Physics 140A-Introduction to Solid State Physics
Winter, 2016
Midterm Exam, February 9, 2016
(4 problems, 100 points total)

Name:_____

Student ID No.:_____

Questions regarding the LBNL tour

Do you want to participate in this optional tour? Yes_____ No_____

If yes, can you participate on these days?

Saturday, February 27_____Saturday, March 6_____

Do you have a car/van/truck/plane? Yes_____ No_____

If Yes, can you take additional people? Yes_____ No_____

If Yes, how many?_____

Some possibly useful constants and equations

$c = 3.00 \times 10^8$ m/s $e = 1.60 \times 10^{-19}$ C 1 eV = 1.60×10^{-19} J 1 Rydberg = 13.606 eV

1 Å = 10^{-10} m = 10 nm $h = 6.63 \times 10^{-34}$ J-s $\hbar = h/2\pi = 1.05 \times 10^{-34}$ J-s $k_B = 1.38 \times 10^{-23}$ J-K^{-}

$k_C \equiv 1/(4\pi\varepsilon_0) = 8.98 \times 10^9$ N-m^2-C^{-2} $a_0 = 0.529$ Å

$m_e = 9.1094 \times 10^{-31}$ kg = 0.5110 MeV/c^2 $m_p = 1.6726 \times 10^{-27}$ kg = 938.27 MeV/c^2

$m_n = 1.6749 \times 10^{-27}$ kg = 939.57 MeV/c^2 $n\lambda = 2d\sin\theta$ $d_{hk\ell} = n/[h^2/a^2+k^2/b^2+\ell^2/c^2]^{1/2}$ $F_{coul} = k_C \dfrac{q_1 q_2}{r^2}$

$\lambda = h/p$ $p = \hbar k$ $\Delta x \Delta p_x \geq \hbar/2$ $\Delta E \Delta t \geq \hbar/2$

$$e^{\pm ix} = \cos x \pm i \sin x \quad \cos x = \frac{1}{2}\left[e^{ix} + e^{-ix}\right] \quad \sin x = \frac{1}{2i}\left[e^{ix} - e^{-ix}\right]$$

$$\sin 2t = 2 \sin t \cos t \quad \cos 2t = \cos^2 t - \sin^2 t = 2\cos^2 t - 1 = 1 - 2\sin^2 t$$

$$E_n = -\frac{Z^2 e^2}{8\pi\varepsilon_0 a_0 n^2} = -\frac{13.6 Z^2}{n^2}(\text{eV}) \quad r_n = \frac{4\pi\varepsilon_0 \hbar^2}{m_e Z e^2} n^2 = a_0 \frac{n^2}{Z} \quad a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2} = 0.529 \text{ Å}$$

$$x = r\sin\theta\cos\phi \quad y = r\sin\theta\sin\phi \quad z = r\cos\theta \quad dV = r^2 dr \sin\theta d\theta d\phi$$

$$\psi_{n\ell m_\ell}(r,\theta,\phi) = R_{n\ell}(r)\Theta_{\ell m_\ell}(\theta)\Phi_{m_\ell}(\phi) = R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi) \quad P_{n\ell}(r) = r^2 R_{n\ell}^2(r) \quad \psi_{\vec{k}}(\vec{r}) = Ce^{i\vec{k}\bullet\vec{r}}$$

