From Last Time…

- Important new Quantum Mechanical Concepts
  - Indistinguishability:
  - Symmetries of the wavefunction: Symmetric and Antisymmetric
  - Pauli exclusion principle: only one fermion per state
  - Spin
- Final concepts needed to understand the hydrogen atom and the periodic table

Today

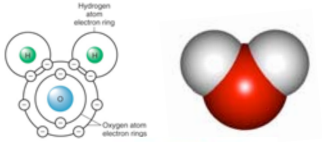
- Molecules, metals and semiconductors

Atoms and Molecules

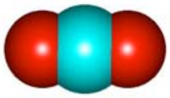
- Have talked about atoms
  - Atoms are a central nucleus with some number of electrons orbiting around it.
  - Number of orbiting electrons determines what element
- Molecules:
  - One or more atoms bonded together.

Simple molecules

- Water: H_2O



- Carbon dioxide: CO_2



- Even these simple molecules can be quite complex.
- Many nuclei, many electrons.
- However some properties can be determined without worrying too much about the details.

Symmetry

- The symmetries of fermions and bosons were a little subtle.
- Symmetries show up in many situations, many times in more direct ways.
- Both water and carbon dioxide have spatial symmetries:

Molecular Symmetries

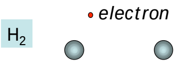
- These symmetries can determine many physical properties.
- Can be related to microscopic quantum mechanical properties such as the wavefunction and the probability.
- These are easiest to see if we start with a very simple molecule
  - Two protons and one electron.

Molecule question

A simple molecule consists of two protons and one electron orbiting around them. This molecule is

A. Helium molecule
[✓ B. Hydrogen molecule]
C. Lithium molecule

ionized hydrogen molecule



Electron must be described as a wave.
Use a wavefunction to do this.
The square of the wavefunction is the probability of finding the electron.

A two atom molecule

One electron orbiting two atoms

What do we expect for the charge density?

If atoms are identical, do we expect more charge on right, left?

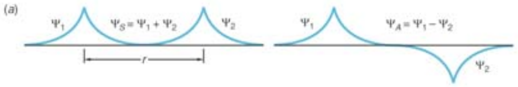
No reason to expect electron to reside on one atom over the other.

What wavefunction is consistent with electron not preferring one atom over the other?

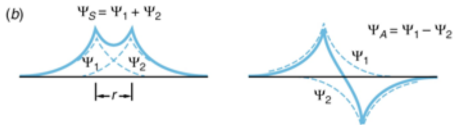
- In quantum mechanics, we can have BOTH.
- Wavefunction is an equal superposition of electron on left atom and electron on right atom.
- Two ways to superimpose states

$\left|\textit{Elec on left atom}\right\rangle + \left|\textit{Elec on right atom}\right\rangle$ $\left|\textit{Elec on left atom}\right\rangle - \left|\textit{Elec on right atom}\right\rangle$

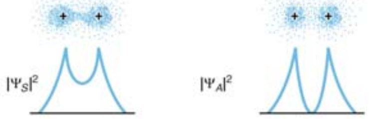
Symmetric Antisymmetric



Two possible wavefunctions



- These are obtained by adding or subtraction quantum states on either atom.
- Both give symmetric charge density…

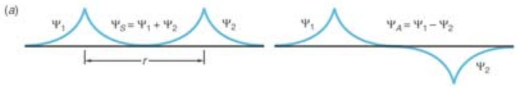


…but details slightly different.

Question

Which state has the lower energy?

Symmetric Antisymmetric



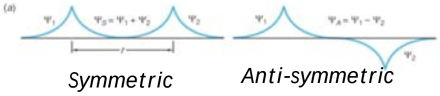
A. Symmetric

B. Antisymmetric

C. Both same

Symmetry of the wavefunction

Two-atom molecule



Symmetric *Anti-symmetric*

Compare particle in a box

$\lambda = 2L$
One half-wavelength

momentum
$p = \frac{h}{\lambda} = \frac{h}{2L}$

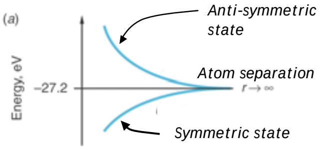
$\lambda = L$
Two half-wavelengths

momentum
$p = \frac{h}{\lambda} = \frac{h}{L}$

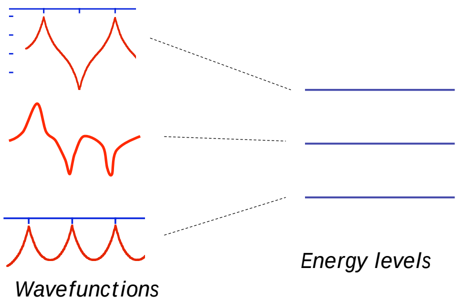
Quantum state energies

- Symmetric state is the 'ground state'.
- Antisymmetric state is the excited state.
  - Wavelength half as large
  - momentum twice as large
  - Larger momentum -> larger kinetic energy

