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.

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Silicon

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

Lead

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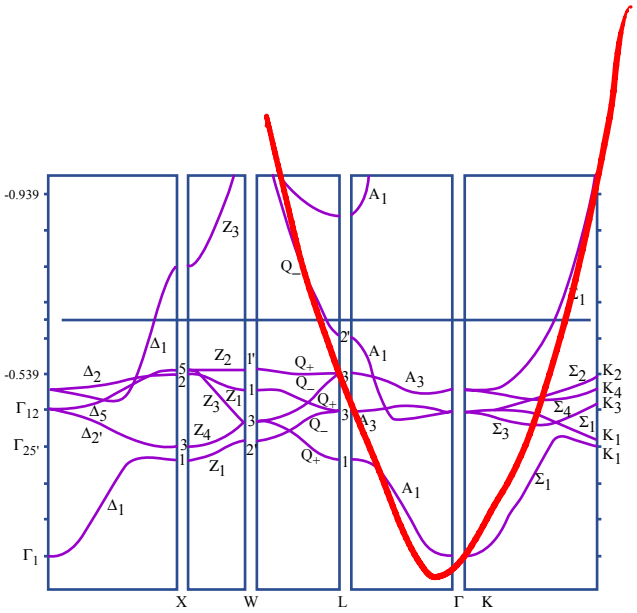
Please see any band gap diagram of lead, such as
http://www.bandstructure.jp/Table/BAND/band_png/pb4800b.ps.png

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

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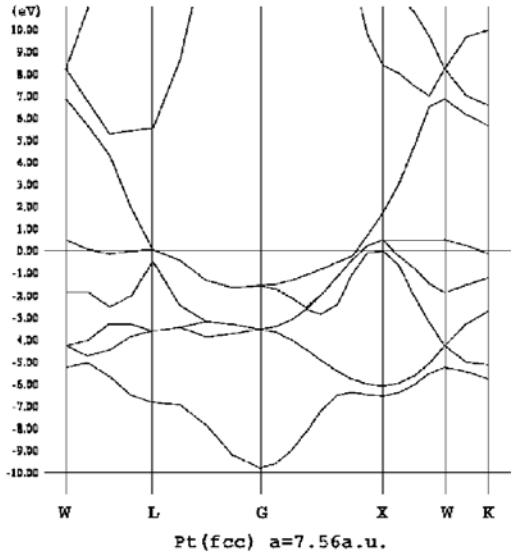
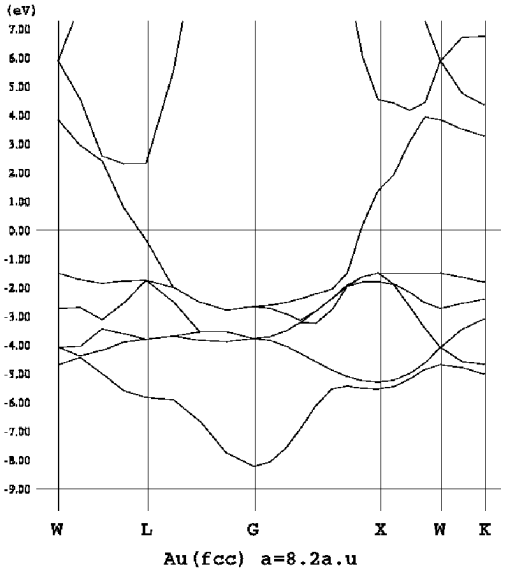
Platinum