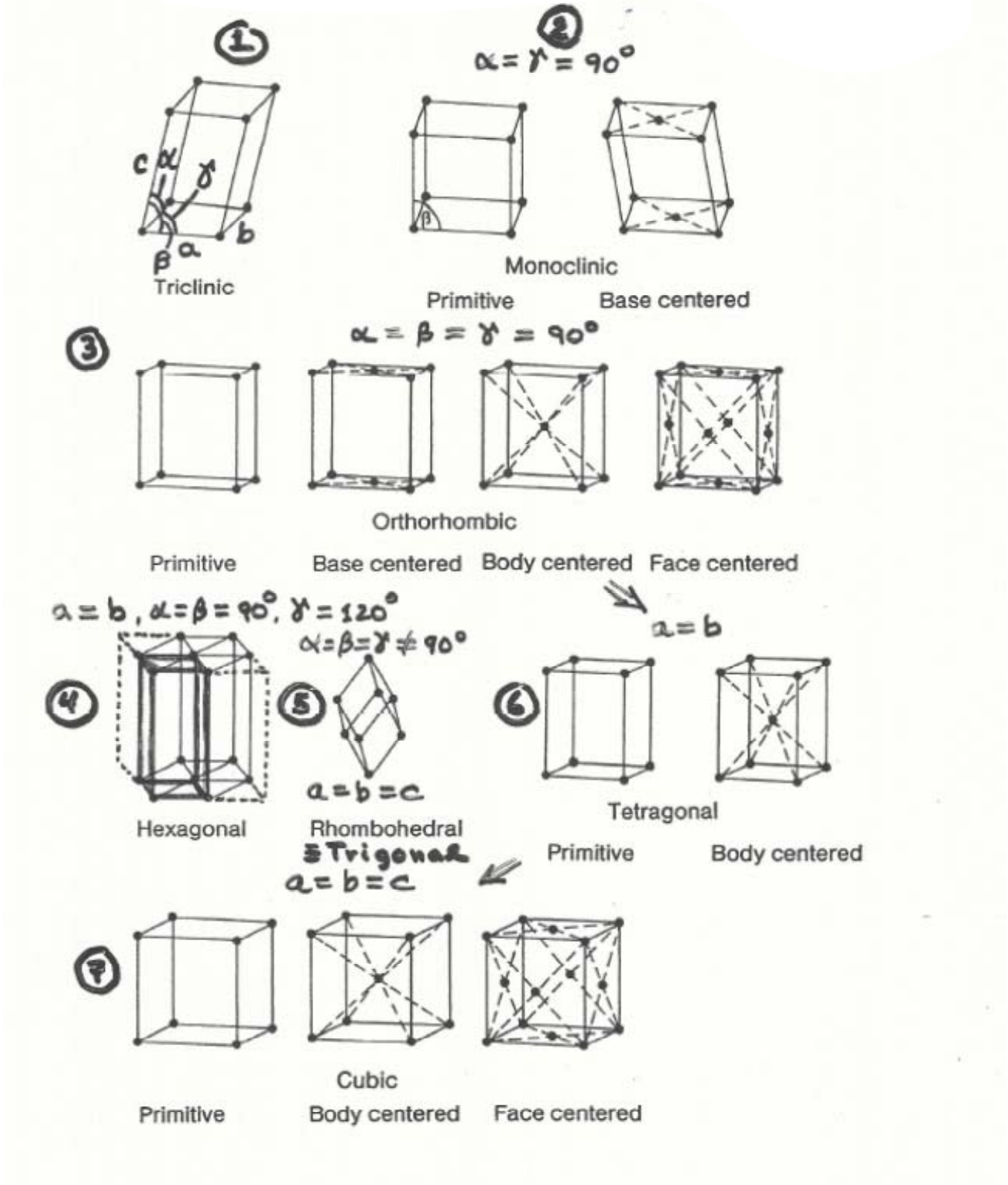
$$V = -\frac{C}{r^6} \quad V = \sum_{i=1}^{\infty} \frac{(+\text{or}-)n_i q_i}{4\pi\varepsilon_0 r_i} + \frac{A}{r_1^n} \quad F_{FD}(E) = \frac{1}{\exp[(E - E_F)/k_B T] + 1}$$

$$\varphi_j^{MO}(\vec{r}) = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} C_{Ai,j}\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A) \qquad \varphi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\bullet\vec{r}} = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} e^{i\vec{k}\bullet\vec{R}_A} C_{Ai,\vec{k}}\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A);\ u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{R}_\ell^{(c)})$$

$$\vec{R}_\ell^{(c)} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \vec{s} = \vec{k} - \vec{k}_0 = \vec{G} \quad f_a = \int_0^R 4\pi r^2 \rho(r)\frac{\sin(sr)}{sr}dr \quad F = \sum_j f_a e^{i\vec{s}\bullet\vec{\delta}_j} \quad S = \sum_\ell e^{i\vec{s}\bullet\vec{R}_\ell^{(c)}}$$

$$\vec{G} = h\vec{a}^* + k\vec{b}^* + \ell\vec{c}^* \quad \vec{a}^* = \frac{2\pi(\vec{b}\,x\,\vec{c})}{\vec{a}\bullet(\vec{b}\,x\,\vec{c})} \quad \vec{b}^* = \frac{2\pi(\vec{c}\,x\,\vec{a})}{\vec{a}\bullet(\vec{b}\,x\,\vec{c})} \quad \vec{c}^* = \frac{2\pi(\vec{a}\,x\,\vec{b})}{\vec{a}\bullet(\vec{b}\,x\,\vec{c})}$$

The seven 3D crystal systems and 14 Bravais Lattices



[1] (15 points) The following are a set of short questions that you should answer in a qualitative or semi-quantitative way with brief sentences or equations:

(a) (5 points) Which of these two elements would you expect to be more purely metallic (as opposed to mixed metallic-covalent) in its bonding: K $4s^1$ or Fe $3d^6 4s^2$ and why?

