1.021, 3.021, 10.333, 22.00 : Introduction to Modeling and Simulation : Spring 2012

Part II – Quantum Mechanical Methods : Lecture 8

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

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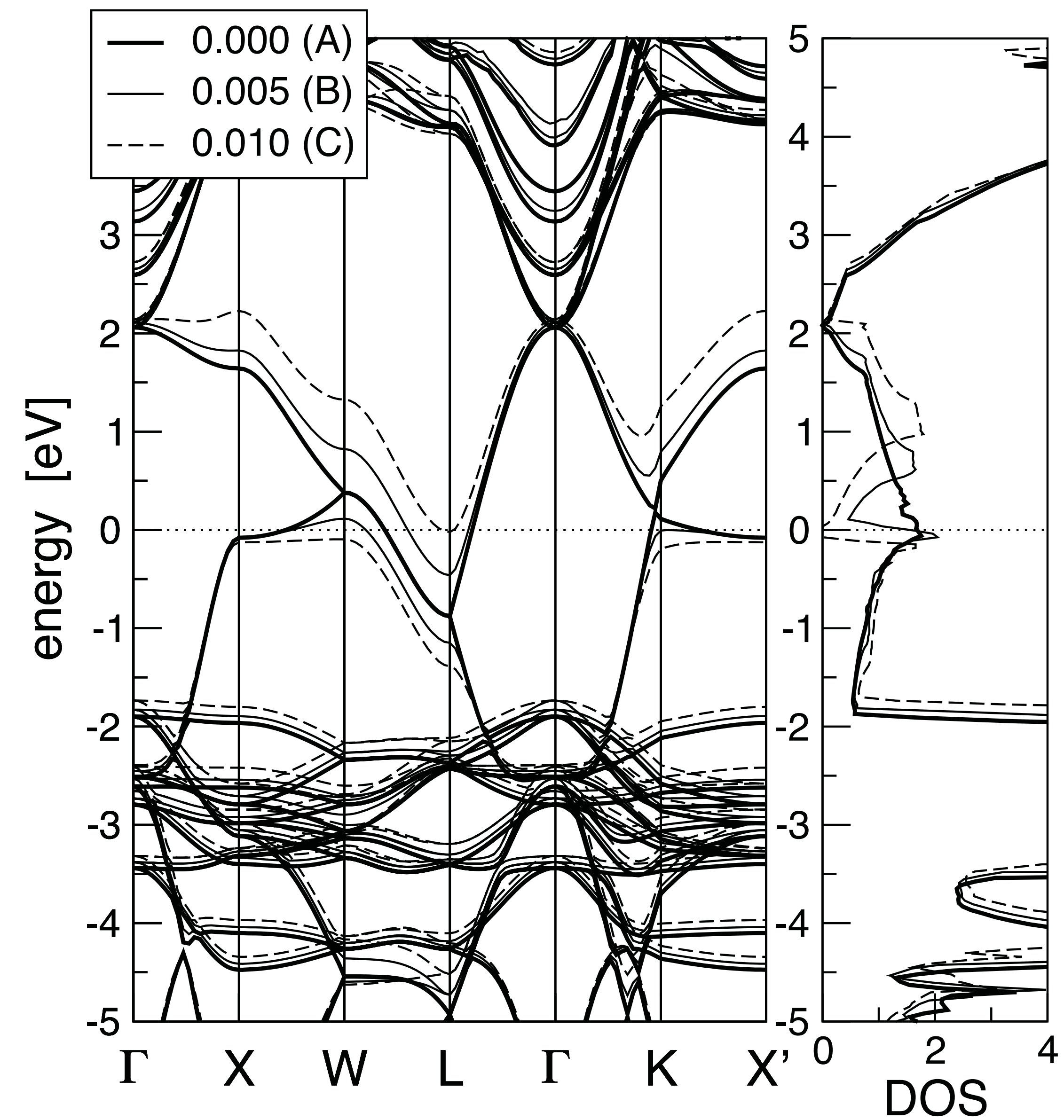
Part II Topics

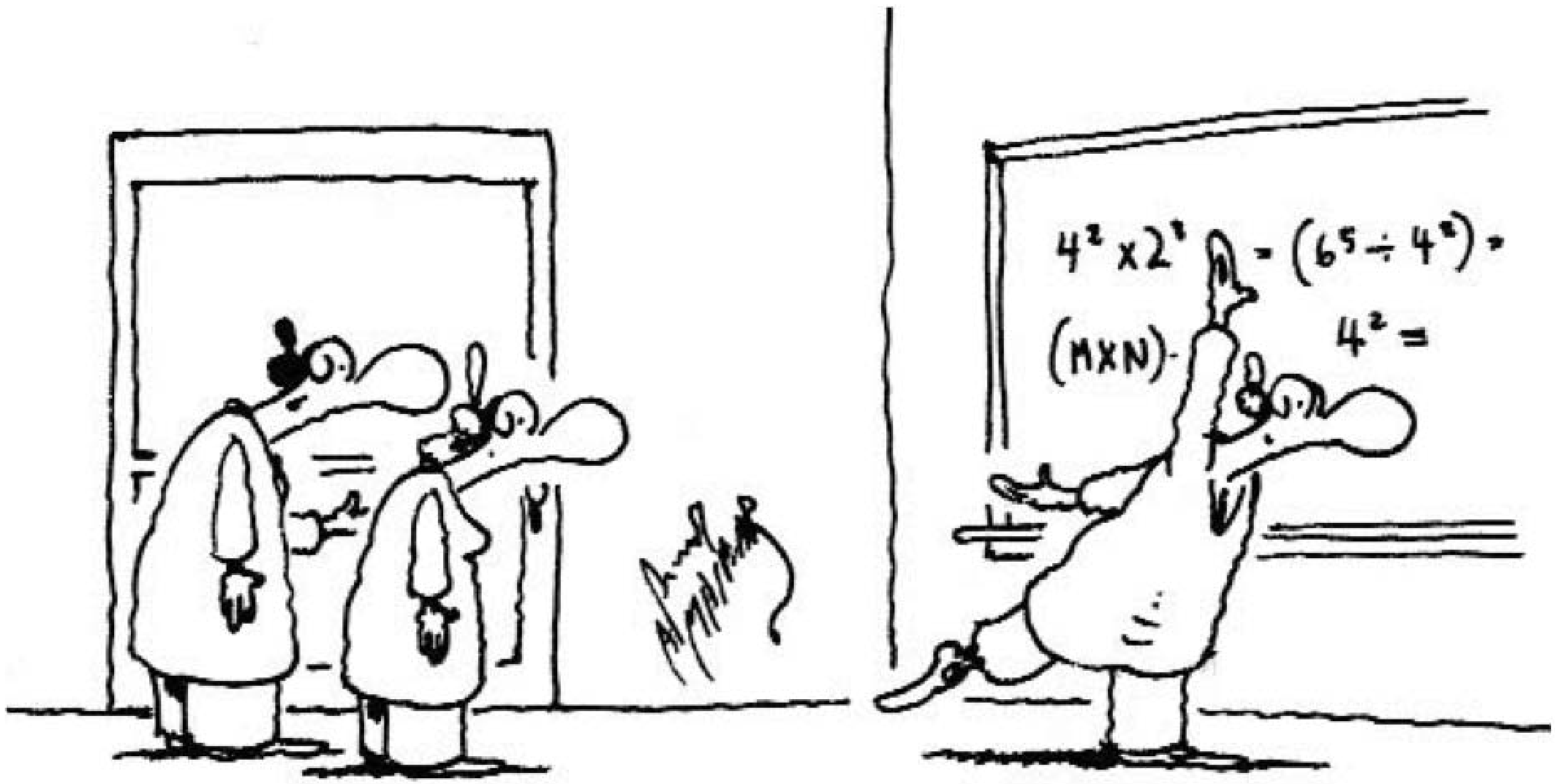
1. It's a Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. From Many-Body to Single-Particle; Quantum Modeling of Molecules
4. Application of Quantum Modeling of Molecules: Solar Thermal Fuels
5. Application of Quantum Modeling of Molecules: Hydrogen Storage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



