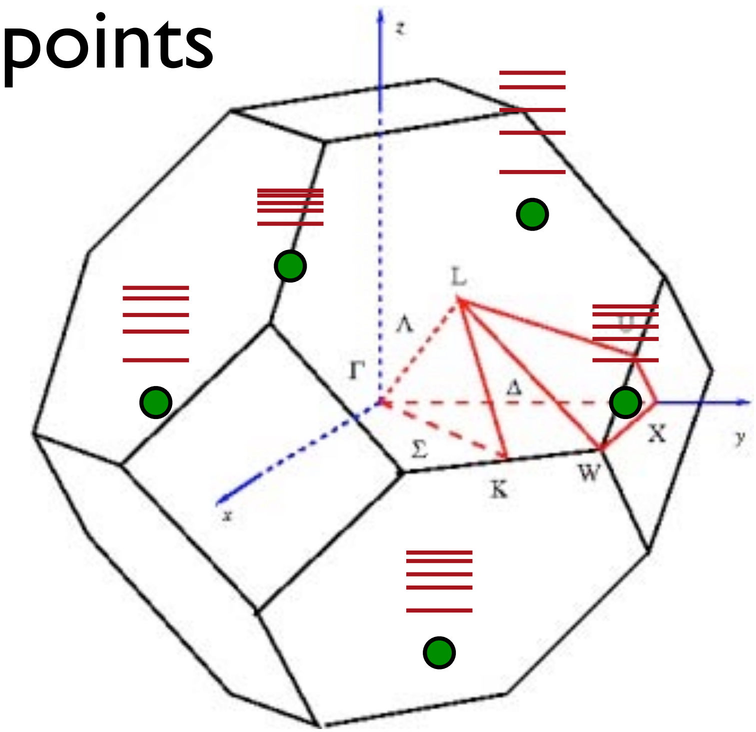
unit cells in
the periodic
domain (N)

Review: inverse lattice

Distribute all electrons over the lowest states.

N k-points

You have
(electrons per unit cell)*N
electrons to distribute!