Gold



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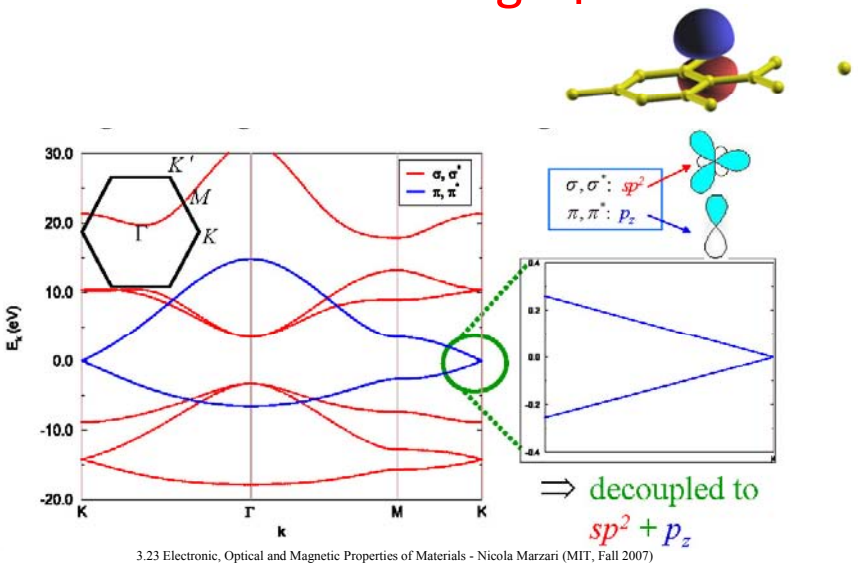
Band structure of graphene



Courtesy Hongki Min. Used with permission.

Band structure of graphene

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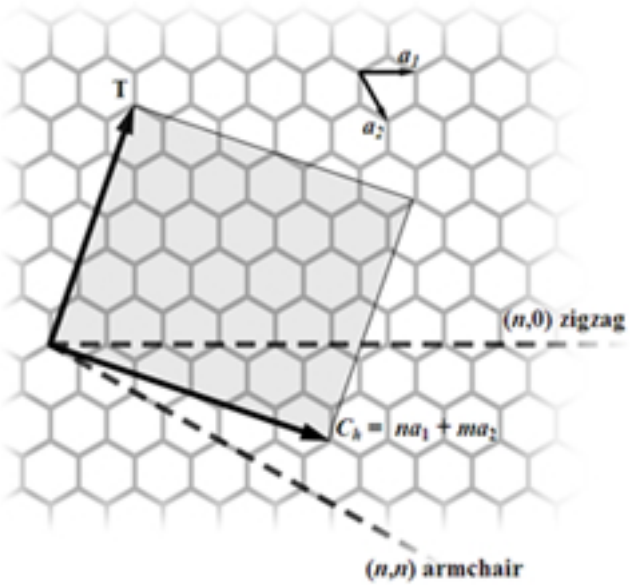
Minot, Ethan. "Tuning the Band Structure of Carbon Nanotubes." PhD dissertation, Cornell University, 2004.

Carbon nanotubes



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Zone folding: Band structure of nanotubes

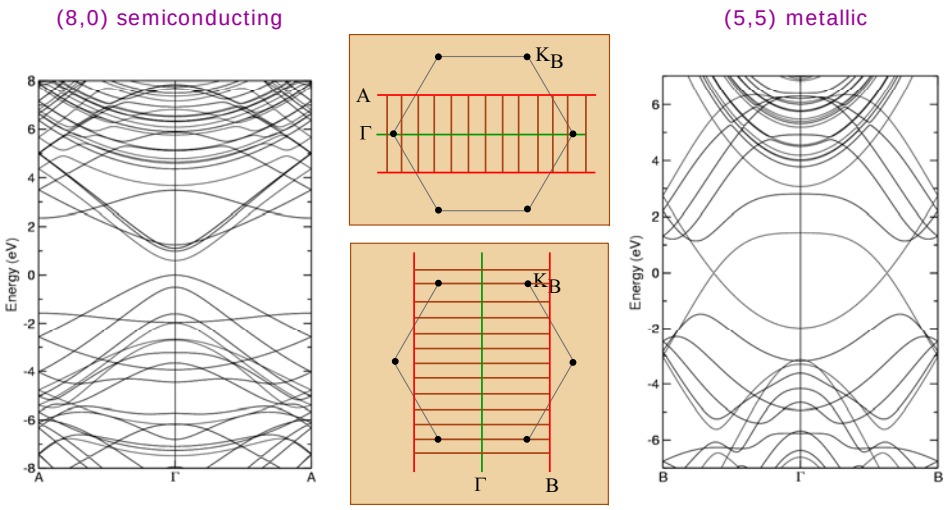


Figure by MIT OpenCourseWare.