Keeping Relevant



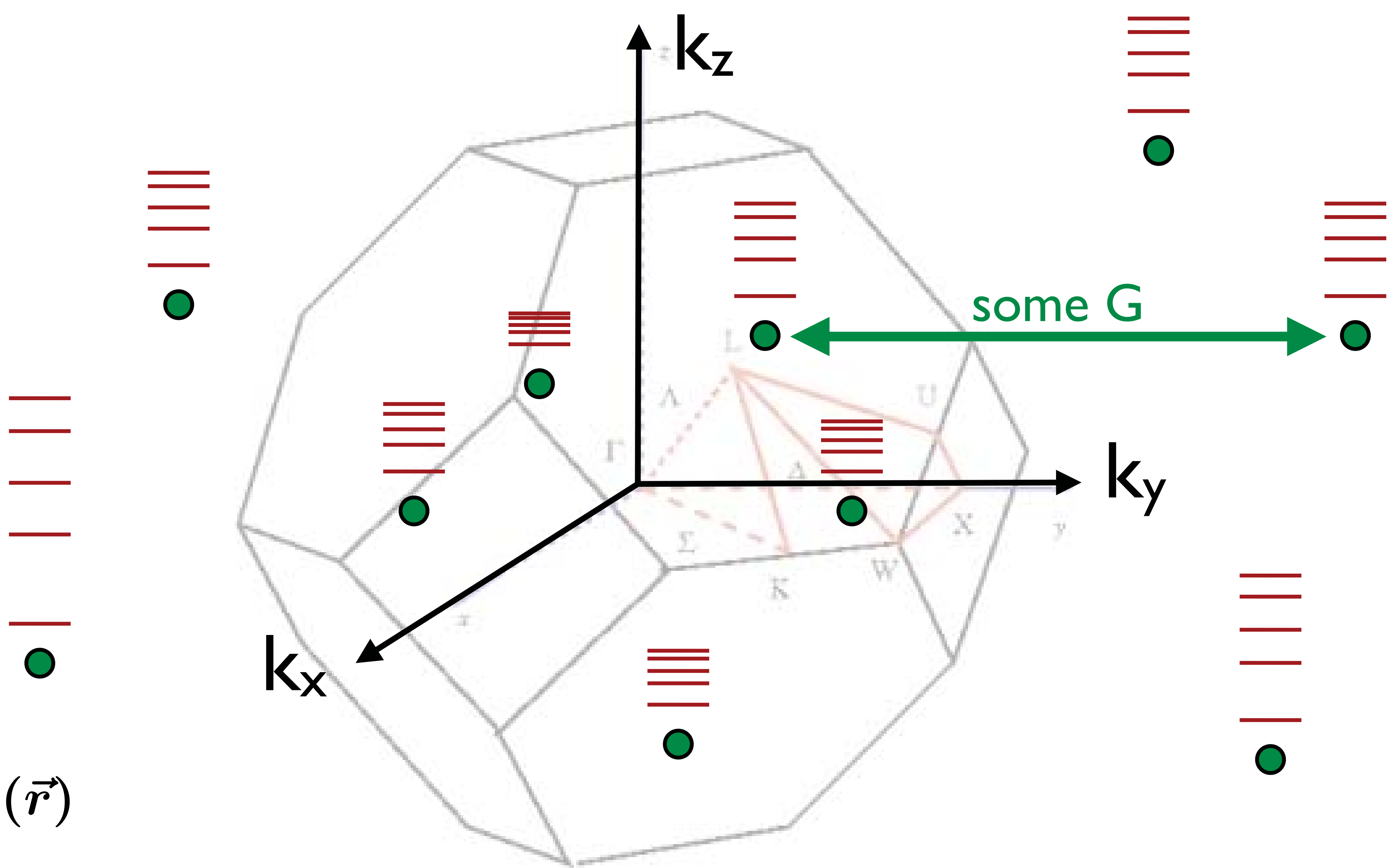
"At some point his theory becomes so abstract it can only be conveyed using interpretive dance."

May/June 2001, Bulletin of the Atomic Scientists

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 $[H, T] = 0$	→	$\psi_{n,\vec{k}}(\vec{r})$

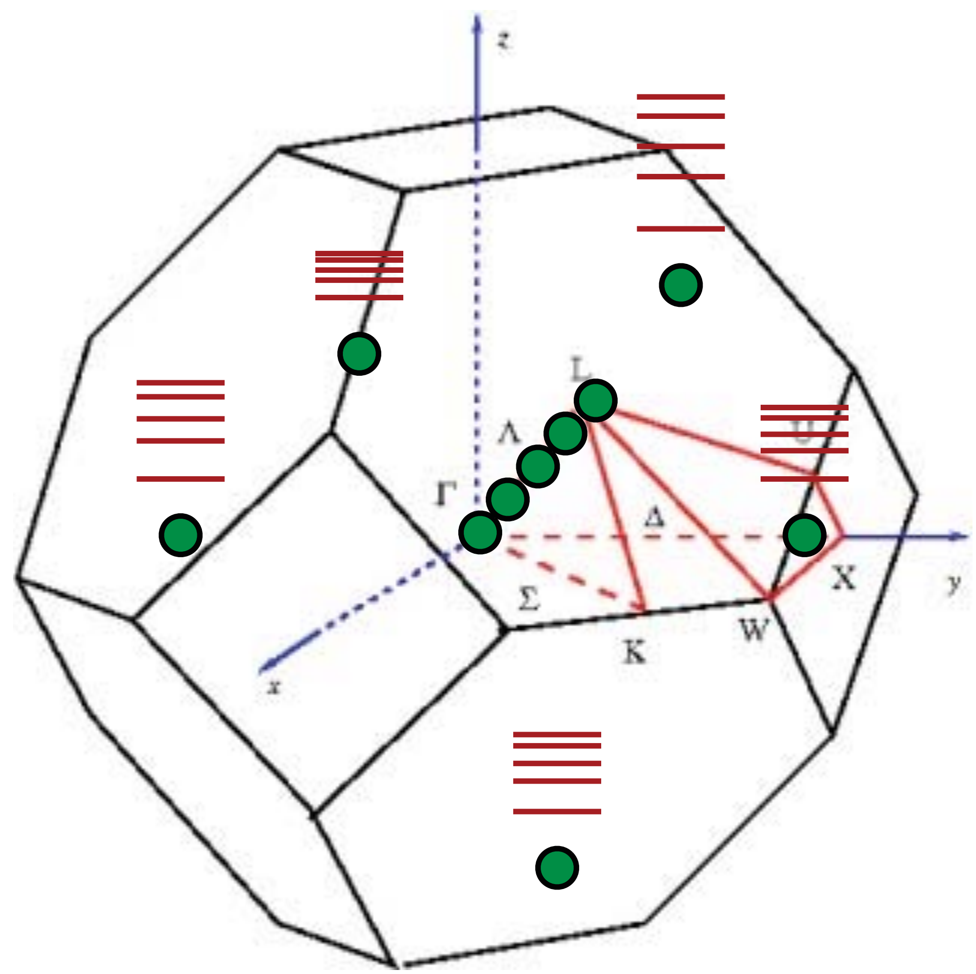
Review: inverse lattice



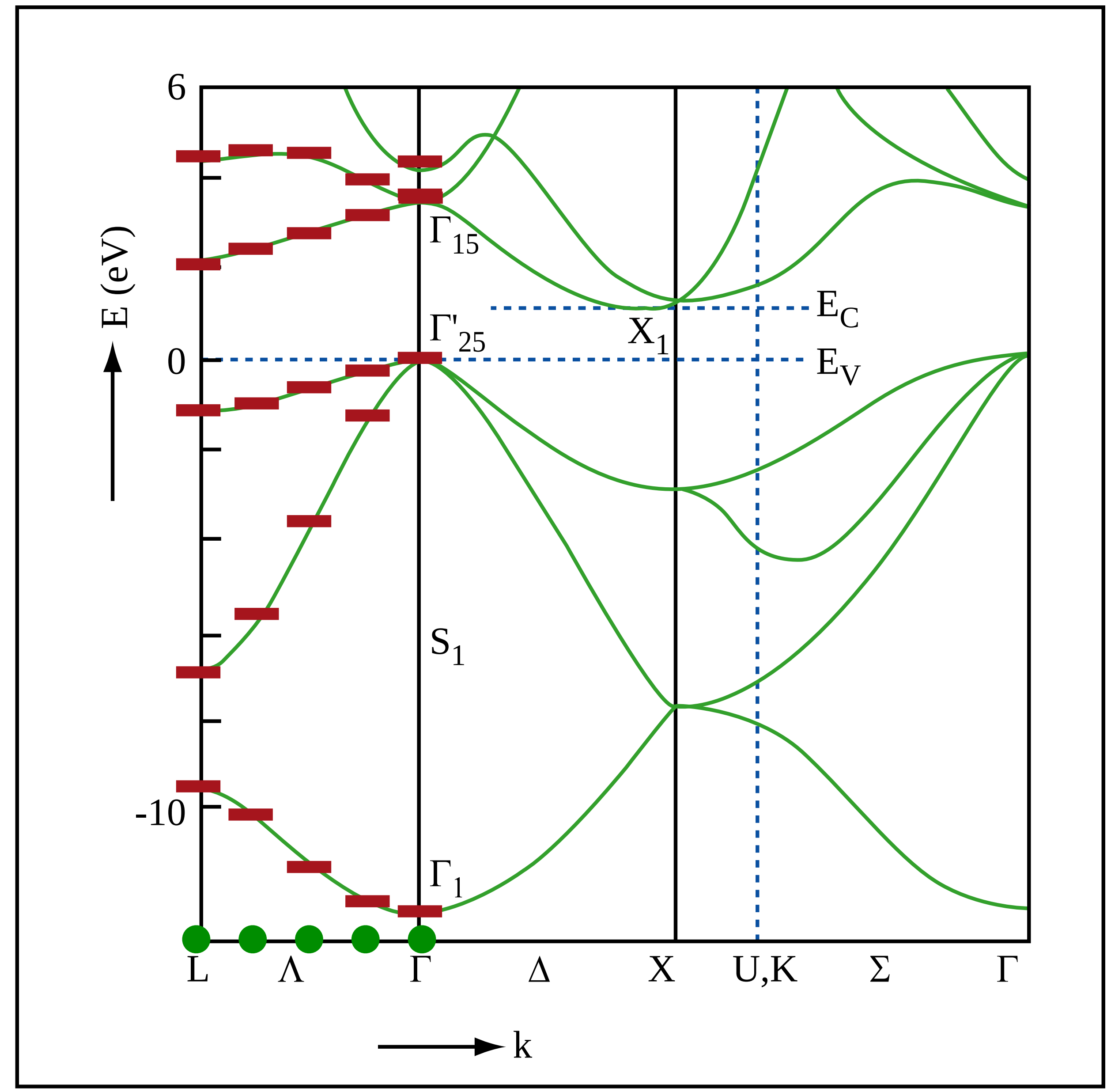
$$\psi_{\vec{k}}(\vec{r}) \longrightarrow \psi_{\vec{k}+\vec{G}}(\vec{r})$$