K = potassium will more purely metallic, as it has a lone 4s electron outside of an inert gas shell, which is easily removed to populate a free-electron-like band in the solid. By contrast, Fe has both an open 3d shell for covalent bonding, and 4s electrons that can contribute to metallic bonding--like all the transition metals.

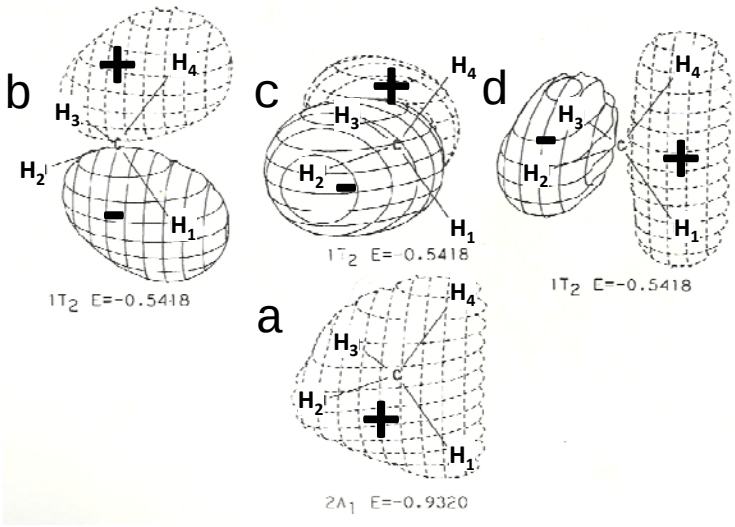
(b) (5 points) What is the origin of the Van der Waals interaction and how does it vary with distance?

Instantaneous dipole fluctuations on one atom which induce a dipole on the other atom, and a net attractive interaction that scales as $1/r^6$.

(c) (5 points) Qualitatively describe what is meant by the Fermi hole, and why it leads to one of Hund's rules for filling atomic subshells.

The Fermi hole is due to the antisymmetry of electron (or any fermion) wave functions, which implies that two electrons with the same spin (↑↑ or ↓↓) will have zero probability of being found at the same point in space. Thus, they stay out of one another's way better than electrons with opposite spins (↓↑ or ↑↓), and the net coulombic repulsion is reduced. [We give the effect of this reduction the name "exchange interaction", but it's really just a quantum-mechanical "adjustment" to the Coulomb interaction caused by anti-symmetry.] Therefore, we get the a lower energy when more spins are coupled parallel, and Hund's first rule results.

[2] (20 points)
The probability contours of the four lowest-energy valence molecular wave functions for tetrahedral methane (CH_4) are shown below, together with their energies in Rydbergs and their overall symmetry designations. Solid contour lines are negative in the wave function, dashed are positive.

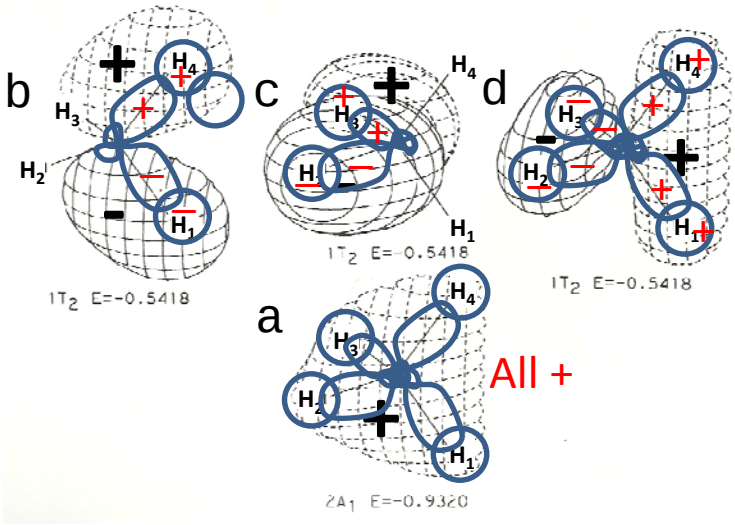


(a) (5 points) Are these bonding or anti-bonding and, if bonding, over which C and H atoms? Specify this for all four of a, b, c, and d.

