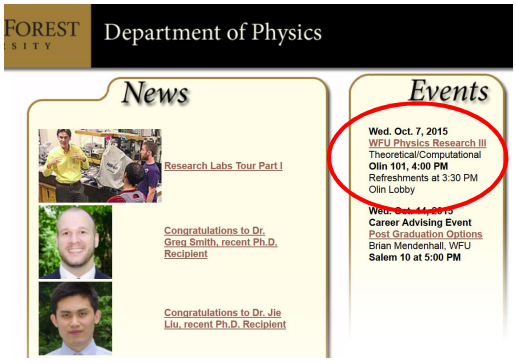
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 19:

Reading: Chapter 6 in GGGPP
Electronic properties of selected materials

1. **Covalent crystals – diamond and graphite**
2. **Metallic crystals**

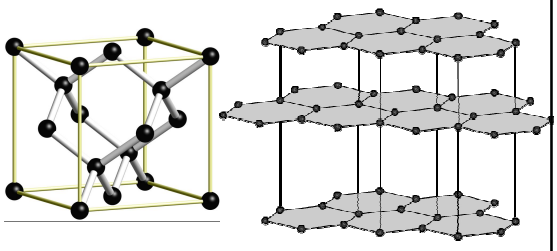
3	Mon, 8/31/2015	Chap. 1.4	Tight binding models	#3
4	Wed, 9/02/2015	Chap. 1.6, 2.1	Crystal structures	#4
5	Fri, 9/04/2015	Chap. 2	Group theory	#5
6	Mon, 9/07/2015	Chap. 2	Group theory	#6
7	Wed, 9/09/2015	Chap. 2	Group theory	#7
8	Fri, 9/11/2015	Chap. 2	Group theory	#7
9	Mon, 9/14/2015	Chap. 2.4-2.7	Densities of states	#8
10	Wed, 9/16/2015	Chap. 3	Free electron model	#9
11	Fri, 9/18/2015	Chap. 4	One electron approximations to the many electron problem	#10
12	Mon, 9/21/2015	Chap. 4	One electron approximations to the many electron problem	#11
13	Wed, 9/23/2015	Chap. 4	Density functional theory	#12
14	Fri, 9/25/2015	Chap. 5	Implementation of density functional theory	#13
15	Mon, 9/28/2015	Chap. 5	Implementation of density functional theory	#14
16	Wed, 9/30/2015	Chap. 5	First principles pseudopotential methods	#15
17	Fri, 10/02/2015	Chap. 6	Example electronic structures	#16
18	Mon, 10/05/2015	Chap. 6	Ionic and covalent crystals	#17
19	Wed, 10/07/2015	Chap. 6	More examples of electronic structures	#18
20	Fri, 10/09/2015	Chap. 1-6	Review	Start exam
	Mon, 10/12/2015		No class	Take-home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
23	Mon, 10/19/2015			



Covalent crystals

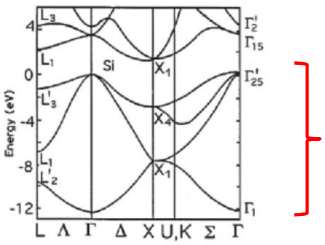
diamond

graphite



Band structure diagram of Si in diamond structure

Si $3s^2\ 3p^2 \rightarrow 3sp^3$



4 bands; accommodates 8 electrons

Band structure of graphene

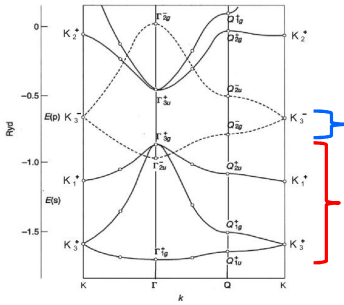


Figure 6.17 Band structure of graphene, obtained with the tight-binding method. Bands which are even and odd under reflection in the plane of graphene are indicated with continuous and broken lines respectively. The energies of the valence states of the carbon atom are also indicated. The values of $\mathbf{k}$ at the points Γ, K, and Q, are $\mathbf{k} = 0$, $\mathbf{k} = (2\pi/a)(2/3, 0)$, and $\mathbf{k} = (2\pi/a)(1/2, \sqrt{3}/6)$, respectively [from F. Bassani and G. Pastori Parravicini, Nuovo Cimento 50 B, 95 (1967); with kind permission from Società Italiana di Fisica].