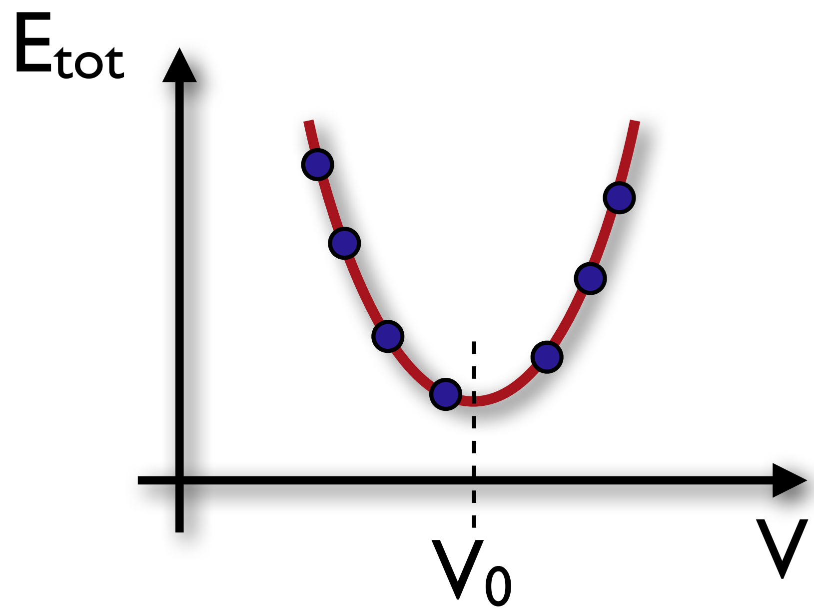


Let’s Do A Few Simulations

http://www.nanohub.org

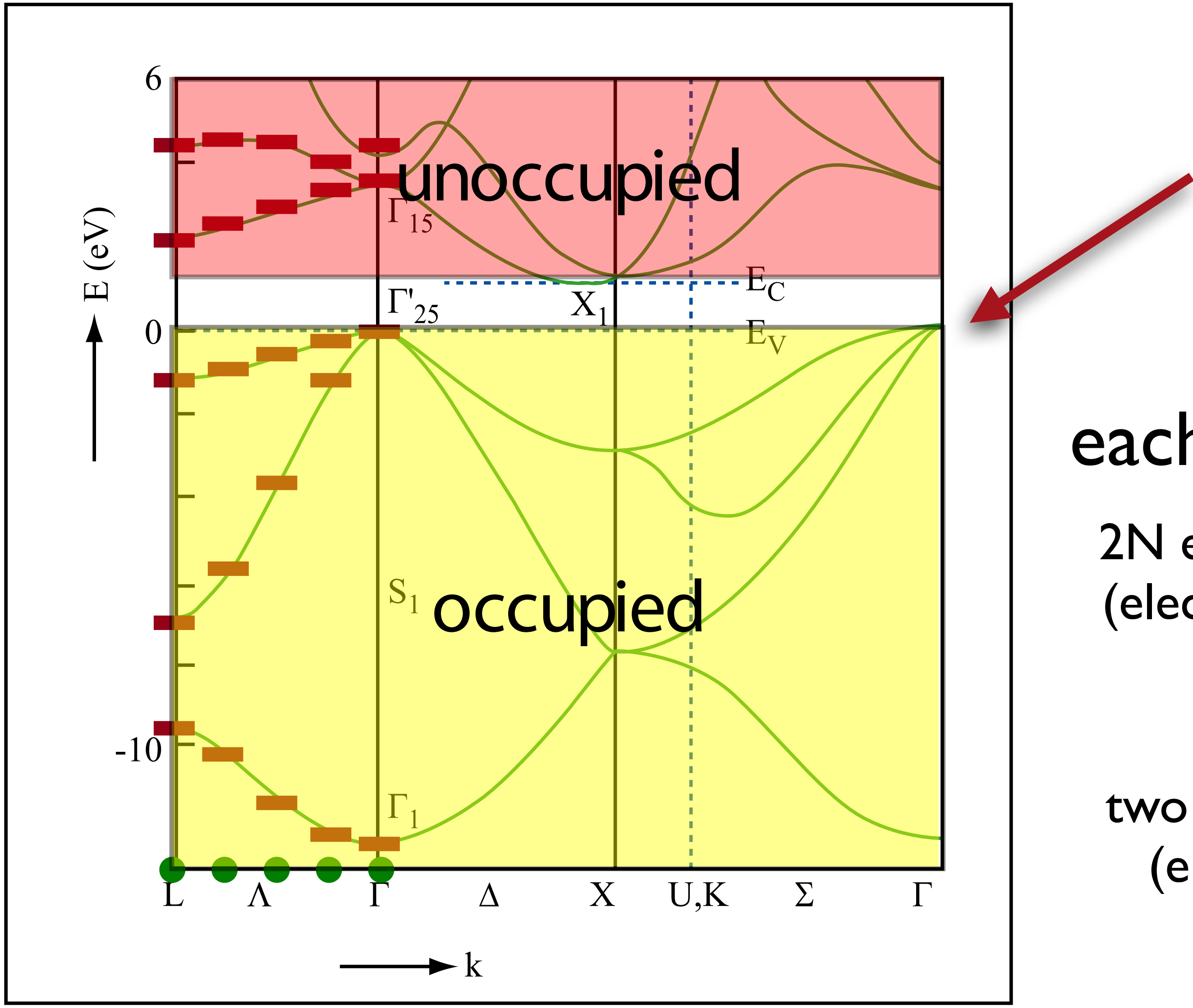
Structural properties

finding the stress/pressure and the bulk modulus



$$p = -\frac{\partial E}{\partial V} \qquad \sigma_{\mathrm{bulk}} = -V\frac{\partial p}{\partial V} = V\frac{\partial^2 E}{\partial V^2}$$

The Fermi energy



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each band can hold:

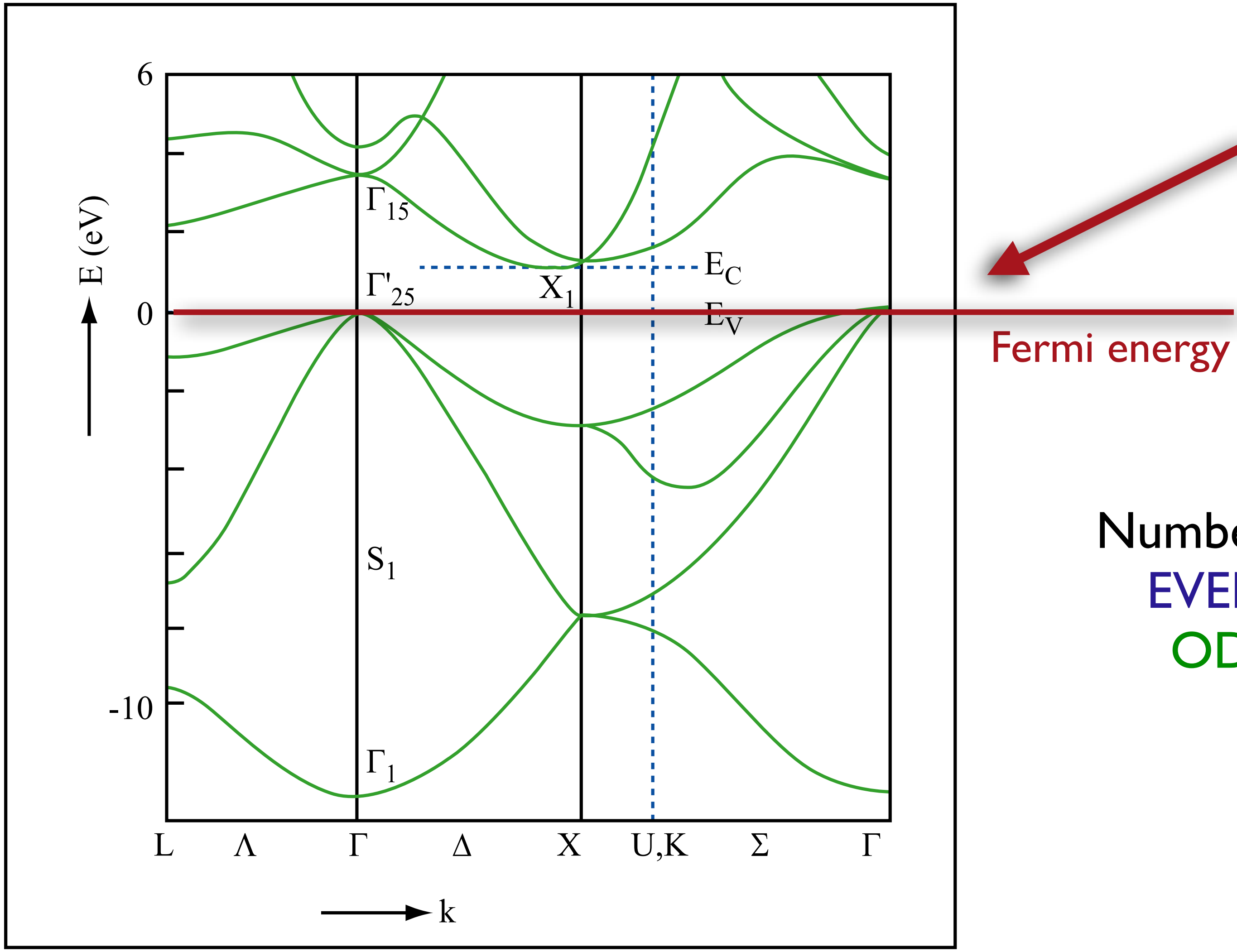
2N electrons and you have (electrons per unit cell)*N

or

two electrons and you have (electrons per unit cell)

Electrical properties

silicon



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Are any bands crossing the Fermi energy?