a Bonding over C and all four hydrogens
b Bonding over C, H_1 and H_4
c Bonding over C, H_2 and H_3
d Bonding over C, H_1, H_4, H_2, and H_3

(b) (10 points) Show with a sketch the atomic-orbital makeup of each of these four wave functions, making use of the correct hybrid orbitals on C and the 1s on H.

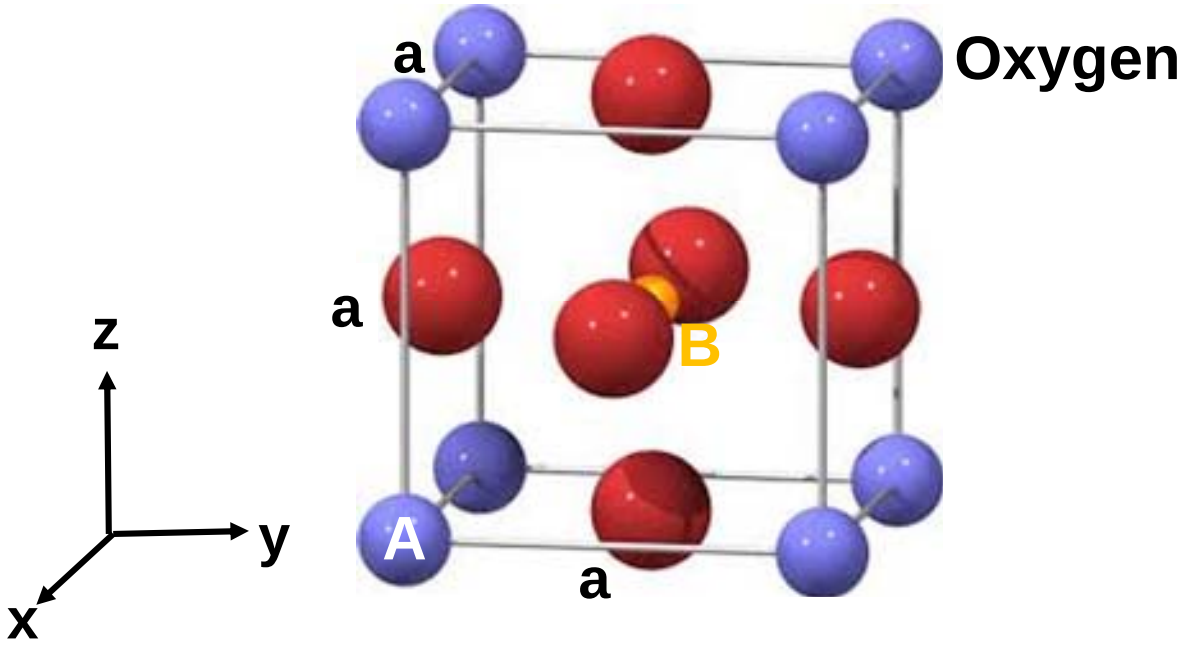
Use tetrahedral sp^3 hybrids on C, adding/subtracting, with H 1s to yield in the overlay sketch below, with the signs of the individual orbitals in red:



(c) (5 points) Wave functions b and c have the same energy of -0.5418 Rydbergs. Explain this in terms of symmetry. (Wave function d also has the same energy, by a more complex symmetry argument.)

Enough to just notice that these two wave functions are equivalent, in that a rotation of wavefunction a by 90 degrees around an axis in the page, and then a rotation by 180 degrees around an axis perpendicular to the page turns it into wave function b. Any equivalent symmetry argument, possibly involving mirror planes, gets full credit.

[3] (45 points) A typical inorganic crystal structure is that of "perovskite" oxide, as depicted below. It has a cubic unit cell and contains three types of atoms, as indicated by A, B, and O = Oxygen below, with B sitting at the center of the cubic unit cell of lattice constant *a* and inside an octahedron of O atoms.