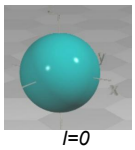
C $2s^2\ 2p^2 \rightarrow 2sp^2 + 2p\pi$

$p\pi$ band

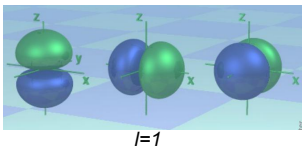
3 bands accommodate 6 electrons

Atomic orbitals for analyzing covalent materials

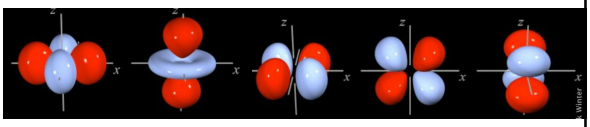
http://winter.group.shef.ac.uk/orbitron/



l=0



l=1



l=2

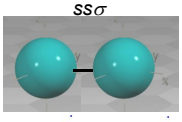
Orbital description of covalent bond --

While, for atoms the "*z*" axis is an arbitrary direction, for diatomic molecules and for describing bonds, it is convenient to take the "*z*" axis as the bond direction.

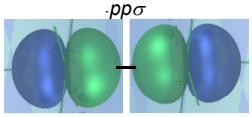
Atom			Bond		
		symbol			*symbol*
l=0	*m=0*	*s*	*l=0*	$\lambda=0$	σ
l=1	*m=0*	*p*	*l=1*	$\lambda=0$	σ
	m= ±1	*p*		$\lambda=1$	π
l=2	*m=0*	*d*	*l=2*	$\lambda=0$	σ
	m= ± 1	*d*		$\lambda=1$	π
	m= ± 2	*d*		$\lambda= 2$	δ

Atomic orbital bond types

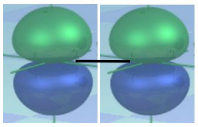
ssσ



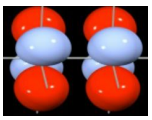
ppσ



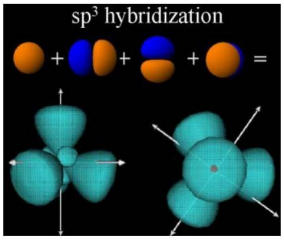
ppπ



ddπ



Linus Pauling's notion of hybrid bonds



http://butane.chem.uiuc.edu/pshapley/GenChem2/A6/index.html

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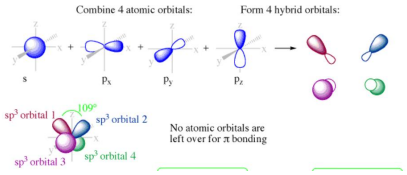
sp^3 hybrid bonds

Sigma Bonds with sp^3 Hybrid Orbitals

Atoms that have 4 bonds, 3 bonds and 1 lone pair, 2 bonds and 2 lone pairs, or 1 bond and 3 lone pairs need four hybrid orbitals 109 degrees apart. Combining an s orbital, a p_x orbital, a p_y orbital, and a p_z orbital makes four, sp^3 orbitals in a tetrahedral array.



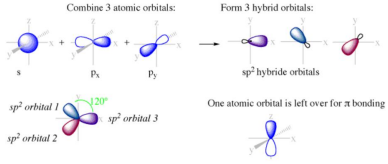
http://butane.chem.uiuc.edu/pshapley/GenChem2/A6/index.html

sp^2 hybrid bonds

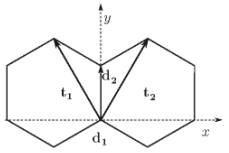
Sigma Bonds from sp and sp^2 Hybrid Orbitals

sp^2 Hybrid Orbitals in Borane

Atoms that have 3 bonds, 2 bonds and 1 lone pair, or 1 bond and 2 lone pairs need 3 orbitals that are 120 degrees apart. Consider the plane of these three orbitals to be the xy plane. Combining an s orbital with a p_x orbital and a p_y orbital makes three sp^2 hybrid orbitals.



Some details of the band structure of graphene, focusing on the pπ bands alone.



$$\mathbf{t}_1 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad \mathbf{t}_2 = a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad \mathbf{d}_1 = 0, \quad \mathbf{d}_2 = a\left(0, \frac{\sqrt{3}}{3}\right);$$

Approximate wavefunction based on linear combination of π orbitals

$$\Phi_{1,2}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{t}_m} e^{i\mathbf{k}\cdot\mathbf{t}_m} \phi_z(\mathbf{r} - \mathbf{d}_{1,2} - \mathbf{t}_m),$$

Hamiltonian in the basis of the π orbitals for sites 1 & 2:

$$\begin{Vmatrix} E_p - E & tF(\mathbf{k}) \\ tF(\mathbf{k})^* & E_p - E \end{Vmatrix} = 0,$$