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

Review: The band structure



k is a continuous variable



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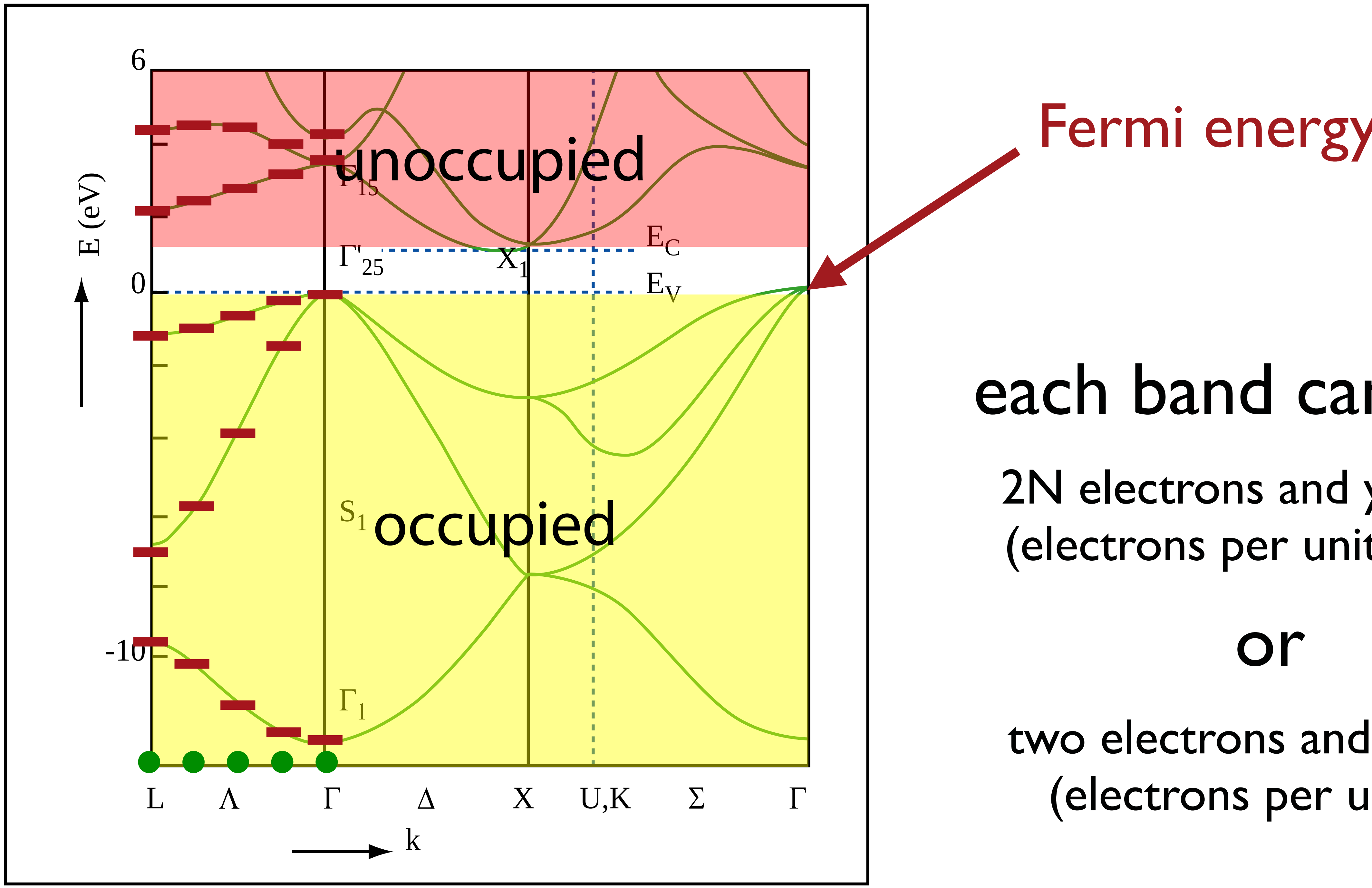
The Fermi energy



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each band can hold:

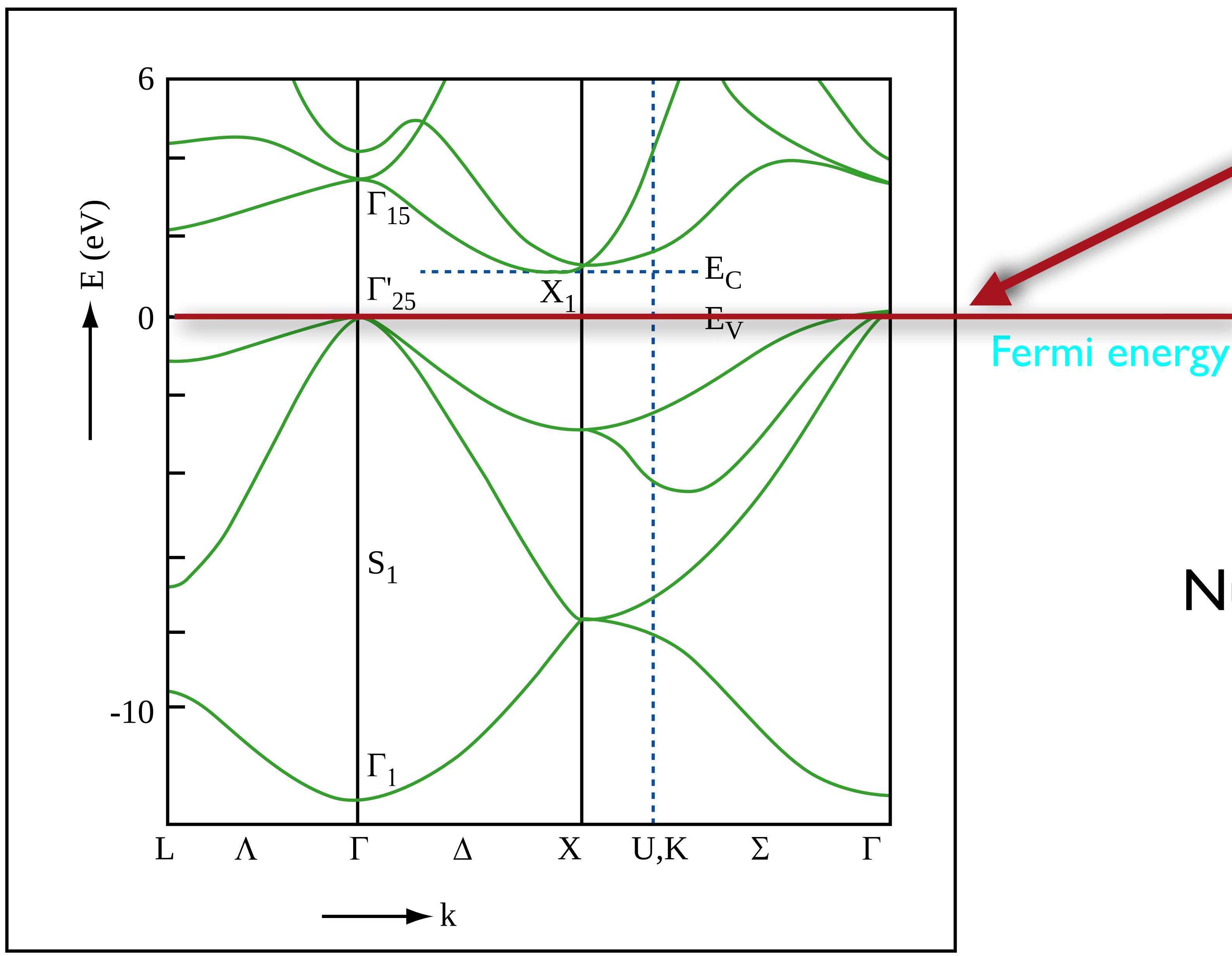
2N electrons and you have (electrons per unit cell)*N

