3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

3.23 Fall 2007 – Lecture 12

SEMICONDUCTORS

Last time

1. Periodic potential: atomic + pertubation
2. Bloch sums of localized orbitals (atomic, or LCAO)
3. Tight-binding formulation (in the case only one orbital has significant overlap)
4. From flat atomic “bands” to dispersive cosines
5. Bandwidths
6. Tight-binding vs. empirical pseudopotential (i.e. a perturbation of the free electron gas)
7. Band structure (DETAILED) of a semiconductor

Ferroelectric perovskites

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King-Smith, R. D., and David Vanderbilt. "First-principles Investigation of Ferroelectricity in Perovskite Compounds." *Physical Review B* 49 (March 1994): 5828-5844.

Ferroelectric perovskites

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King-Smith, R. D., and David Vanderbilt. "First-principles Investigation of Ferroelectricity in Perovskite Compounds." *Physical Review B* 49 (March 1994): 5828-5844.

Silicon

8 VALENCE e
sp^3

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Please see Fig. 2.24 in Yu, Peter Y., and Cardona, Manuel.
Fundamentals of Semiconductors: Physics and Materials Properties.
New York, NY: Springer, 2001.

Lead

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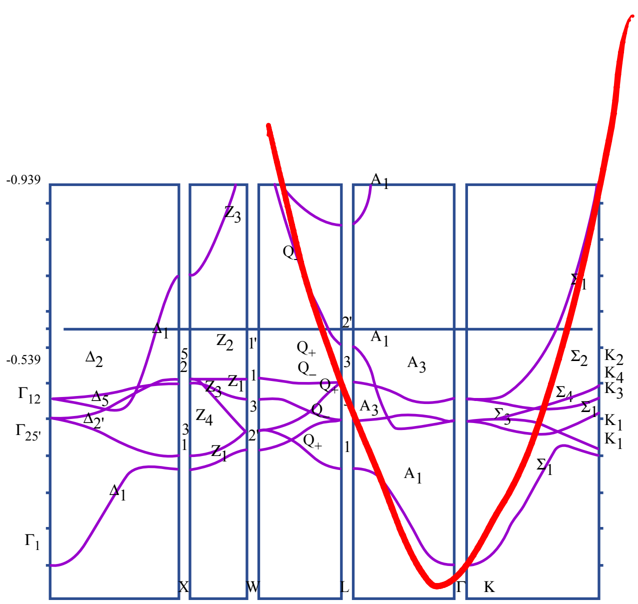
Please see any band gap diagram of lead, such as
http://www.bandstructure.jp/Table/BAND/band_png/pb4800b.ps.png

111 → 100 → 100
110 → Γ
1/2 1/3 0

Copper



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Silver

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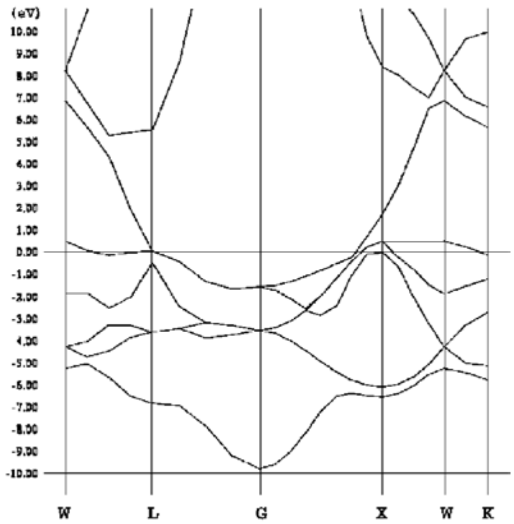
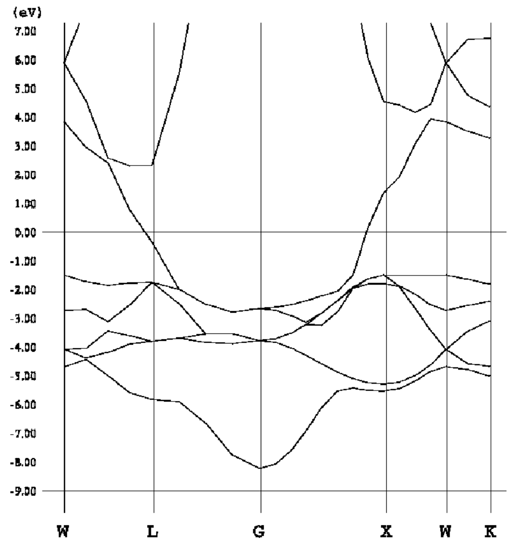
Please see and band gap diagram of silver, such as
http://www.bandstructure.jp/Table/BAND/band_png/ag39275a.ps.png

Platinum   Gold



Pt(fcc) a=7.56a.u.