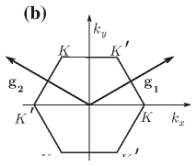
where *t* is a matrix element between sites 1 & 2 and

$$F(\mathbf{k}) = \sum_{\mathbf{t}_l} e^{i\mathbf{k}\cdot\mathbf{t}_l} = 1 + 2\cos\frac{k_x a}{2}\exp\left(-i\frac{\sqrt{3}k_y a}{2}\right);$$

Band structure:

$$E = E_p \pm t\left|F(\mathbf{k})\right|$$

Brillouin zone for graphene



$$K = \frac{4\pi}{3a}\hat{\mathbf{x}}$$

Band structure:

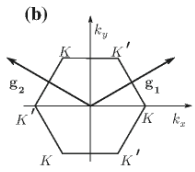
$$E = E_p \pm t\left|F(\mathbf{k})\right|$$

$$F(\mathbf{k}) = 1 + 2\cos\frac{k_x a}{2}\exp\left(-i\frac{\sqrt{3}k_y a}{2}\right);$$

Consider $\mathbf{k}_K = \frac{4\pi}{3a}\hat{\mathbf{x}} + \kappa\left(\cos\phi\hat{\mathbf{x}} + \sin\phi\hat{\mathbf{y}}\right)$

$$F(\mathbf{k}_K) = 1 + 2\cos\left(\frac{2\pi}{3} + \frac{\kappa a}{2}\cos\phi\right)e^{-i\frac{\sqrt{3}\kappa a \sin\phi}{2}}$$

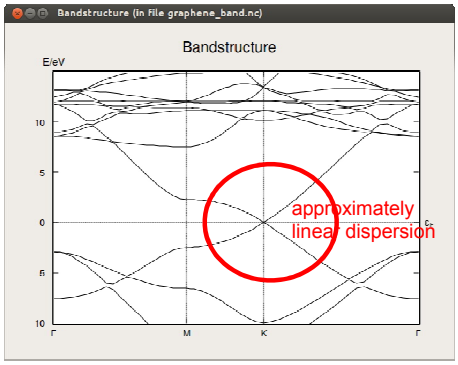
Brillouin zone for graphene



$$F(\mathbf{k}_K) = 1 + 2\cos\left(\frac{2\pi}{3} + \kappa a\cos\phi\right)e^{-i\frac{\sqrt{3}\kappa a\ \sin\phi}{2}}$$

$$\approx -\frac{\sqrt{3}\kappa a}{2}(\cos\phi - i\sin\phi) = -\frac{\sqrt{3}\kappa a}{2}e^{-i\phi}$$

$$E = E_p \pm t\left|F(\mathbf{k}_K)\right| \approx E_p \pm \frac{\sqrt{3}}{2}\kappa a t$$



Examples of bands from your textbook

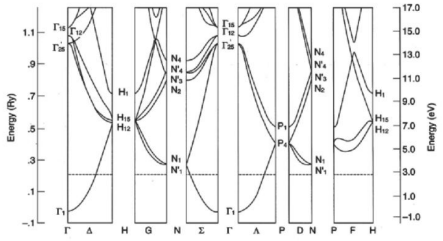


Figure 6.11 Band structure of sodium. The Fermi energy is indicated by a dotted line [from D. A. Papaconstantopoulos "Handbook of the Band Structure of Elemental Solids" (Plenum, New York, 1986); with kind permission from Springer Science and Business Media B. V.].

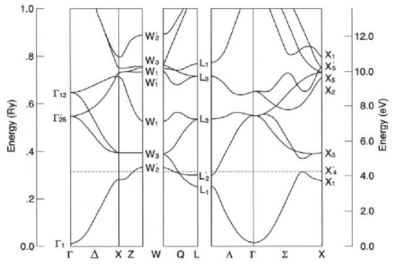


Figure 6.12 Band structure of calcium. The Fermi energy is indicated by a dotted line [from D. A. Papaconstantopoulos "Handbook of the Band Structure of Elemental Solids" (Plenum, New York, 1986); with kind permission from Springer Science and Business Media B. V.].

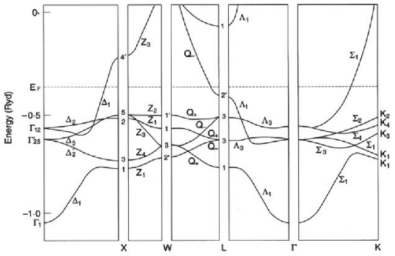


Figure 6.13 Band structure of copper [With permission from Fig. 3, Phys. Rev. *129*, 138 (1963)].

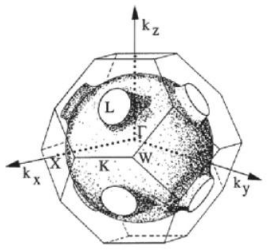


Figure 6.14 Brillouin zone for the face-centered cubic lattice and Fermi surface of copper.