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

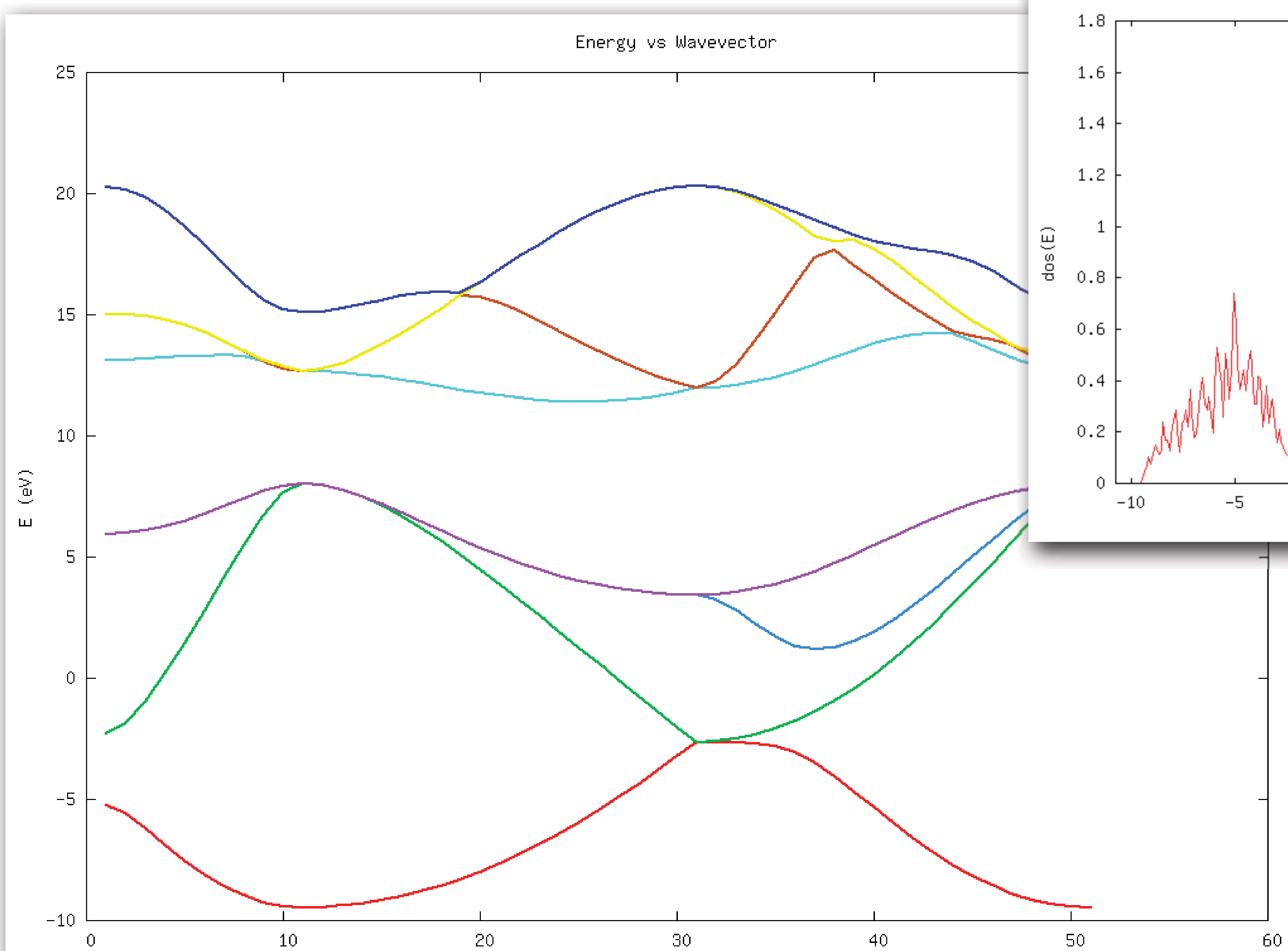
NO: INSULATOR

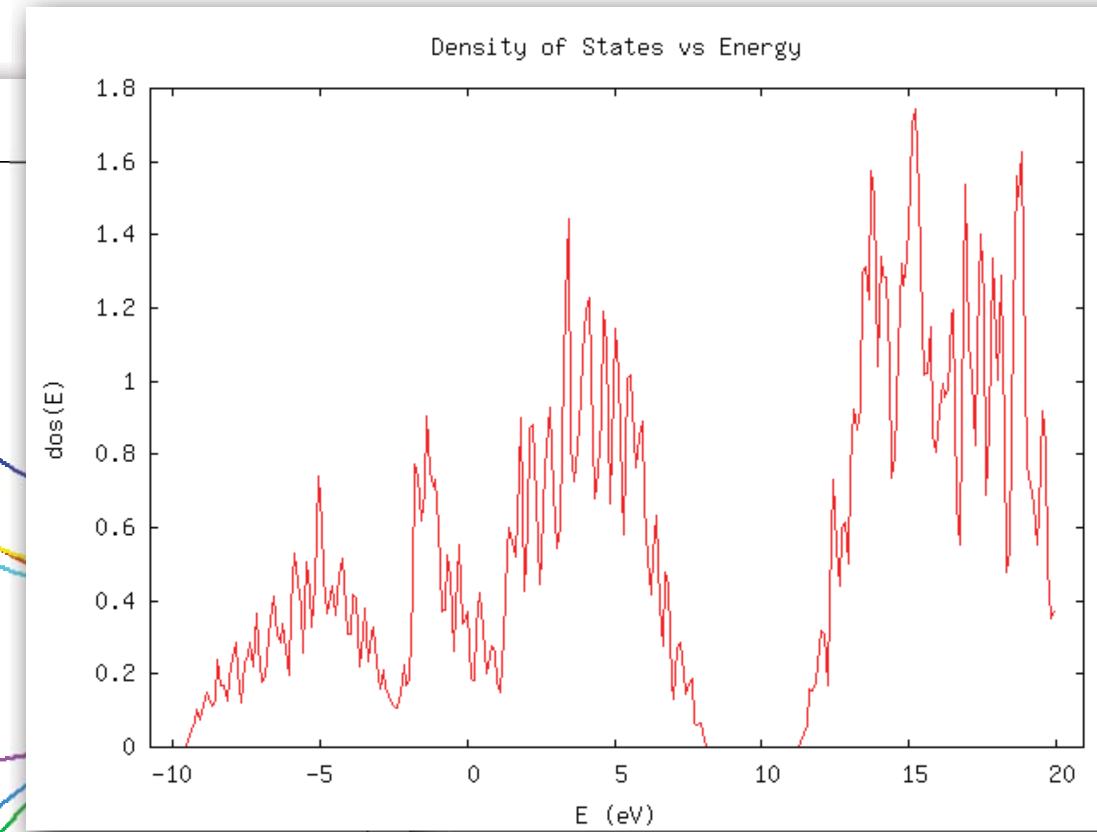
Number of electrons in unit cell:

EVEN: MAYBE INSULATOR

ODD: FOR SURE METAL

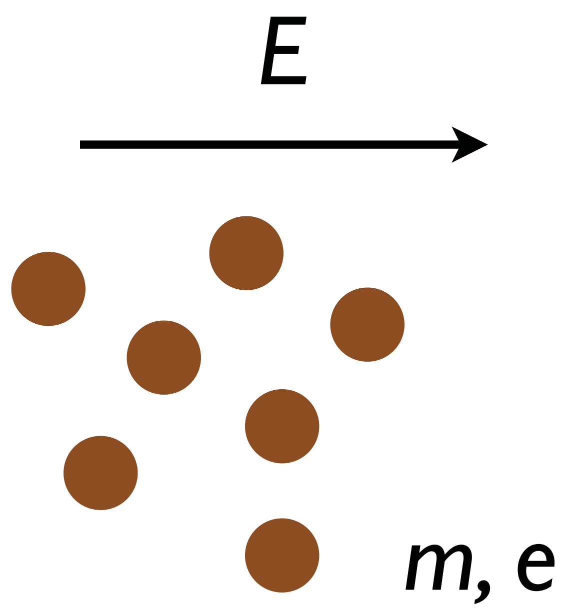
Electrical properties





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

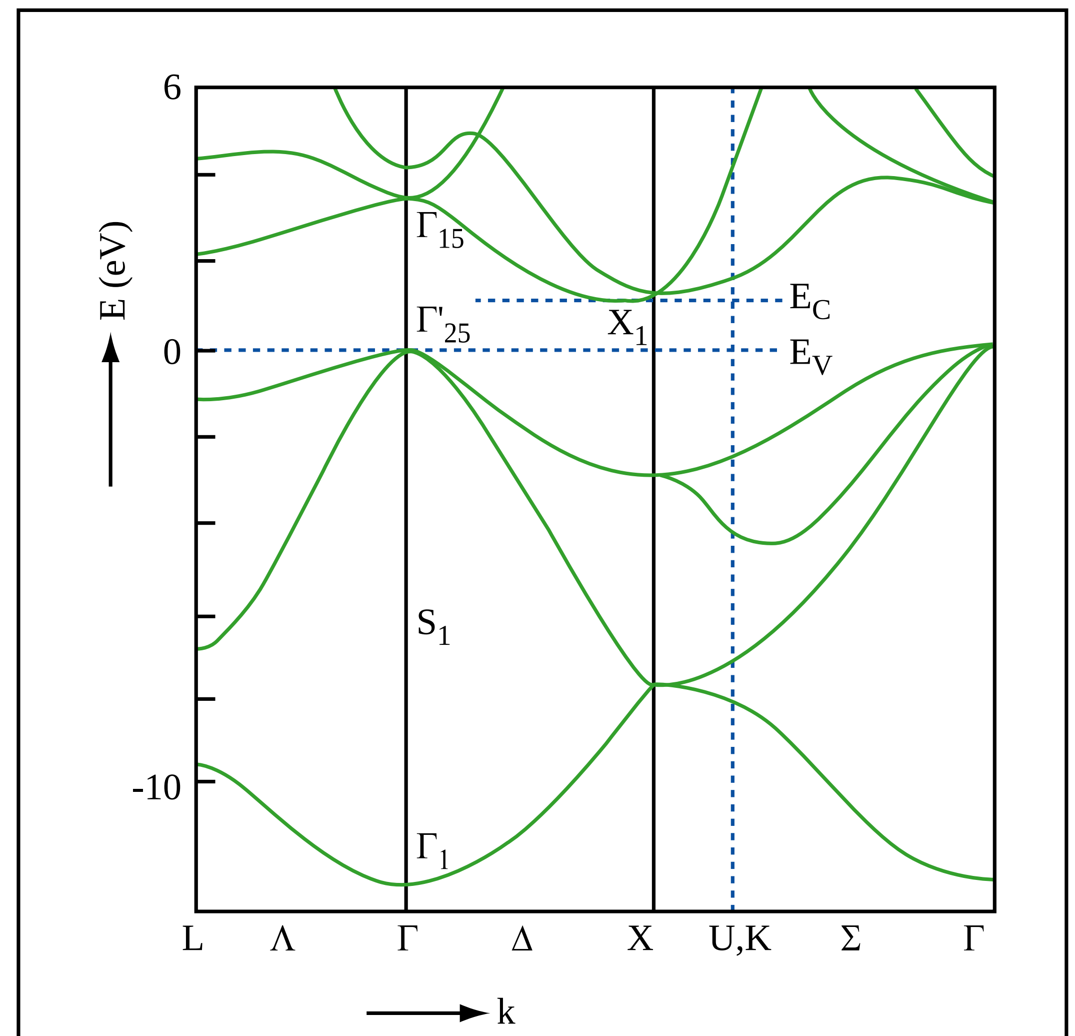
Calculating σ from band structure

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



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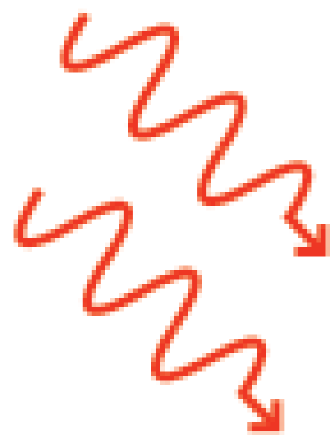
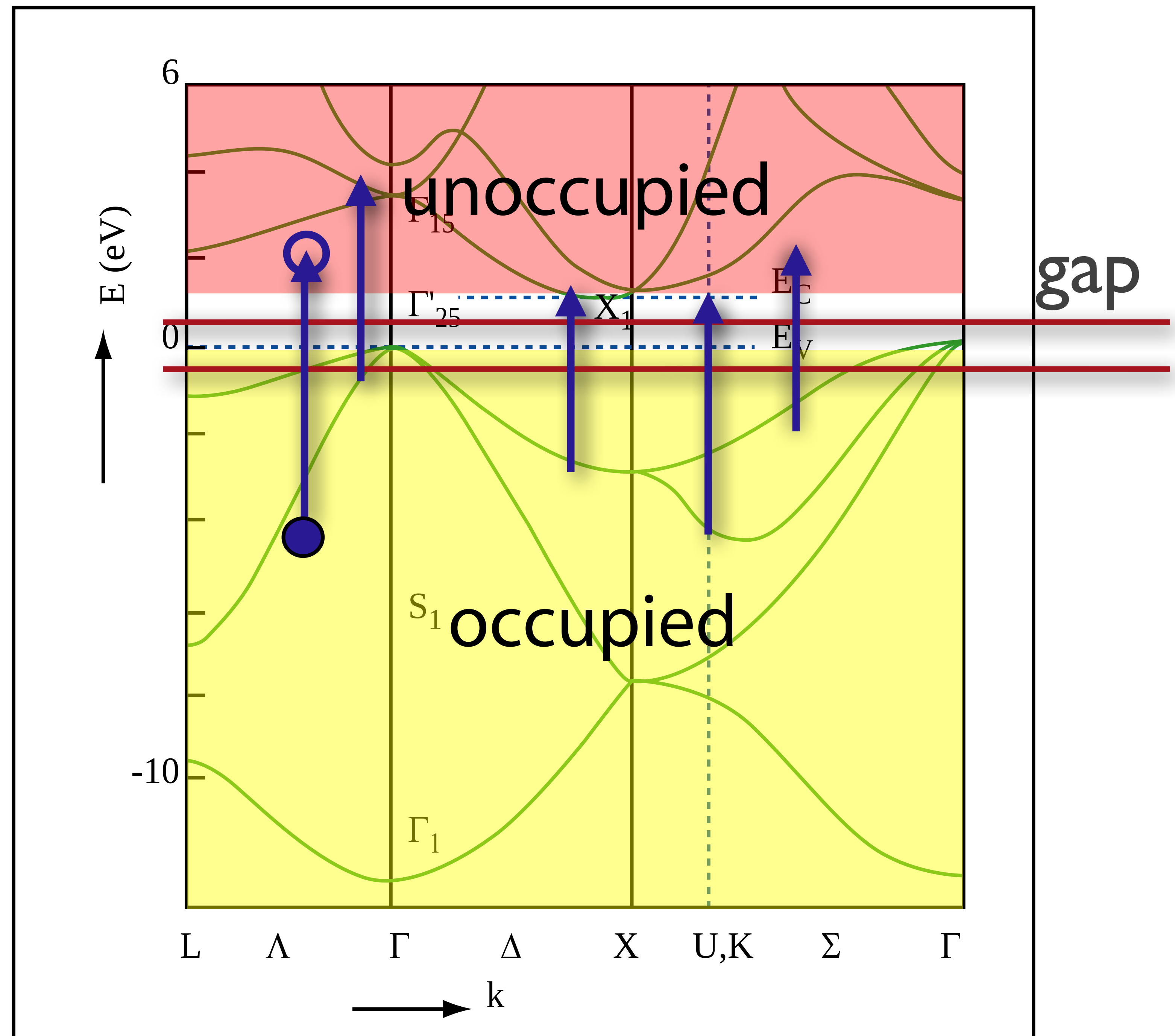
Simple optical properties

E=hν





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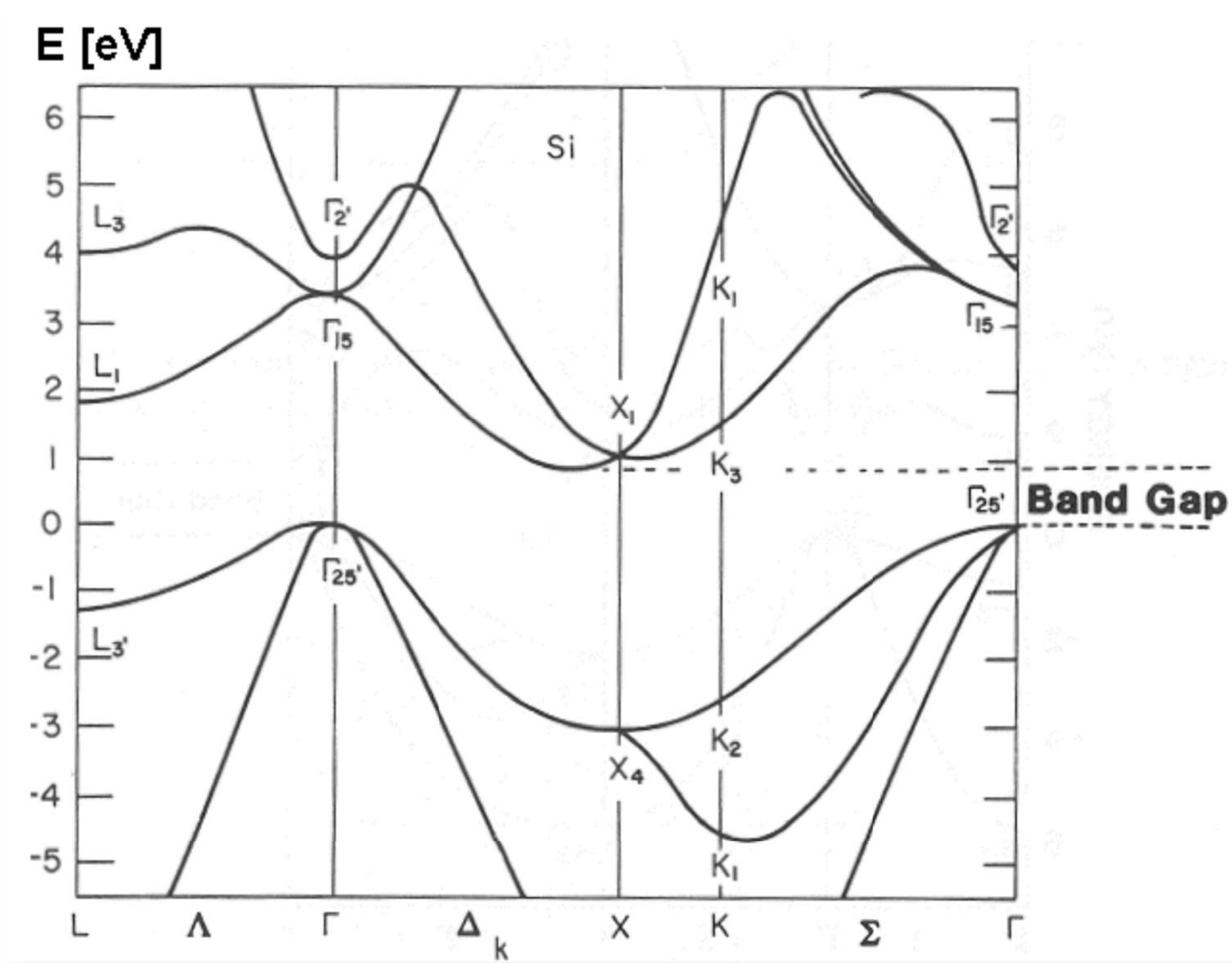
photon has almost no momentum: only vertical transitions possible

energy conversation and momentum conversation apply

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

It's all in the band-structure!