The independent-electron gas

- Hamiltonian

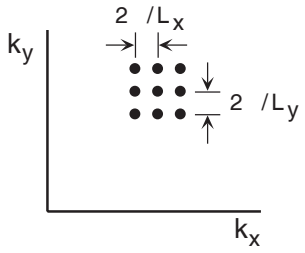
- Eigenvalues and eigenfunctions

The independent-electron gas

- BvK boundary conditions

The independent-electron gas

- Counting the states



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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

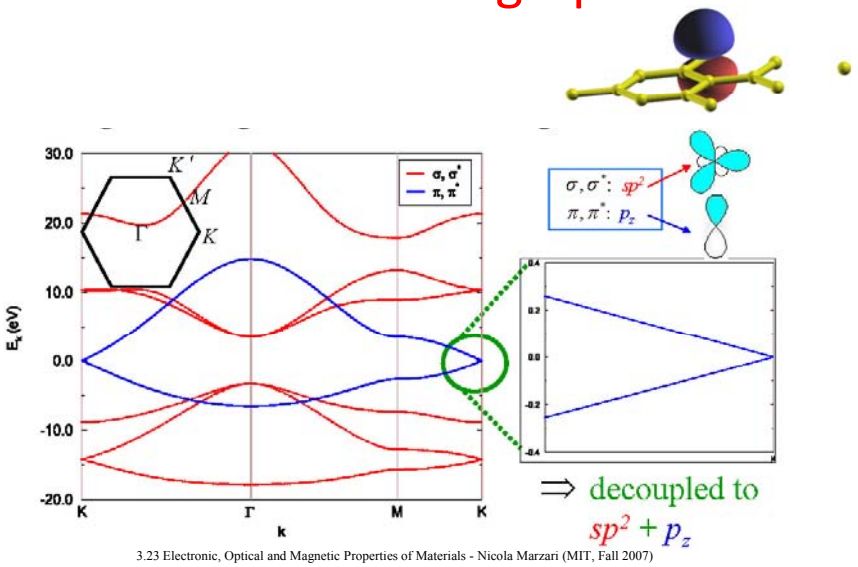
The independent-electron gas

- Energy density

Density of states (for any solid)

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

Band structure of graphene



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Massive vs massless bands

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

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

- 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 $\varepsilon^{(d-l)/l}$

Statistics of classical and quantum particles

	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

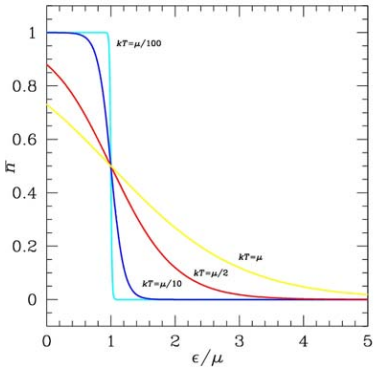
	1	2	3
1	AA		
2		AA	
3			AA
4	A	A	
5	A		A
6		A	A

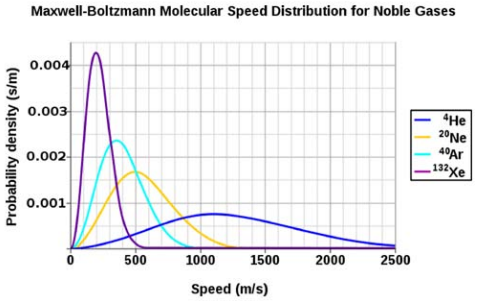
	1	2	3
1	A	A	
2	A		A
3		A	A

Probability and Partition Function

Chemical potential

Fermi-Dirac distribution





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