(a) (5 points) What is the chemical formula for this type of crystal? Show your reasoning.

8 A atoms on corners x 1/8 = 1
6 O atoms on faces x ½ = 3
1 B atom in center x 1 =1

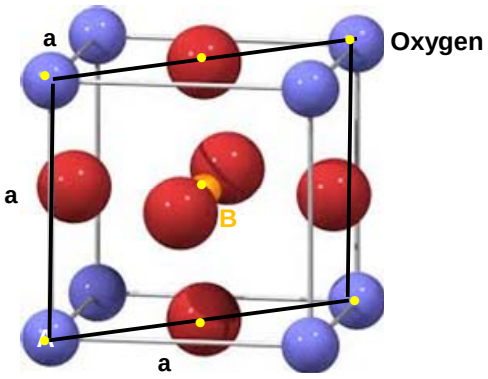
Therefore, ABO_3

(b) (5 points) Now assume ionic bonding. If the O is present as O^{-2}, and B is present as B^{+2}, what must the ionic charge be on A?

Just require overall neutrality, so 3 O^{-2} = -6, then B = +2, and A must be +4.

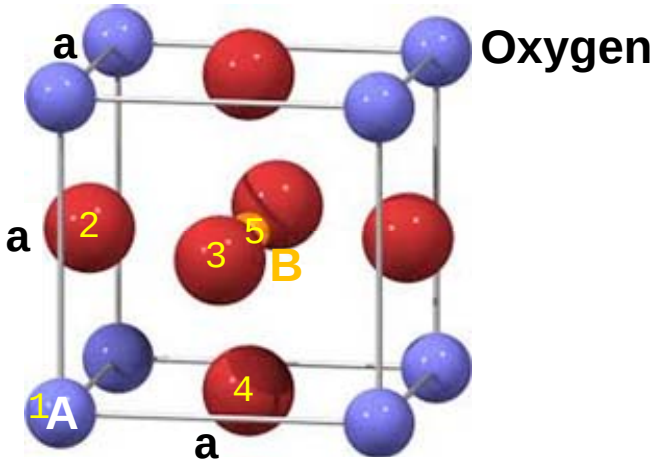
(c) (10 points) Sketch the (110) plane of this crystal, indicating clearly any A,B, and O atoms present.

The (110) plane is outlined in black below, and the seven atoms with the yellow dot will be in this plane.



(d) (5 points) What is the Bravais lattice of this crystal, and what is one suitable choice of the atomic basis for it? [There may be more than one choice of atomic basis that works.]

Simple cubic, and one basis that has all of the five atomic positions needed in it is the one below:



(e) (10 points) Now consider the packing of the ions in this crystal, and what conditions must hold among the three ionic radii r_A, r_B, and r_O for them to be

considered touching one another. Write down the <u>two independent equations</u> that must hold among these three radii.

$[r_B + r_O] = a/2$ and $r_A+r_O = \sqrt{2}a/2$

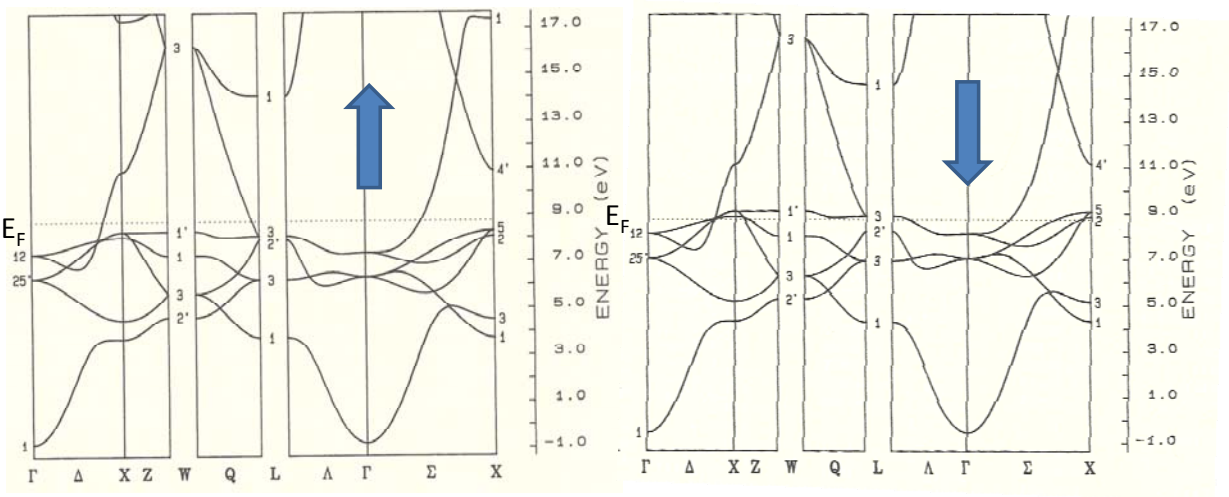
or $a = 2[r_B + r_O] = 2/\sqrt{2}[r_A+r_O]$

