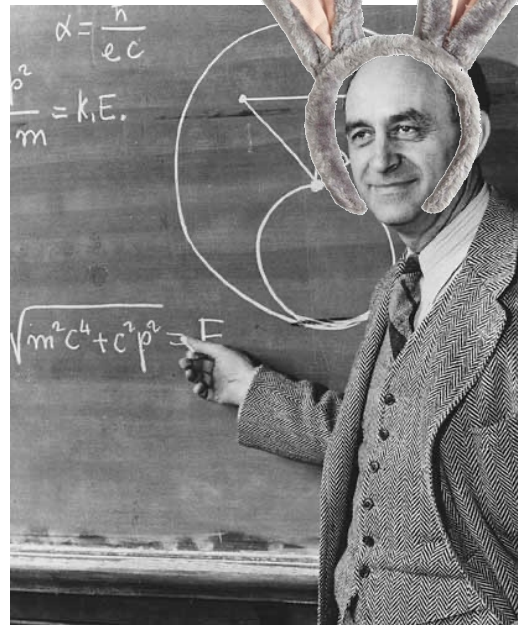


“Dr. Fermi, I presume?”

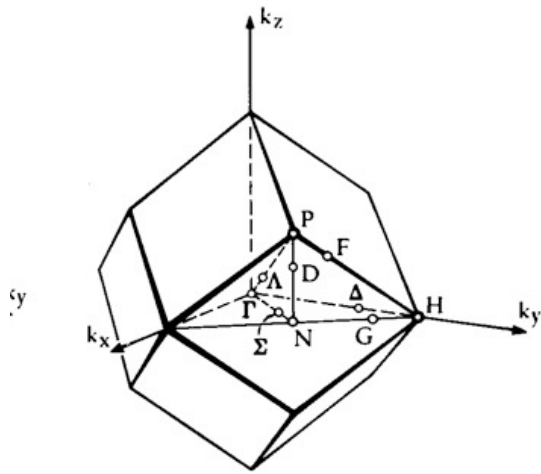


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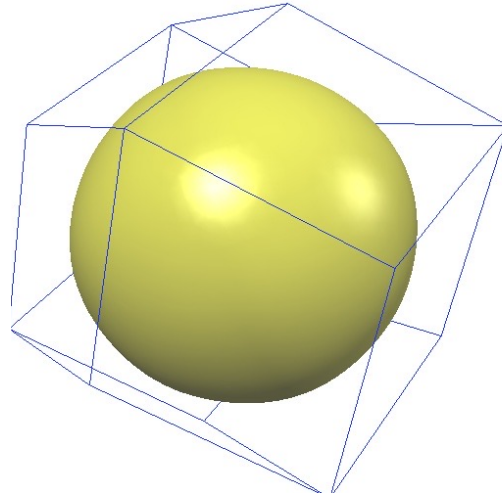
Last week

- Diamond/zincblende lattices and their BZs – special points and paths
- Band structures and ARPES
- Diamond and zincblende semiconductors
- Free electron gas and silicon; silicon vs lead; silicon vs germanium vs GaAs (also, OSSCAR)
- Valence and conduction band minima/maxima – discussion in Si/Ge/GaAs along a path or in 3D BZ
- Band gaps (values), and direct/indirect
- Perovskites, coinage metals, localized vs delocalized
- Group velocity and effective mass