YES: METAL

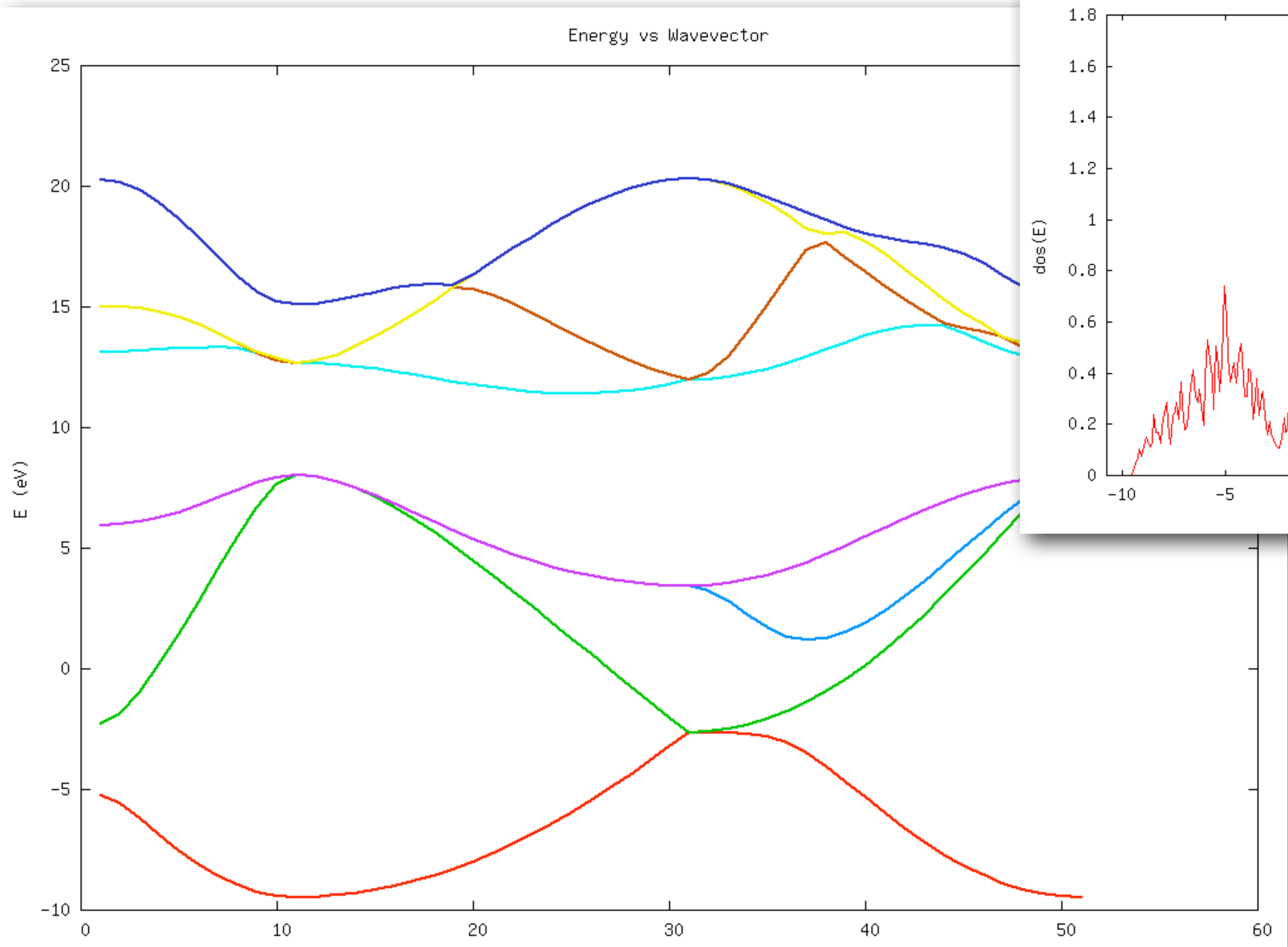
NO: INSULATOR

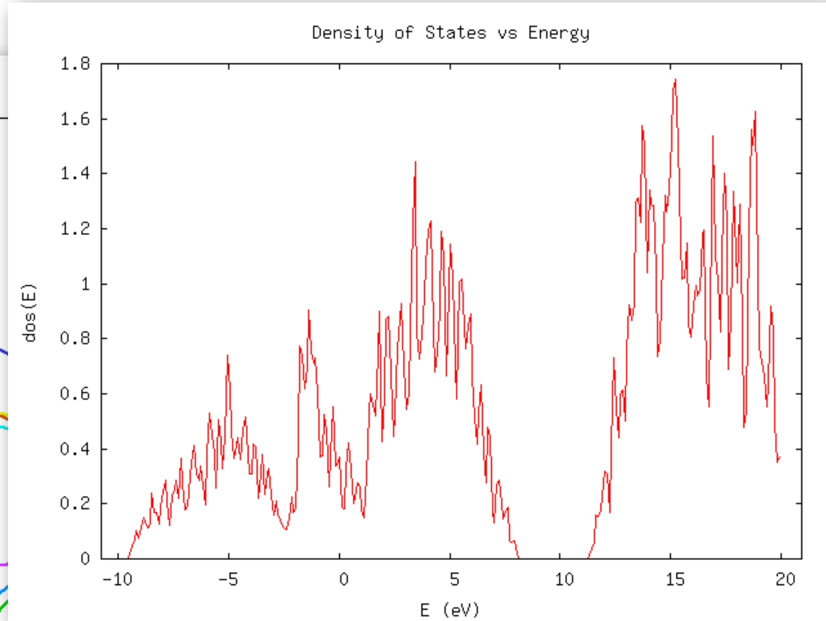
Number of electrons in unit cell:

EVEN: MAYBE INSULATOR

ODD: FOR SURE METAL

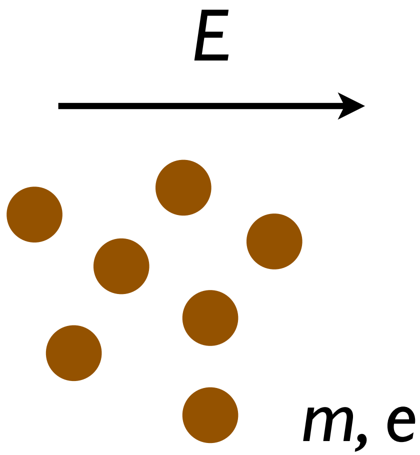
Electrical properties





diamond:
insulator

Electron Transport



E-field

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

At equilibrium

$$v = \frac{e\tau E}{m}$$

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

Electric current

Electrical conductivity

$$\sigma = \frac{ne^2\tau}{m}$$

Electron Transport

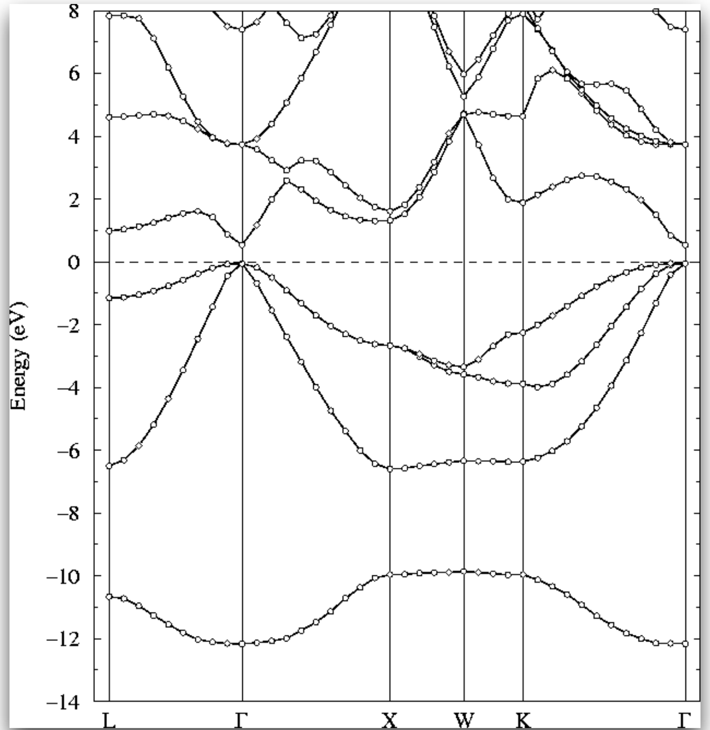
Calculating σ from band structure

Fermi function

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

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

Curvature of band structure



Simple optical properties

E=hv

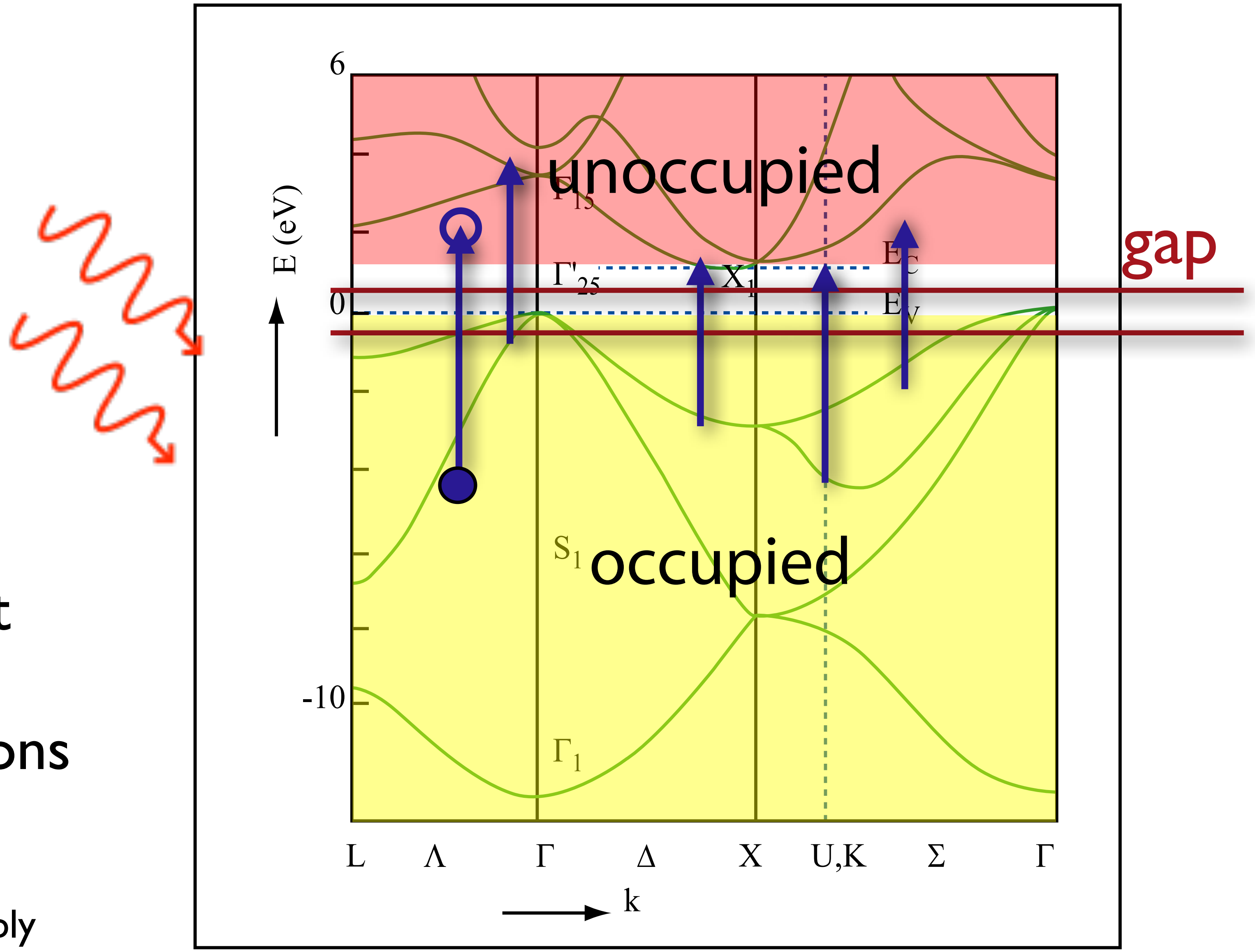


Image by MIT OpenCourseWare.