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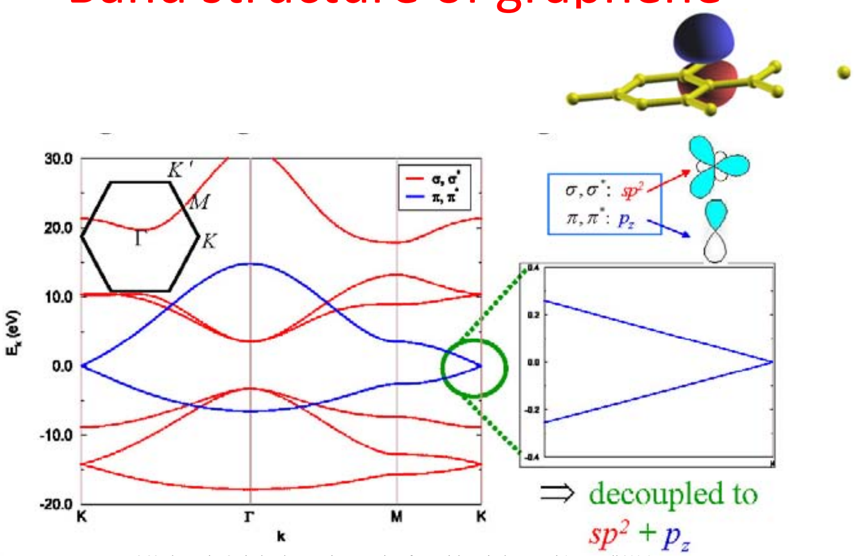
Au(fcc) a=8.2a.u

Band structure of graphene



Courtesy Hongki Min. Used with permission.

Band structure of graphene

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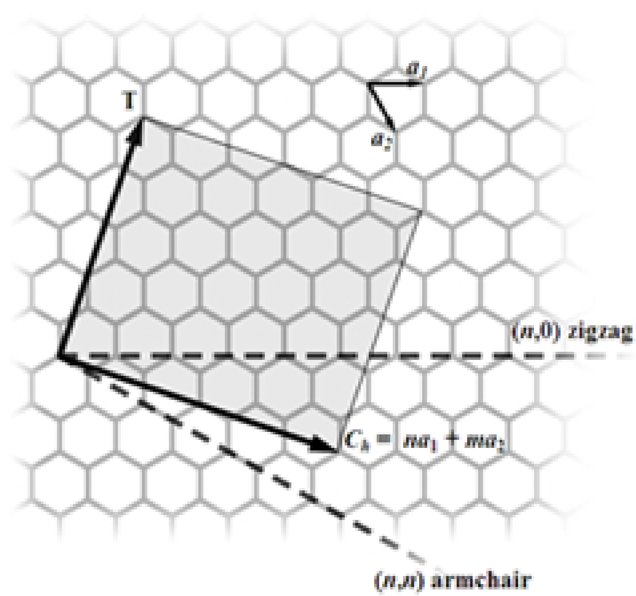
Minot, Ethan. "Tuning the Band Structure of Carbon Nanotubes." PhD dissertation, Cornell University, 2004.

Carbon nanotubes



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Zone folding: Band structure of nanotubes