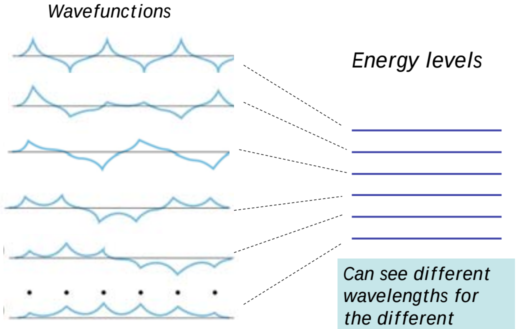
- Since momentum depends on 'size of box' (atomic separation)…
- … energy difference increases as atom separation decreases.



A three-atom molecule



A six-atom molecule



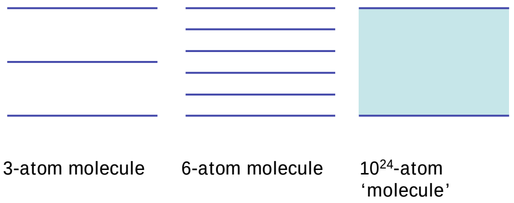
Can see different wavelengths for the different molecular states

Solids

- Solids consist of many atoms bonded together
- Many possible ways to combine atomic wavefunctions to get charge density with correct symmetry.
- All these quantum states have slightly different energies.
- Solid is similar to atom or molecule, except quantum states are extremely close together in energy.

Energy levels in a solid

- Solids consists of ~10^{24} atoms
- Energy levels spaced *extremely* close together

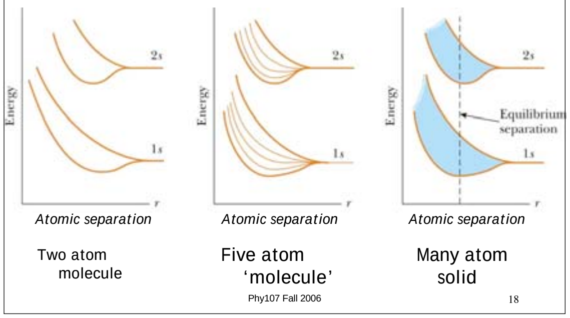


Energy bands in a solid

- This energy region of densely packed quantum states in called an **energy band**.
- Each quantum state on an individual atom (for instance, 1s, 2s, etc) leads to one of these energy bands.
- The detailed arrangement of these energy bands is called the band structure.

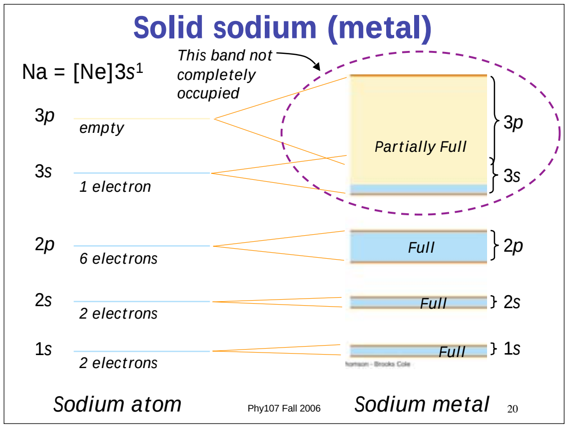
Band structure

- Atomic orbitals interact to form new energy levels



Occupation of quantum states

- These quantum states are filled with electrons just as atomic states get filled one by one, lowest energy first, just like an atom.
- Dramatically more electrons to fill the states!
- But since each band arises from an atomic quantum state,
- But due to details in which atomic states broaden into bands, sometimes bands overlap and and are not completely full or empty.