and if the "accommodation ratio" = $t = [r_B + r_O]/\sqrt{2}[r_A+r_O] \approx 1$, the perovskite structure is favored.

(f) (10 points) Now, assume that *a* = 3.9 Å and that an x-ray beam of 1.2 Å wavelength is incident on the full crystal. Predict the angles of first-order Bragg reflection from the (100) types of planes in this crystal.

For first-order Bragg reflection $\lambda = 2d_{hk\ell} \sin\theta$, with the d_{100} spacing given by $d_{hk\ell} = n/[h^2/a^2+k^2/b^2+\ell^2/c^2]^{1/2} = 1/[1/a^2 + 0 + 0]^{1/2} = a$, really a result you can just see from the unit cell. So $\sin\theta = \lambda/2d_{hk\ell} = 1.2/[2(3.9)] = 8.84°$.

[4] (20 points) Below is shown the electronic structure of a certain elemental solid, plotted in the usual fashion as a function of *k*, and for electrons of the two different spins.



(a) (5 points) What type of solid is this, a metal, a semiconductor, or an insulator, and explain your answer.

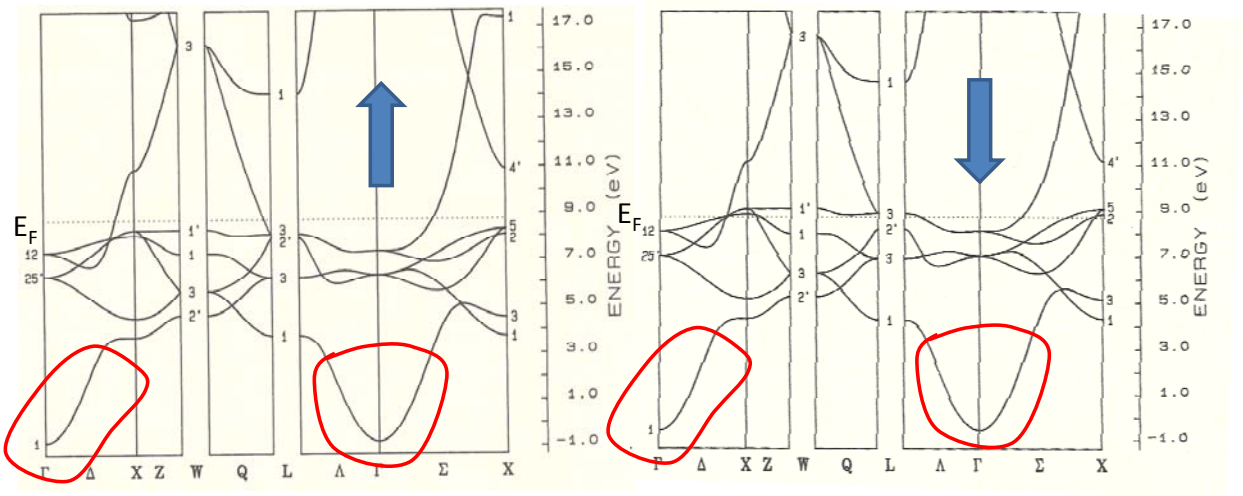
A metal, because it has bands crossing the Fermi level.

(b) (10 points) Is this material magnetic or not? Again explain your answer.

Looking carefully at these bands, you see that the spin-up are lower in energy than the spin-down. Thus, there will be a greater filling of spin-up, generating a net magnetic moment on the atoms, and magnetic order.

(c) (5 points) Do you see any states here that appear to be free-electron like? Indicate their presence by drawing on the above diagrams, and the equation that must represent their energy as a function of k.

The equation is $E(k) = \hbar^2k^2/2m_e$, and the bands circled below look free-electron like.



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