Simple optical properties

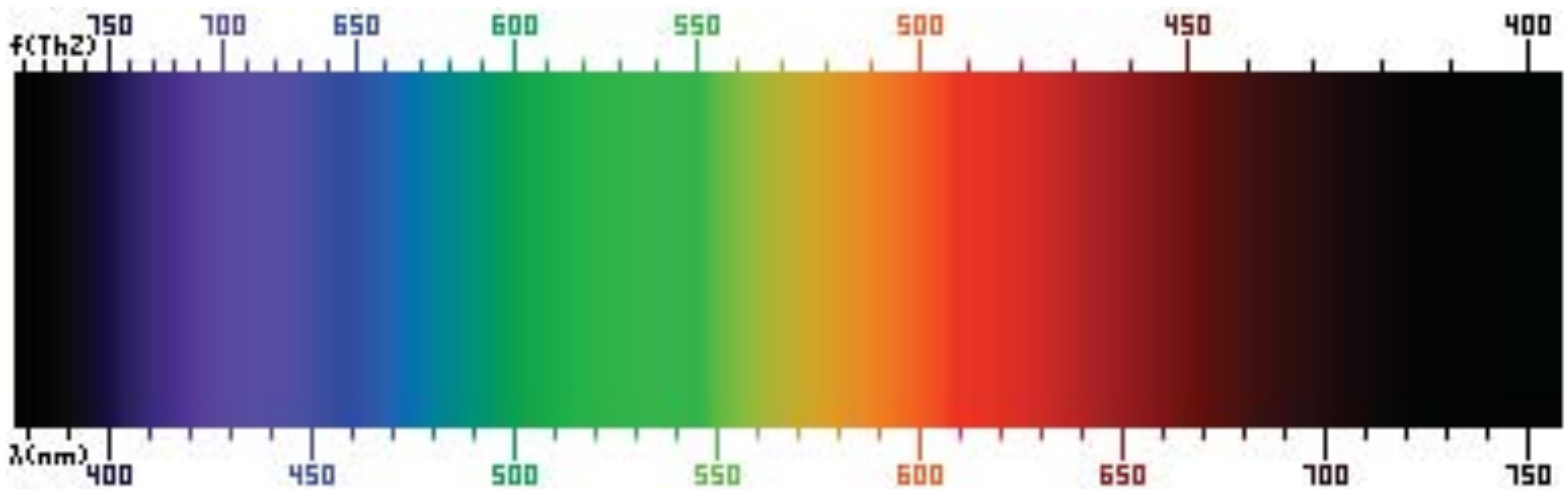


Image in the public domain.

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

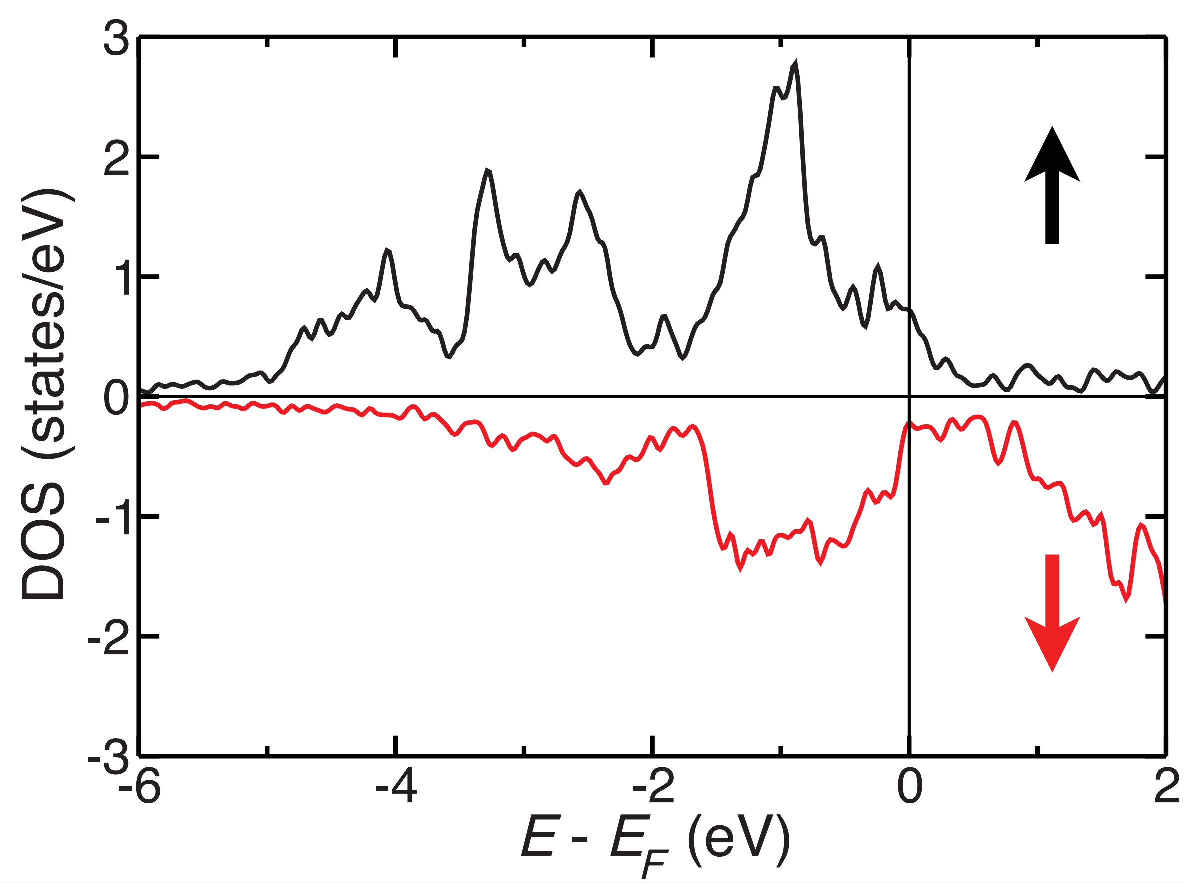
up down

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

Vatican fresco "The School of Athens" by Raphael. Image is in the public domain.

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

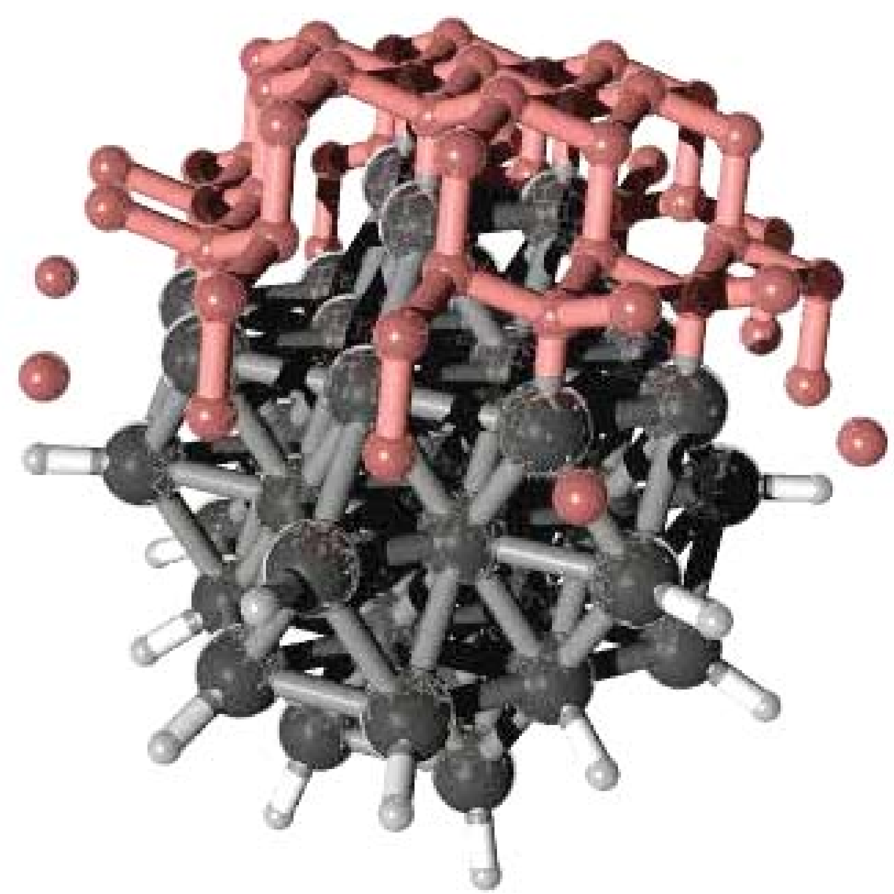
Aristotle depicted by Raphael, holding his Ethics. Image is in the public domain.