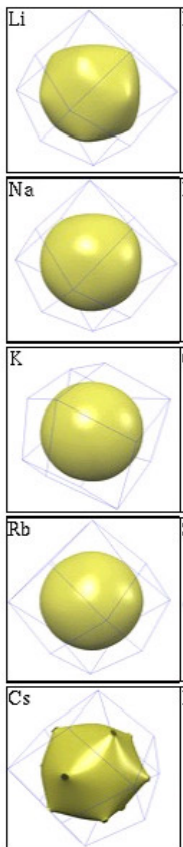
The Fermi surface



BODY CENTERED CUBIC

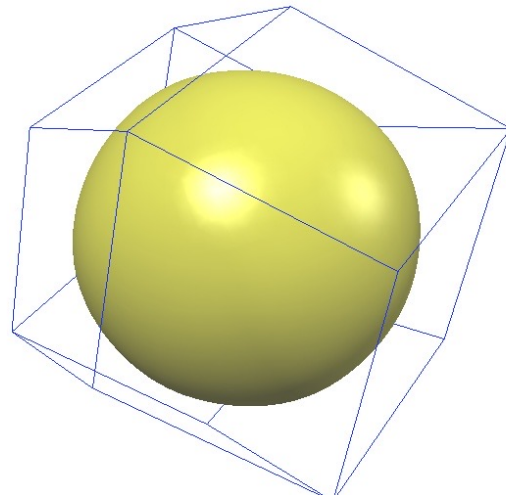


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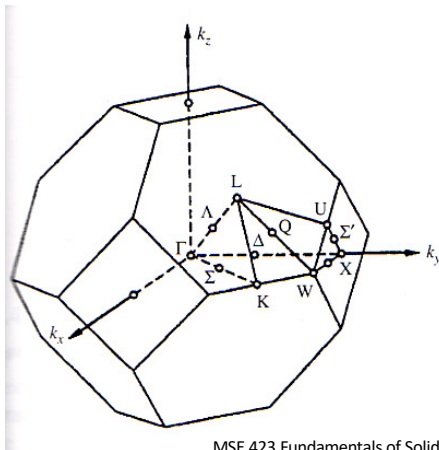
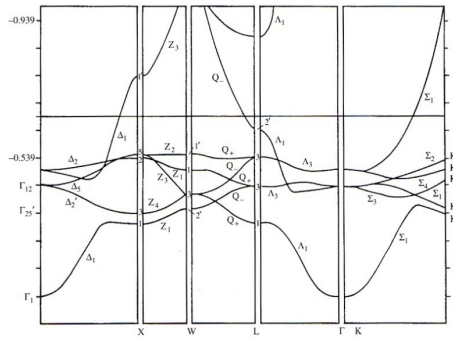
The Fermi surface

K

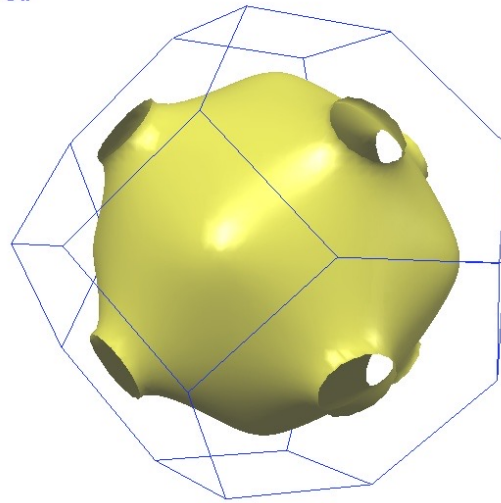


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The Fermi surface (fcc)



Cu



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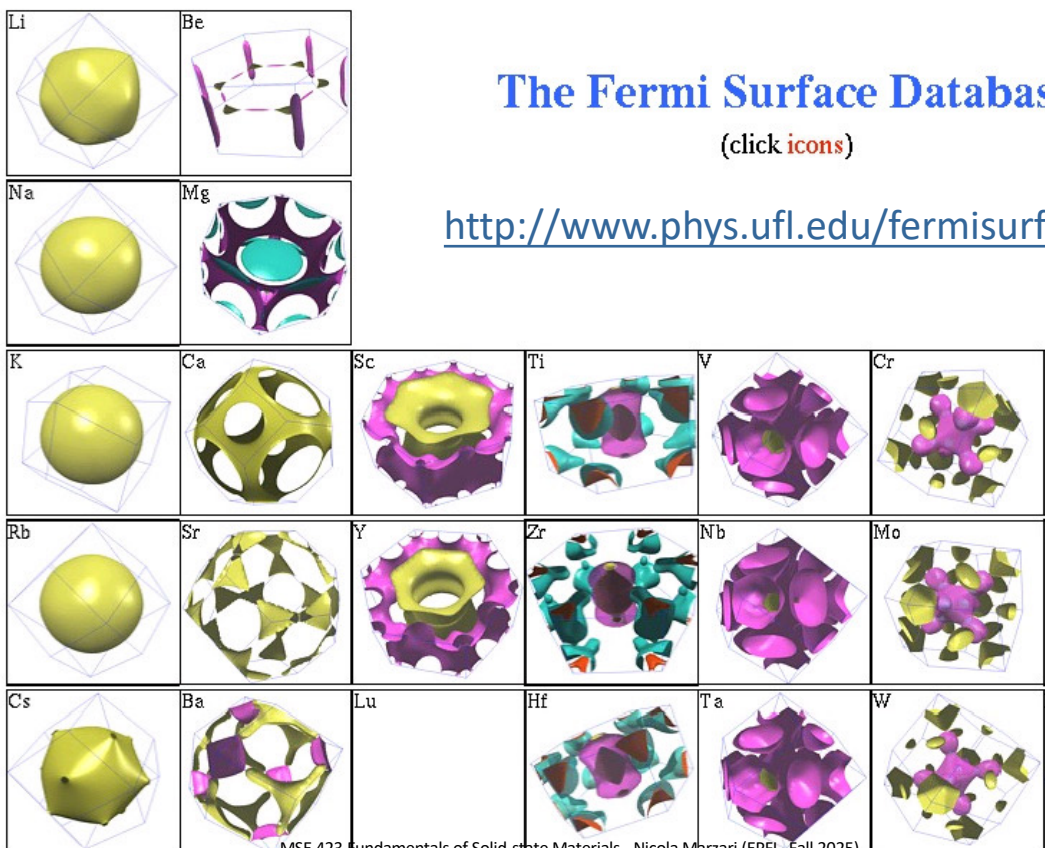
D (VRML) Fermi Surface Database