photon has almost no momentum: only vertical transitions possible

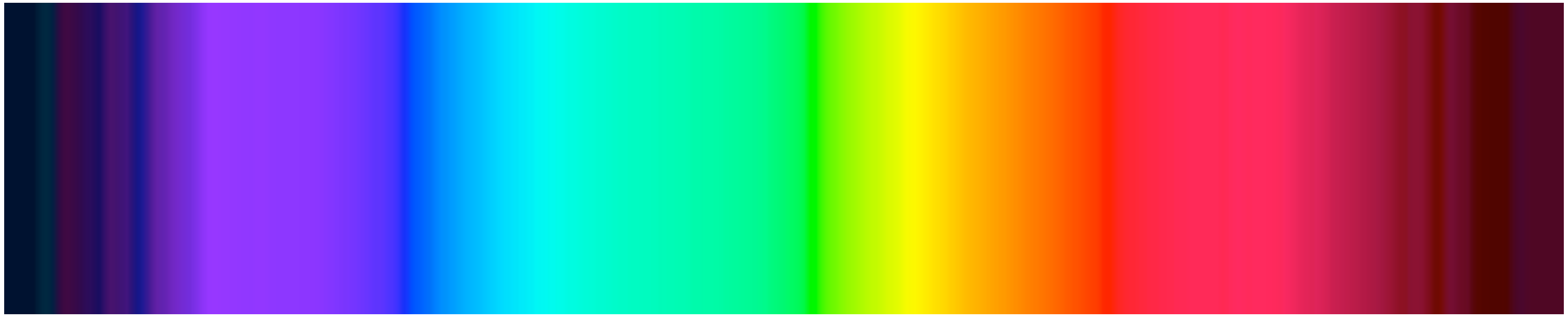
energy conversation and momentum conversation apply

Silicon Solar Cells Have to Be Thick ($$$)

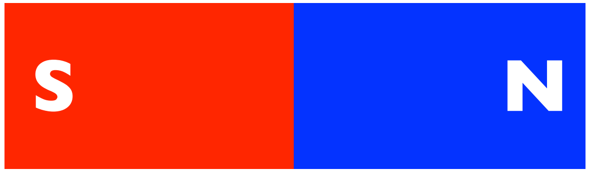
It's all in the band-structure!

Please see graph at http://www.tf.uni-kiel.de/matwis/amat/semi_en/kap_2/illustr/si_banddiagram.gif.

Simple optical properties



Magnetism



Origin of magnetism: electron spin

An electron has a magnetic moment of μ_B, Bohr magneton.

Spin up $n_\uparrow$

Spin down $n_\downarrow$

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

Magnetization

spin-polarized calculation:
separate density for electrons with spin

up

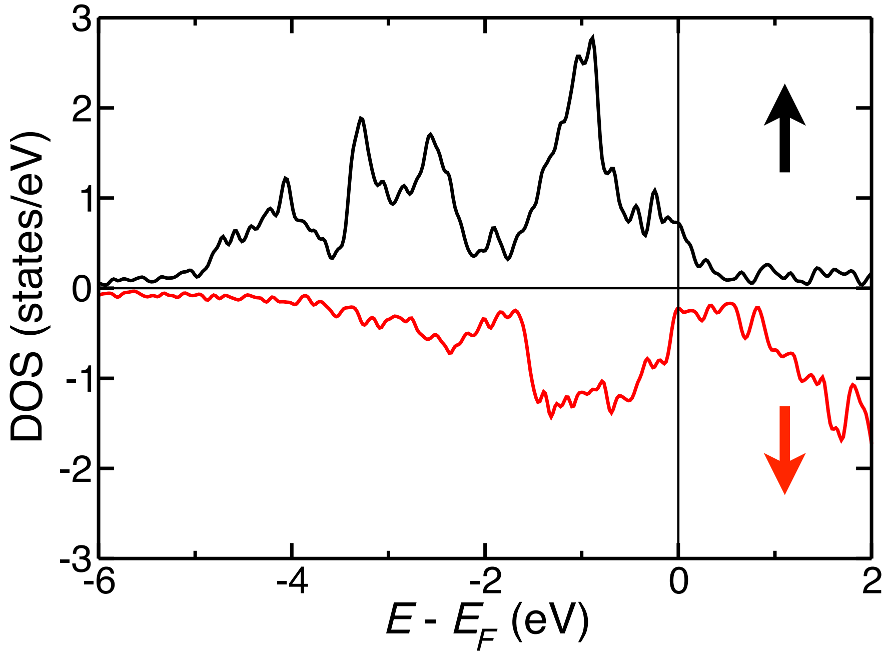
down

Integrated difference between up and down density gives the magnetization.