Solid sodium (metal)

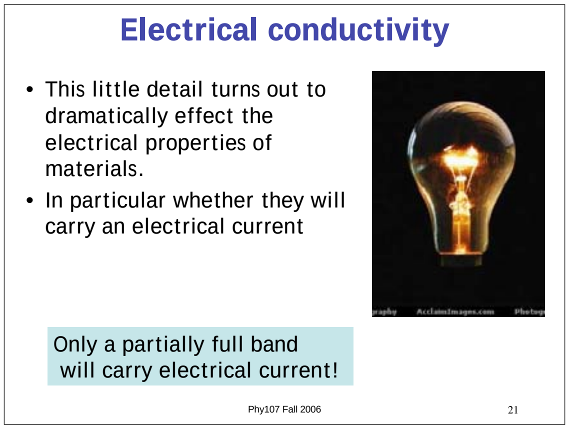
Na = [Ne]3s^1

This band not completely occupied

3*p*	empty			3*p*
3*s*	1 electron	Partially Full		3*s*
2*p*	6 electrons	Full		2*p*
2*s*	2 electrons	Full		2*s*
1*s*	2 electrons	Full		1*s*

homson - Brooks Cole

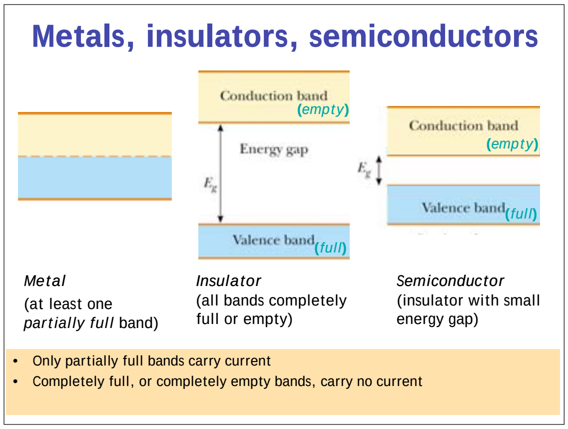
Sodium atom *Sodium metal*



Electrical conductivity

- This little detail turns out to dramatically effect the electrical properties of materials.
- In particular whether they will carry an electrical current

Only a partially full band will carry electrical current!



Metals, insulators, semiconductors

Metal
(at least one *partially full* band)

Insulator
(all bands completely full or empty)

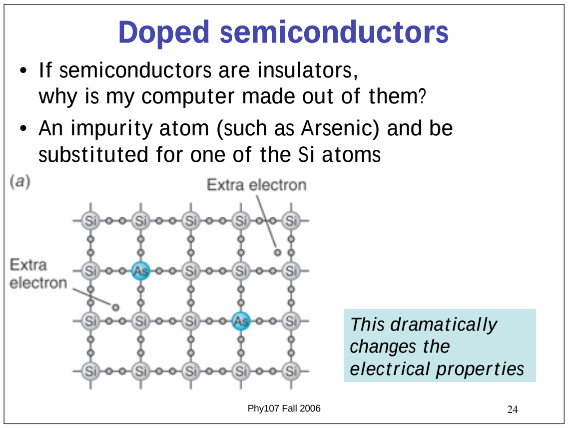
Semiconductor
(insulator with small energy gap)

- Only partially full bands carry current
- Completely full, or completely empty bands, carry no current

Properties of some elements

Metals	**Insulators**	**Semiconductors**
Copper	*Diamond (Carbon)*	*Silicon*
Zinc	*Sulfur*	*Germanium*
Aluminum		
Gold		
Platinum		
Sodium		
Calcium		

Wider variety of insulators, semiconductors can be listed if compounds are included



Doped semiconductors

- If semiconductors are insulators,
  why is my computer made out of them?
- An impurity atom (such as Arsenic) and be substituted for one of the Si atoms

This dramatically changes the electrical properties

Doping a semiconductor

- Elements in same column have same number of ‘outer’ electrons.
- Substitution of element from another column changes band filling

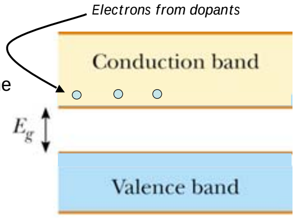
One fewer electron (acceptors)

One extra electron (donors)

Example: Phosphorus-doped silicon

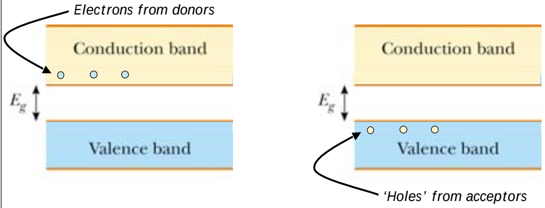
Si = [Ne]3p^2
P = [Ne]3p^3

- P has one extra electron.
- That electron goes into the conduction band
  - Conduction band partially full
  - Valence band full
  - Called an *n*-type semiconductor



Electrons from dopants

n- and *p*-type semiconductors



Electrons from donors

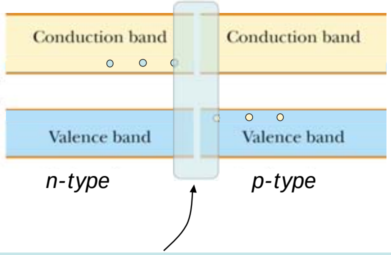
‘Holes’ from acceptors

n-type semiconductor
Donors have one extra electron

p-type semiconductor
Acceptors have one fewer electron

So what?