<http://www.phys.ufl.edu>

The Fermi Surface Databas

(click icons)

<http://www.phys.ufl.edu/fermisurface/>



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The independent-electron gas

- Hamiltonian
- Eigenvalues and eigenfunctions

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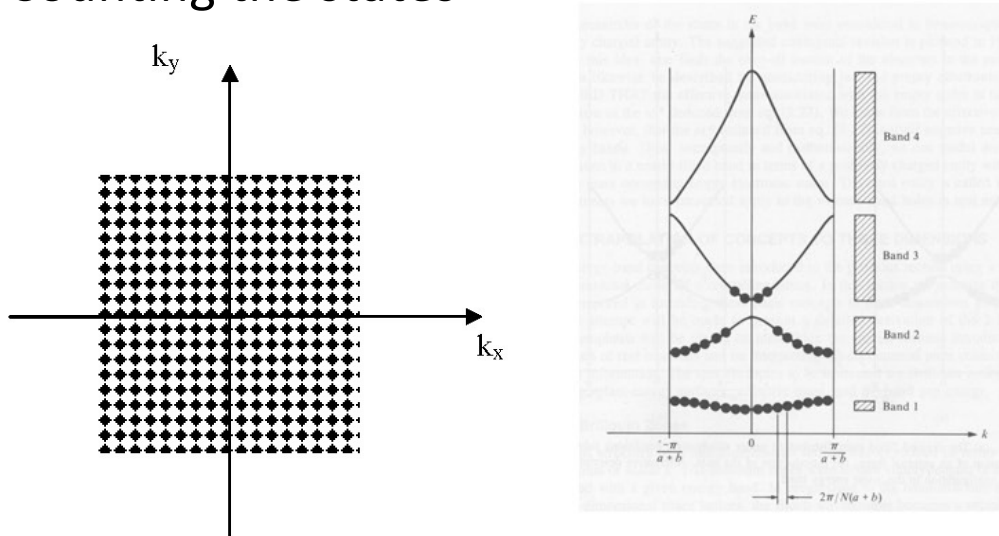
The independent-electron gas

- BvK boundary conditions

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The independent-electron gas

- Counting the states



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The independent-electron gas

- Particle density

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The independent-electron gas

- Energy density

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Density of states (for any solid)

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

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

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Massive vs massless bands

Dimensions	d=1	d=2	d=3
Massless ($E \approx k$)	const	E	E^2
Massive ($E \approx k^2$)	$1/\text{sqrt}(E)$	const	$\text{sqrt}(E)$

$$g_n(\epsilon) = 2 \int \frac{1}{8\pi^3} \frac{1}{|\nabla \epsilon_n(\vec{k})|} dS$$

- S goes as k^{d-1} , where d is the dimensionality
- $\frac{1}{|\nabla \epsilon(\vec{k})|}$ 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 $\epsilon^{(d-l)/l}$

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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

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Probability and partition function