Magnetism

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

bcc Fe



$$\mu = \mu_B \int^{E_F} dE[g_{\uparrow}(E) - g_{\downarrow}(E)]$$

Quantum Molecular Dynamics

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

F=ma

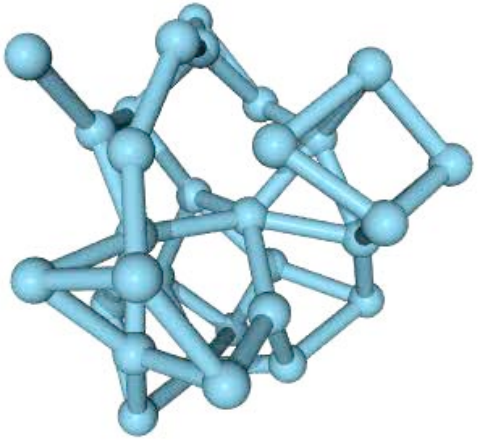
Use Hellmann-Feynman!

$$\frac{\partial E_n}{\partial \lambda} = \int \psi_n^* \frac{\partial \hat{H}}{\partial \lambda} \psi_n d\tau$$

Carbon Nanotube Growth

Carbon nanotube growth: http://en.wikipedia.org/wiki/Carbon_nanotube.

Silicon Nanocluster Growth



Water

Henry Cavendish was the first to describe correctly the composition of water (2 H + 1 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).

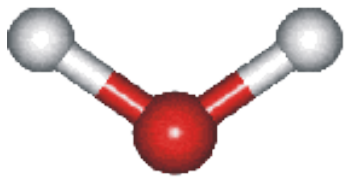
Cavendish was a pretty neat guy.

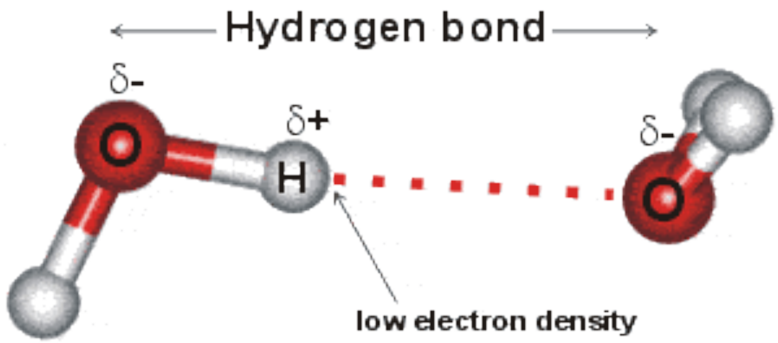
A University dropout, he also compared the conductivities of electrolytes and expressed a version of Ohm's law.

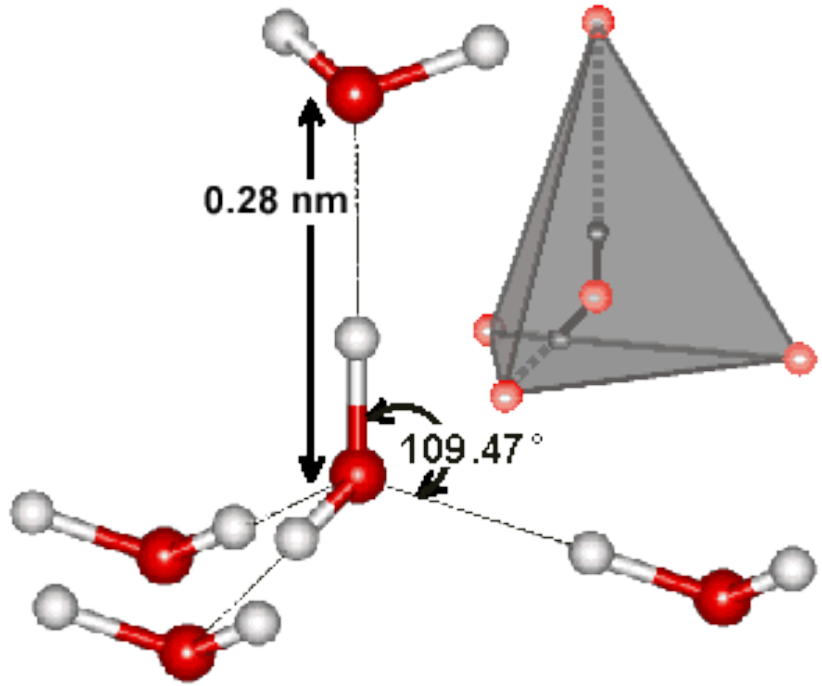
His last major work was the first measurement of Newton's gravitational constant, with the mass and density of the Earth. The accuracy of this experiment was not improved for a century.