- Real usefulness comes from combining *n* and *p*-type semiconductors



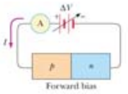
n-type

p-type

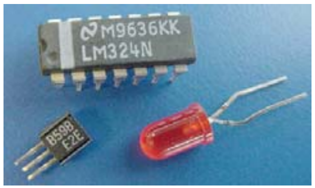
Junction develops a ‘built-in’ electric field at the interface due to charge rearrangement.

Semiconductor devices

- This built-in electric field has a direction, so the diode behaves differently in different directions.
- Many devices made from a junction between *n*- and *p*-type materials.
  - Diodes, transistors, LEDs (light-emitting diodes), diode lasers, solar cells etc

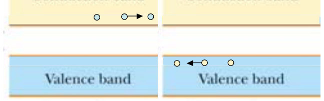


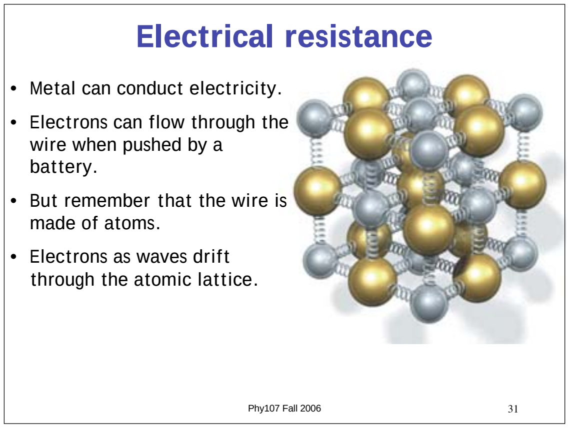
Junction Diode



Light emitting diode

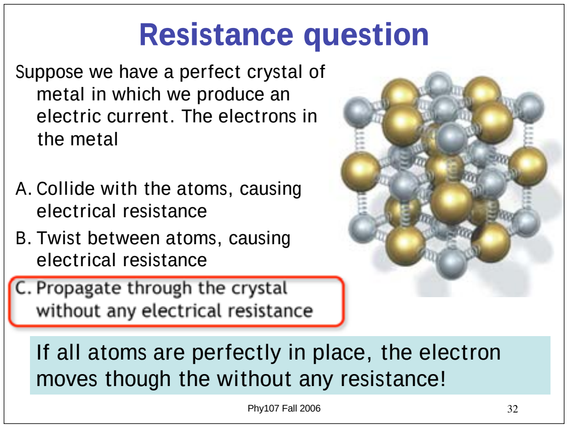
- Battery causes electrons and holes to flow toward *pn* interface
- Electrons and holes recombine at interface (electron drops down to lower level)
- Photon carries away released energy.
- Low energy use - one color!





Electrical resistance

- Metal can conduct electricity.
- Electrons can flow through the wire when pushed by a battery.
- But remember that the wire is made of atoms.
- Electrons as waves drift through the atomic lattice.



Resistance question

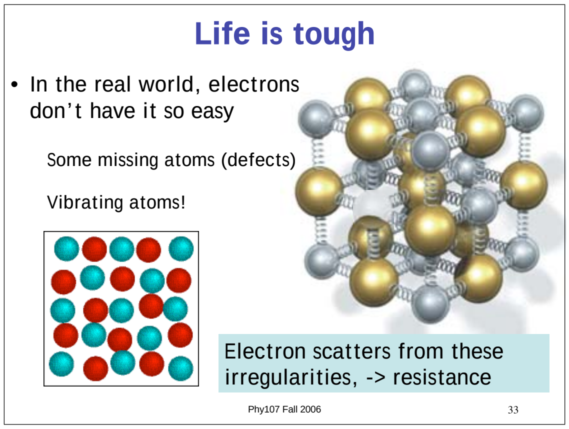
Suppose we have a perfect crystal of metal in which we produce an electric current. The electrons in the metal

A. Collide with the atoms, causing electrical resistance

B. Twist between atoms, causing electrical resistance

[✓ C. Propagate through the crystal without any electrical resistance]

If all atoms are perfectly in place, the electron moves though the without any resistance!