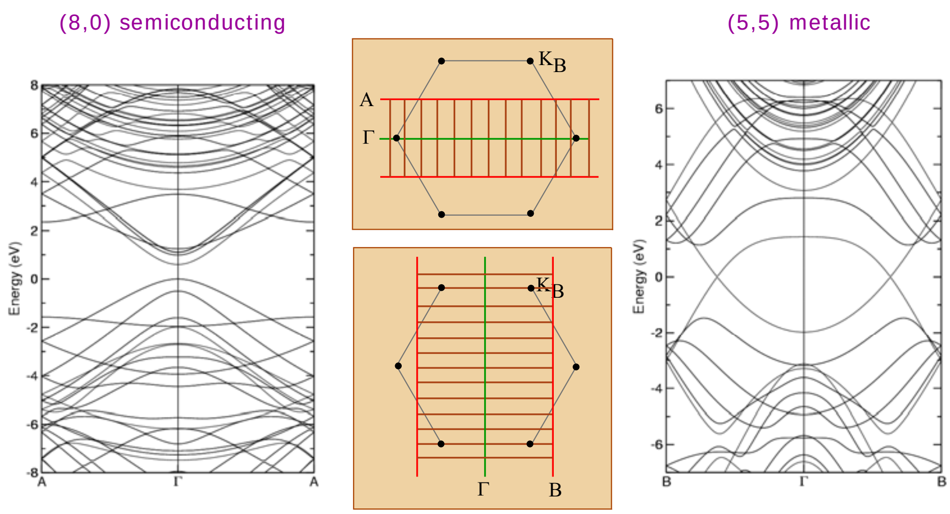

Figure by MIT OpenCourseWare.

The independent-electron gas

- Hamiltonian

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2$$

- Eigenvalues and eigenfunctions

$$\psi^{1e} = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

$$\varepsilon_k = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$\psi^{\text{MANY } e} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(r_1) & \cdots & \varphi_1(r_n) \\ \vdots & & \\ \varphi_n(r_1) & \cdots & \varphi_n(r_n) \end{vmatrix}$$

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The independent-electron gas

- BvK boundary conditions

$e^{i(k_x,0,0)\cdot\vec{r}}$

$$\psi_k(x+Na,y,z)=\psi_k(x,y,z)$$

$\Downarrow$ BLOCH'S

$$e^{ik_x Na}=1 \qquad k_x Na = 0, 2\pi, 4\pi \ldots$$

n_x

$$k_x=\frac{2\pi}{a}n_x \quad \text{INTEGER}$$

The independent-electron gas

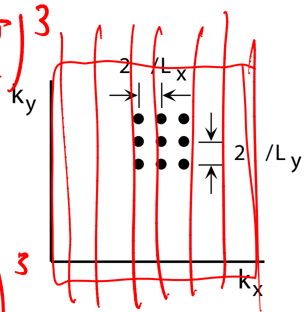
- Counting the states

$d\Omega =$

$= \left(\frac{2\pi}{L}\right)^3$

N^3

$\left(\frac{L}{2\pi}\right)^3$



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Please see any diagram of free electron band gaps, such as
http://leung.uwaterloo.ca/CHEM/750/Lectures%202007/SSNT-5-Electronic%20Structure%20II_files/image008.jpg.

The independent-electron gas

- Particle density

FERMI MOMENTUM $\hbar k_F$

$$N_{el} = 2 \, \frac{4\pi}{3} k_F^3 \left(\frac{L}{2\pi}\right)^3 = \frac{2}{3} \frac{4\pi}{(2\pi)^3} k_F^3 V$$

$$\boxed{n = \frac{N_{el}}{V} = \frac{k_F^3}{3\pi^2}}$$

The independent-electron gas

- Energy density

$$E = 2 \sum_{\|k\| < \|k_F\|} \frac{\hbar^2}{2m} k^2 = \int_{\substack{BZ \\ \|k\| < \|k_F\|}} d^3k \, \frac{L^3}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} =$$