Water

Which of the following is the correct picture for H_2O?







Cool water site: http://www.lsbu.ac.uk/water/

Classical or Quantum?

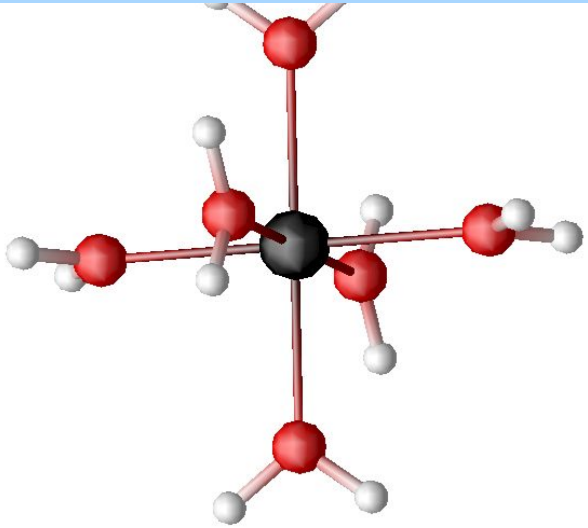
Please see the second table at
http://www.science.oregonstate.edu/~hetheriw/astro/rt/info/water/water_models.html.

More than 50 classical potentials in use today for water.

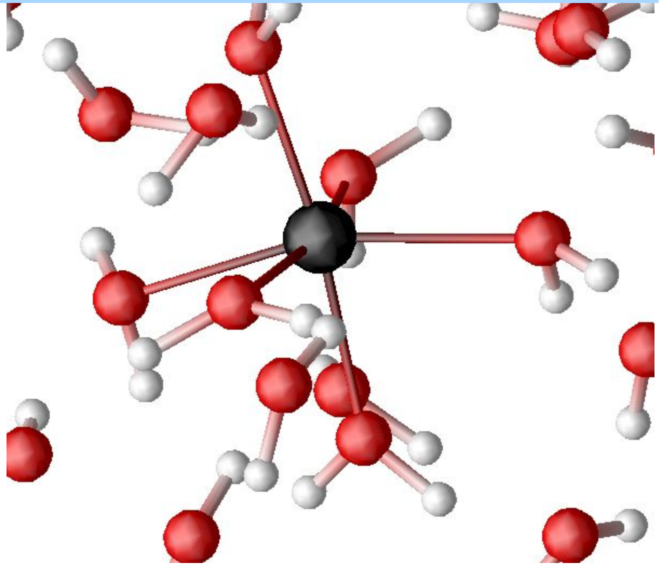
Which one is best?

Mg++ in Water

classical



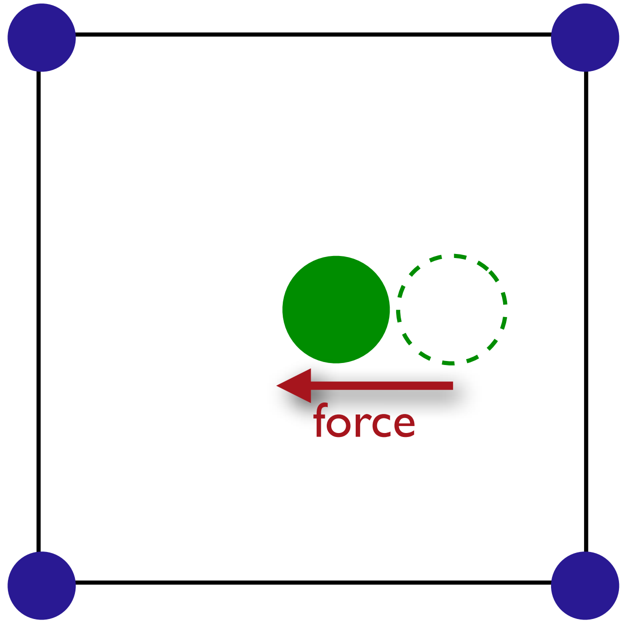
quantum



Important Differences!

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

Literature

- Charles Kittel, Introduction to Solid State Physics
- Ashcroft and Mermin, Solid State Physics
- wikipedia, "phonons", "lattice vibrations", ...