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Chemical potential

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Fermi-Dirac distribution

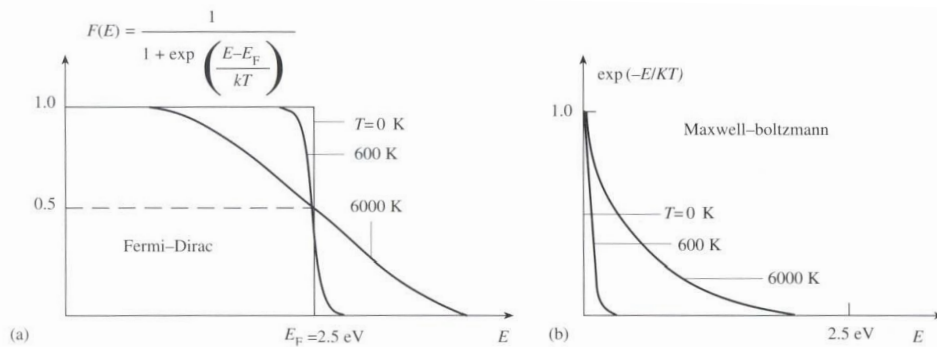


Fig. 6.1
(a) The Fermi-Dirac distribution function for a Fermi energy of 2.5 eV and for temperatures of 0 K, 600 K, and 6000 K.
(b) The classical Maxwell-Boltzmann distribution function of energies for the same temperatures.

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Tight-binding (LCAO for solids)

- Hamiltonian $\hat{H} = \hat{H}_{at} + \Delta\hat{U}(\vec{r})$

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Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

$$\Psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{R}} \exp(i\vec{k} \cdot \vec{R}) \varphi_n(\vec{r} - \vec{R})$$

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Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

$$\Psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{R}} \exp(i\vec{k} \cdot \vec{R}) \phi(\vec{r} - \vec{R})$$

$$\phi(\vec{r}) = \sum_n b_n \varphi_n(\vec{r})$$

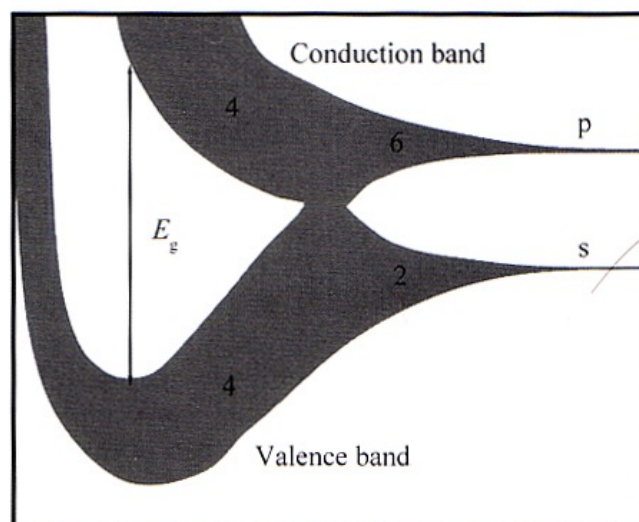
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From levels to bands

$$\varepsilon(\vec{k}) = E_m - \beta - \sum_{\substack{\text{nearest} \\ \text{neighb.}}} \gamma(\vec{R}) \cos(\vec{k} \cdot \vec{r})$$

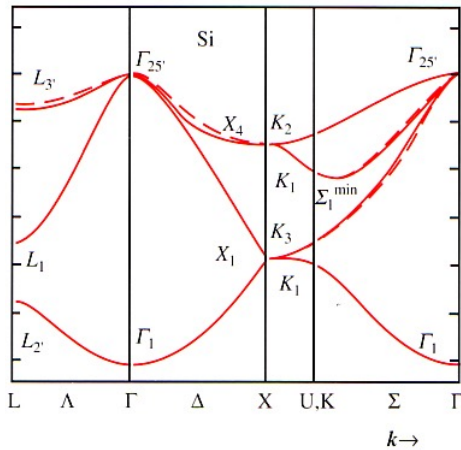
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From levels to bands



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How many bands in silicon ?