$$= \frac{V}{\pi^2} \frac{\hbar^2 k_F^5}{10 m}$$

$$\boxed{\frac{E}{N} = \frac{3}{5} \varepsilon_F}$$

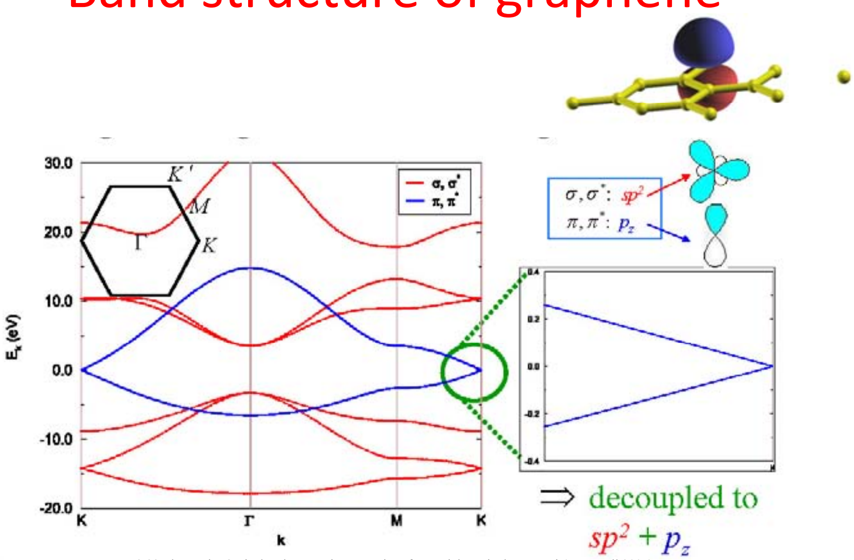
Density of states (for any solid)

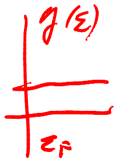
$$g_n(\varepsilon) = 2\int \frac{1}{8\pi^3}\,\delta(\varepsilon - \varepsilon_n(\vec{k}))\,d\vec{k}$$

$$\Downarrow$$

$$g_n(\varepsilon) = \frac{2}{8\pi^3}\int_{S_n(\varepsilon)} dS\,\frac{1}{\|\nabla\varepsilon_n(k)\|}$$

Band structure of graphene





Massive vs massless bands

Dimensions	d=1	d=2	d=3
Massless (E≈k)	const	E	E²
Massive (E≈k²)	1/sqrt(E)	const	sqrt(E)

$$g_n(\varepsilon) = 2\int \frac{1}{8\pi^3} \frac{1}{\left|\nabla \varepsilon_n(\vec{k})\right|} dS$$

k^{d-1} $k^{-(l-1)}$ k^{d-l}

- S goes as k^{d-1} , where d ~~is the~~ dimensionality
- $\frac{1}{\left|\nabla \varepsilon(\vec{k})\right|}$ for a band that has k^l dispersions goes as $k^{-(l-1)}$,
- the integral goes as k^{d-l}
- energy is proportional to k^l, the integral goes as $\boxed{\varepsilon^{(d-l)/l}}$

Statistics of classical and quantum particles

DISTINGUISHABLE

	1	2	3
1	AB		
2		AB	
3			AB
4	A	B	
5	A		B
6		A	B
7	B	A	
8	B		A
9		B	A

CLASSICAL

INDISTINGUISHABLE

	1	2	3
1	AA		
2		AA	
3			AA
4	A	A	
5	A		A
6		A	A

BOSE-EINSTEIN

	1	2	3
1	A	A	
2	A		A
3		A	A

FERMI-DIRAC

Probability and Partition Function

$(k_B T)^{-1}$

$$P_s = \frac{e^{-\beta E_s}}{\sum\limits_{\substack{\text{ALL STATES } s \\ \text{WITH ENERGY } E_s}} e^{-\beta E_s}}$$

$\frac{\text{PARTITION}}{\text{FUNCTION}}$ Z

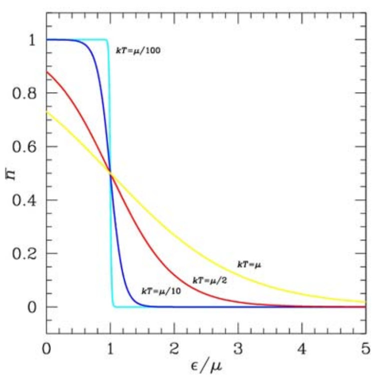
$$F = -k_B T \ln Z$$

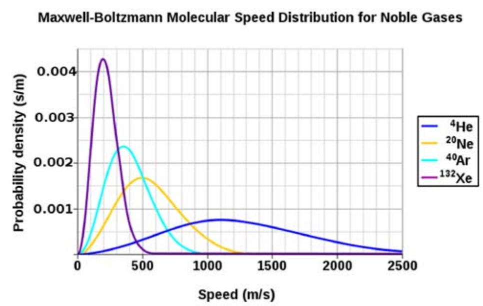
Chemical potential

$$\mu \simeq F(N+1) - F(N) = \frac{dF}{dN}$$

$$\bar{n}_s = \frac{1}{1 + \exp\left(\frac{\varepsilon_s - \mu}{kT}\right)}$$

Fermi-Dirac distribution





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