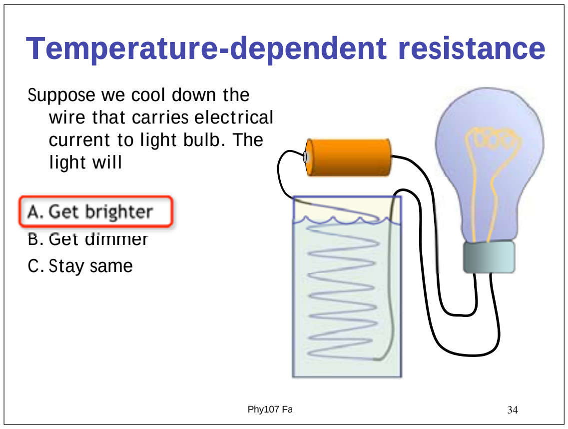
Life is tough

- In the real world, electrons don't have it so easy

Some missing atoms (defects)

Vibrating atoms!

Electron scatters from these irregularities, -> resistance



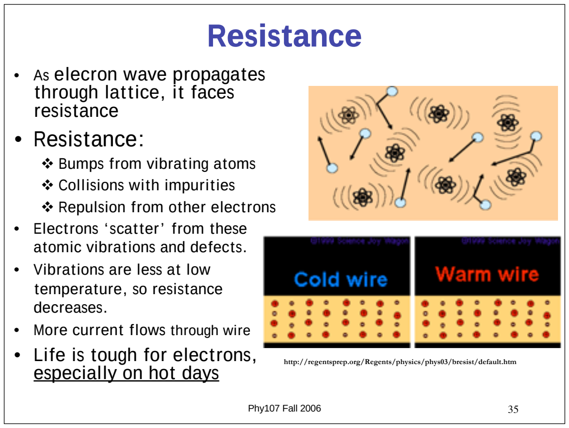
Temperature-dependent resistance

Suppose we cool down the wire that carries electrical current to light bulb. The light will

[✓ A. Get brighter]

B. Get dimmer

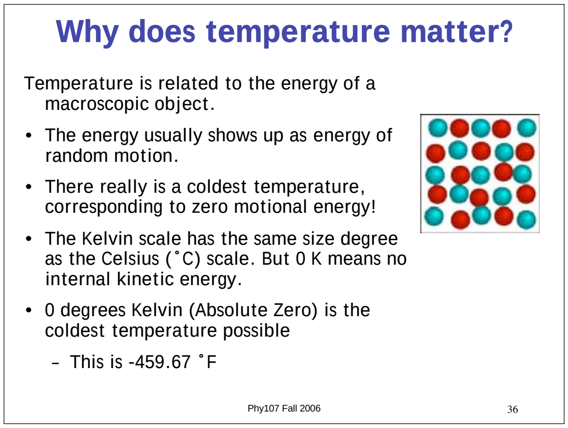
C. Stay same



Resistance

- As elecron wave propagates through lattice, it faces resistance
- Resistance:
  - ❖ Bumps from vibrating atoms
  - ❖ Collisions with impurities
  - ❖ Repulsion from other electrons
- Electrons 'scatter' from these atomic vibrations and defects.
- Vibrations are less at low temperature, so resistance decreases.
- More current flows through wire
- Life is tough for electrons, <u>especially on hot days</u>

http://regentsprep.org/Regents/physics/phys03/bresist/default.htm



Why does temperature matter?

Temperature is related to the energy of a macroscopic object.

- The energy usually shows up as energy of random motion.
- There really is a coldest temperature, corresponding to zero motional energy!
- The Kelvin scale has the same size degree as the Celsius (˚C) scale. But 0 K means no internal kinetic energy.
- 0 degrees Kelvin (Absolute Zero) is the coldest temperature possible
  - This is -459.67 ˚F

Temperature scales

- Kelvin (K):
  - **K = C + 273.15**
  - **K = 5/9 F + 255.37**

Fahrenheit	Celsius	Kelvin	comments
212	100	373.15	water boils
32	0	273.15	water freezes
-300.42	-195.79	77.36	liquid nitrogen boils
-452.11	-268.95	4.2	liquid helium boils
-459.67	-273.15	0	absolute zero

Low temperature properties

- Next time - what happens at very low temperatures