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Tight-binding vs. empirical psp

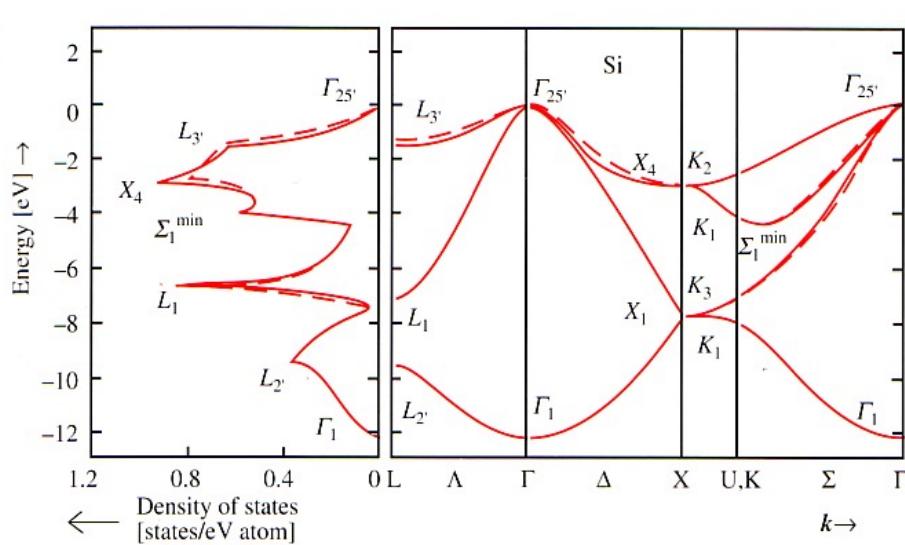


Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (*broken curves*) and by the empirical pseudopotential method (*solid lines*) [2.19]

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Tight-binding vs. empirical psp

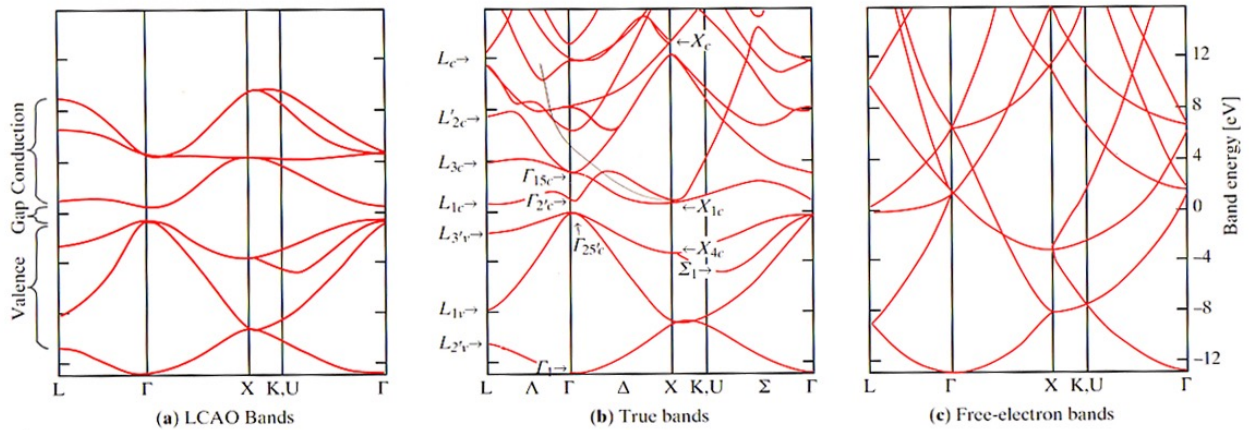
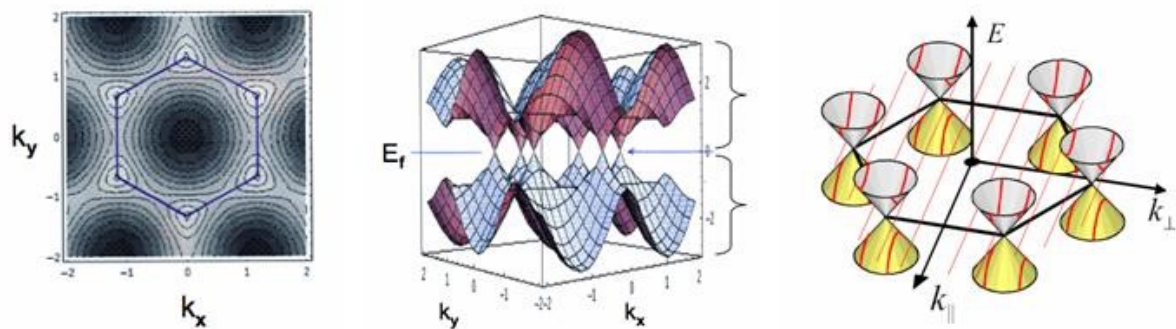