F=ma

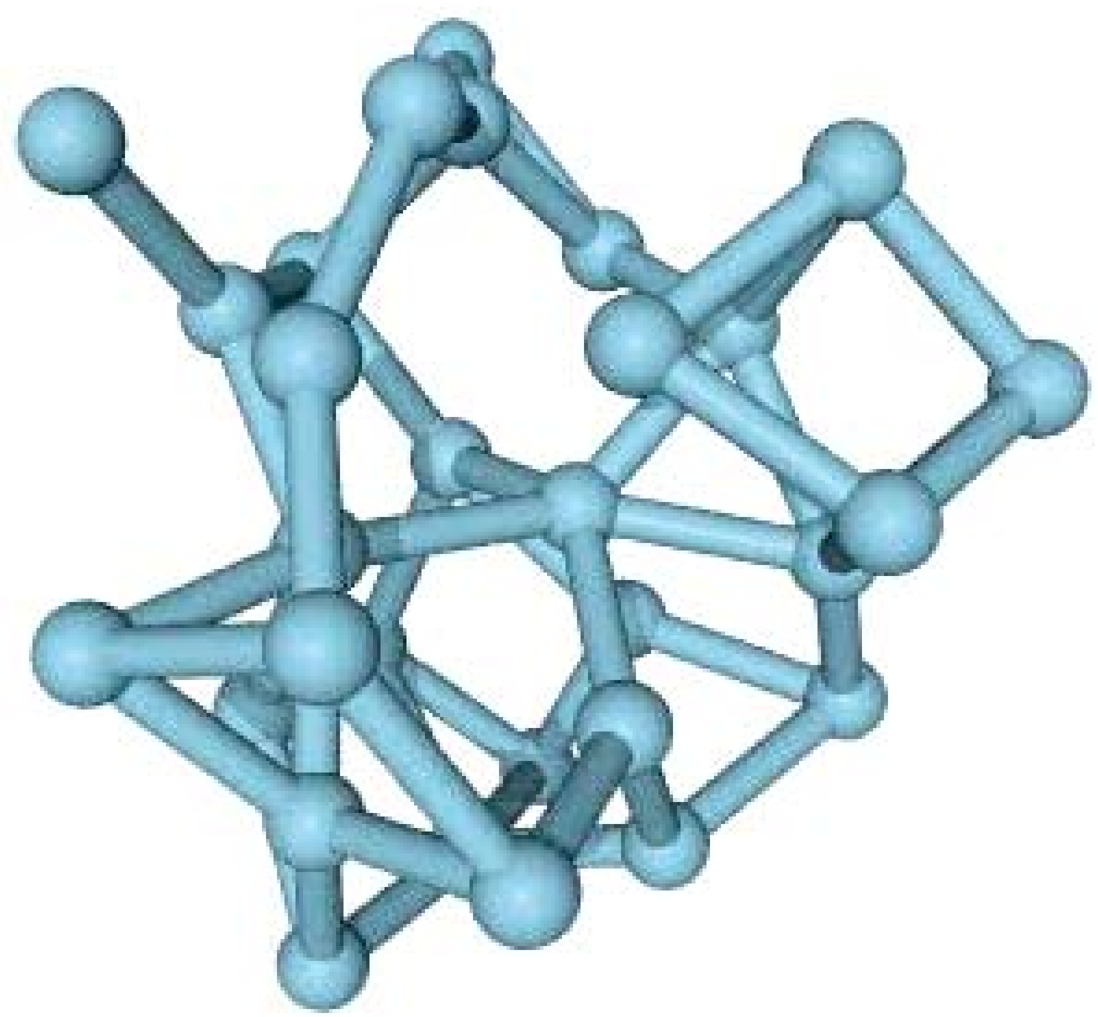
Use Hellmann-Feynman!

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

Carbon Nanotube Growth



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).

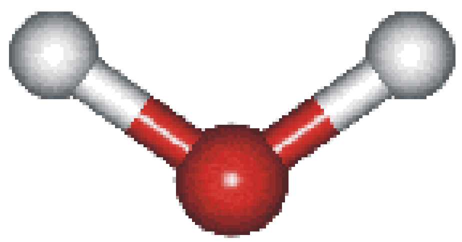
Cavendish was a pretty neat guy.

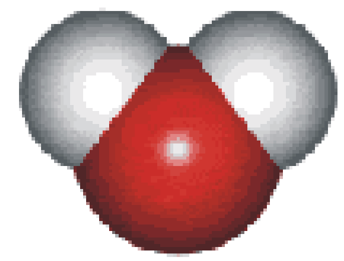
A University dropout, he also compared the conductivities of electrolytes and expressed a version of Ohm's law.

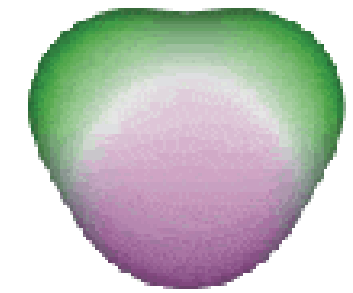
His last major work was the first measurement of Newton's gravitational constant, with the mass and density of the Earth. The accuracy of this experiment was not improved for a century.

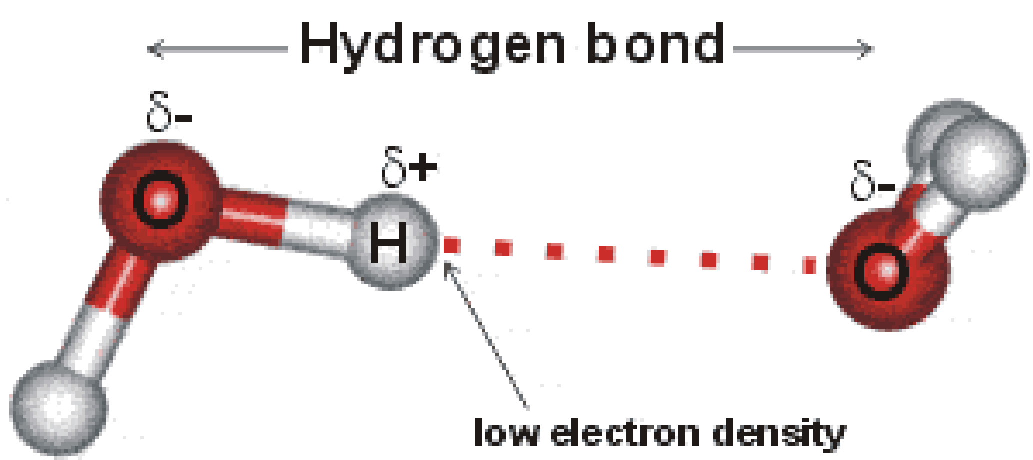
Water

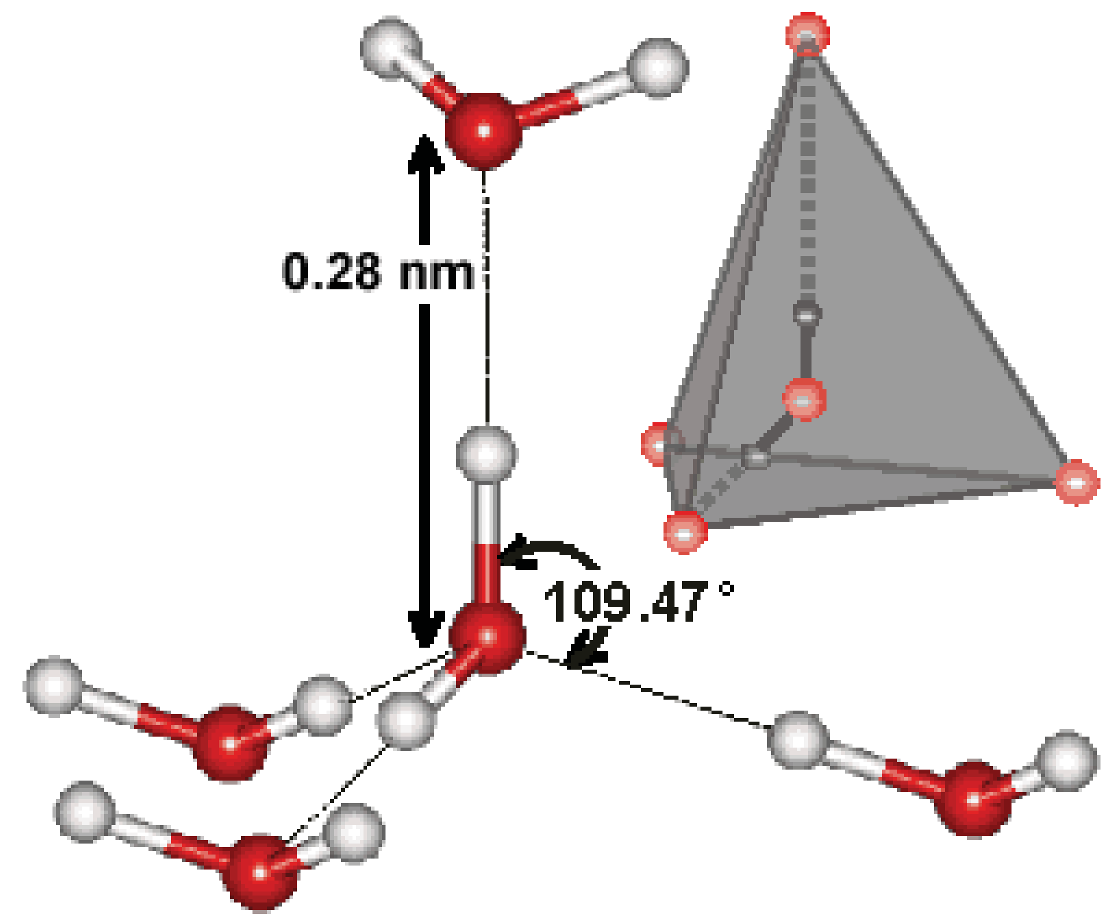
Which of the following is the correct picture for H_2O?











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

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

Classical or Quantum?