Fig. 2.25. A comparison between the band structure of Ge calculated by (a) the tight-binding method, (b) the empirical pseudopotential method, and (c) the nearly free electron model [Ref. 2.18, p. 79]

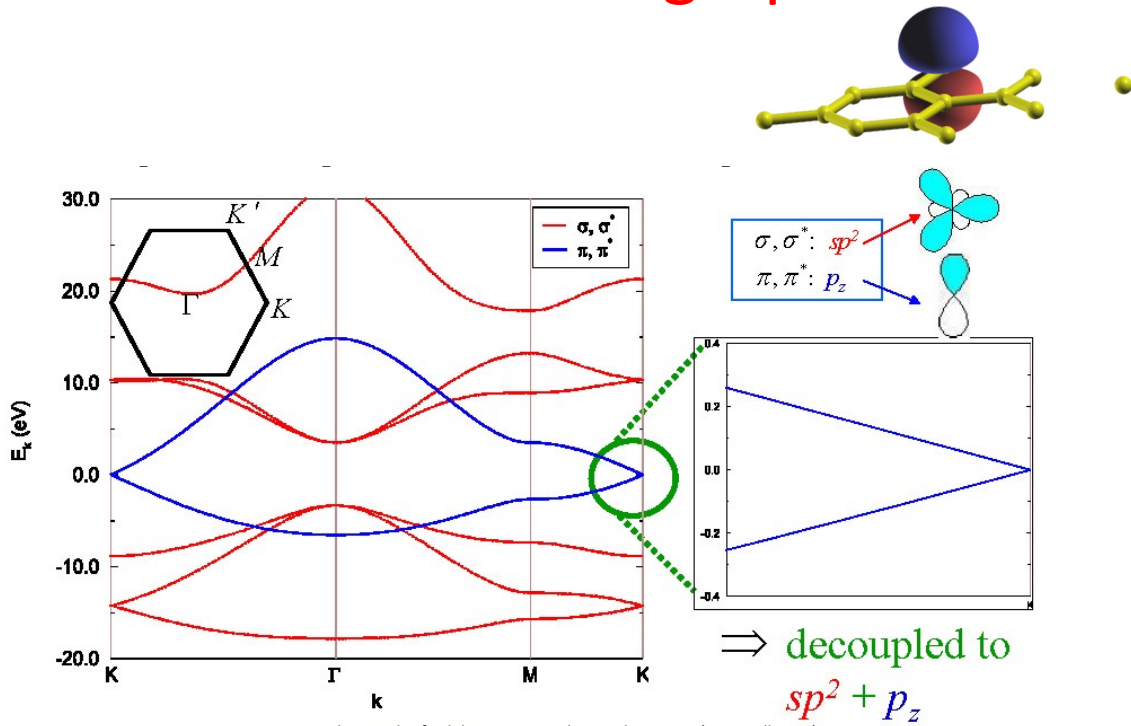
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Band structure of graphene

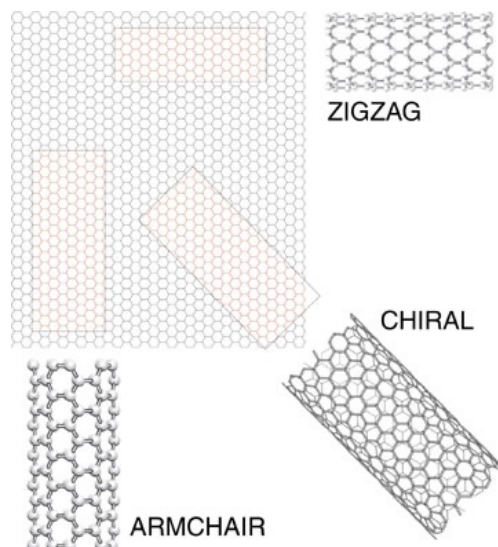


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Band structure of graphene



Carbon nanotubes



Zone folding: Band structure of nanotubes