Model	Dipole moment	Dielectric constant	Self diffusion, 10^{-5} cm^2/s	Average configurational energy, kJ mol^{-1}	Density maximum, °C	Expansion coefficient, 10^{-4} $°C^{-1}$
SSD	2.35 [511]	72 [511]	2.13 [511]	-40.2 [511]	-13 [511]	-
SPC	2.27 [181]	65 [185]	3.85 [182]	-41.0 [185]	-45 [983]	7.3 [704] **
SPC/E	2.35 [3]	71 [3]	2.49 [182]	-41.5 [3]	-38 [183]	5.14 [994]
SPC/Fw	2.39 [994]	79.63 [994]	2.32 [994]	-	-	4.98 [994]
PPC	2.52 [3]	77 [3]	2.6 [3]	-43.2 [3]	+4 [184]	-
TIP3P	2.35 [180]	82 [3]	5.19 [182]	-41.1 [180]	-91 [983]	9.2 [180]
TIP3P/Fw	2.57 [994]	193 [994]	3.53 [994]	-	-	7.81 [994]
TIP4P	2.18 [3, 180]	53[a] [3]	3.29 [182]	-41.8 [180]	-25 [180]	4.4 [180]
TIP4P-FQ	2.64 [197]	79 [197]	1.93 [197]	-41.4 [201]	+7 [197]	-
TIP4P/2005	2.305 [984]	60 [984]	2.08 [984]	-	+5 [984]	2.8 [984]
SWFLEX-AI	2.69 [201]	116 [201]	3.66 [201]	-41.7 [201]	-	-
COS/G3 **	2.57 [704]	88 [704]	2.6 [704]	-41.1 [704]	-	7.0 [704]
GCPM	2.723 [859]	84.3 [859]	2.26 [859]	-44.8 [859]	-13 [859]	-
SWM4-NDP	2.461 [933]	79 [933]	2.33 [933]	-41.5 [933]	-	-
TIP5P	2.29 [180]	81.5 [180]	2.62 [182]	-41.3 [180]	+4 [180]	6.3 [180]
TIP5P-Ew	2.29 [619]	92 [619]	2.8 [619]	-	+8 [619]	4.9 [619]
POL5/TZ	2.712 [256]	98 [256]	1.81 [256]	-41.5 [256]	+25 [256]	-
Six-site*	1.89 [491]	33 [491]	-	-	+14 [491]	2.4 [491]
Expt.	2.95	78.4	2.30	-41.5 [180]	+3.984	2.53

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

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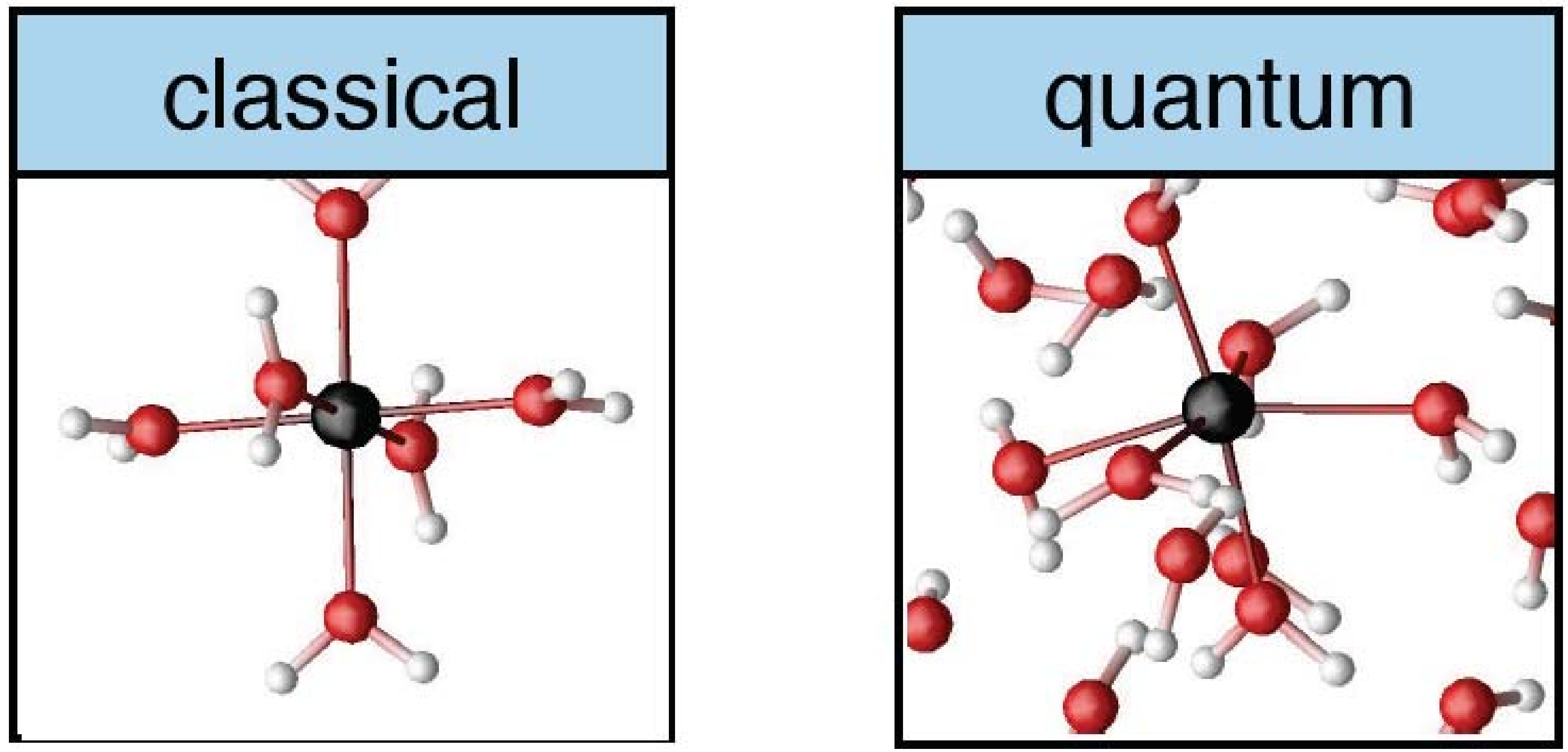
More than 50 classical potentials in use today for water.

Which one is best?

Mg++ in Water



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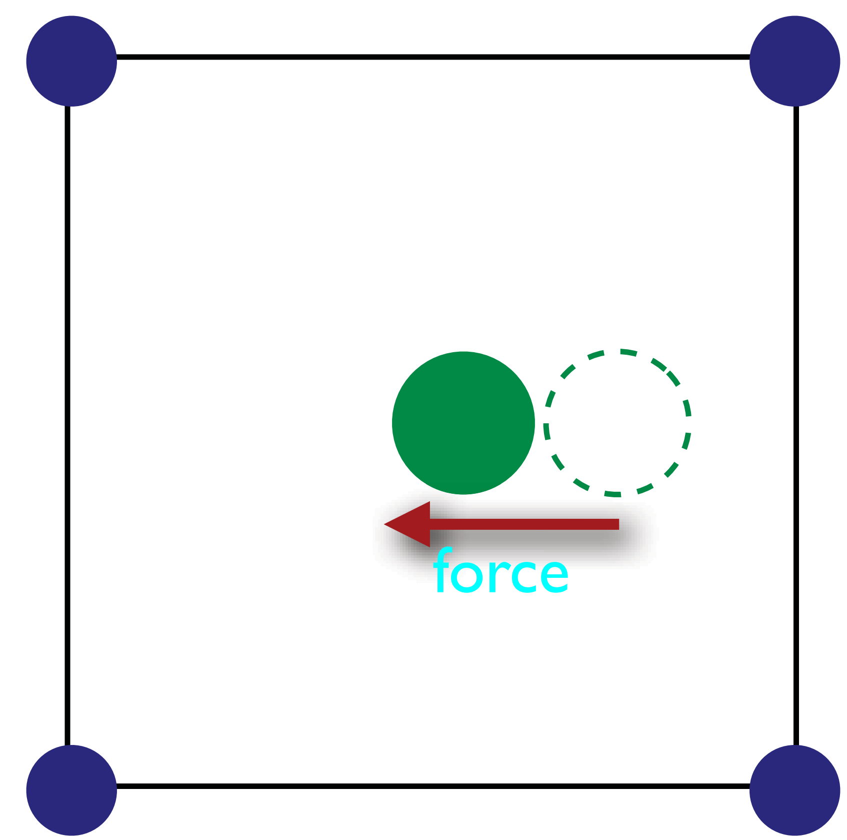
Important Differences!

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

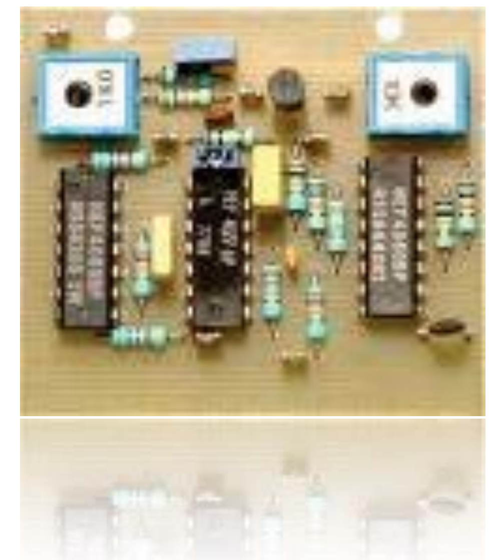
structural properties

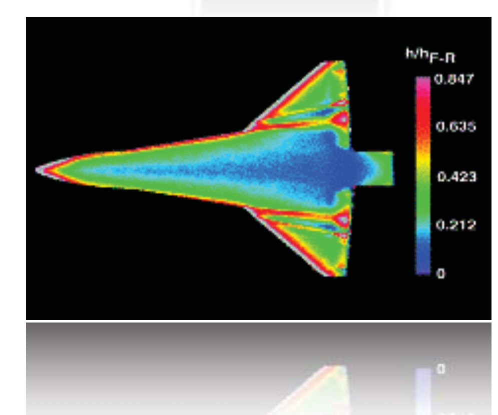
electrical properties

optical properties

magnetic properties

vibrational properties





Literature

- Charles Kittel, Introduction to Solid State Physics
- Ashcroft and Mermin, Solid State Physics
- wikipedia, "phonons", "lattice vibrations", ...
- solar PV: tons of web sites, e.g.: http://pveducation.org/pvcdrom