# Materials 218/UCSB: Assignment V


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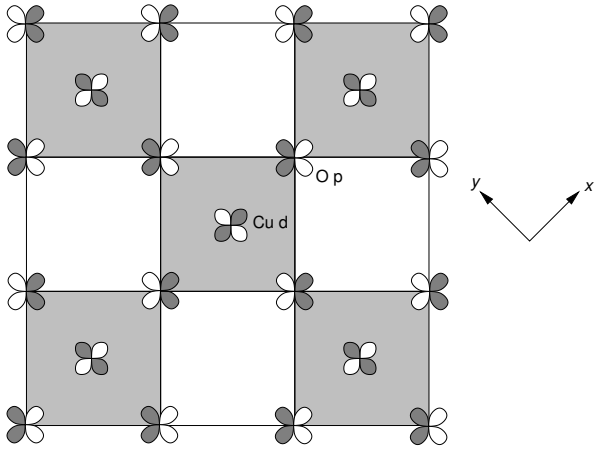
## Due date: February 27th 2003 (EXTRA TIME)

1. In class, we examined the band structure of a square lattice of $s$ orbitals. Sketch out the band structure of a *rectangular* lattice of $s$ orbitals with $a$ and $b$ as the lattice parameters and $a < b$. Remember that $X(0, \frac{\pi}{a})$ and $Y(\frac{\pi}{b}, 0)$ will not be degenerate. Sketch the DOS alongside.

2. Sketch the band structure of square lattice of $p_x$ and $p_y$ orbitals, with the DOS alongside.

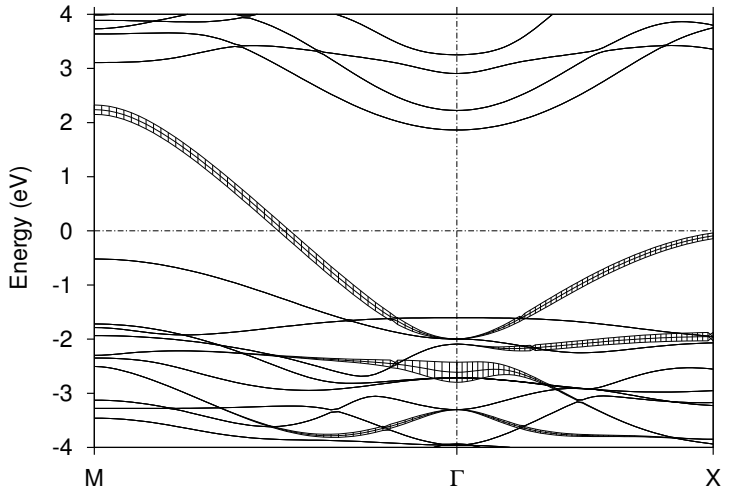
3. The Physics of High-$T_C$ superconductors:

   The essential electronic structural features of High-$T_C$ copper oxide superconductors are summarized in the sketch below, with perovskite $CuO_2$ planes represented by a chessboard. The black tiles on the chessboard have a copper atom with a $d_{x^2-y^2}$ orbital at the center. At the corner of every tile is an oxygen atom with a $p_x$ and a $p_y$ orbital.




   Sketch out the band structure of such a 2D lattice, concentrating on the band formed through the metal-oxygen-metal network (nearest neighbors). Suggest why similar compounds formed from *early* transition metals such as Ti or V would not have bands that are as disperse.[1].

   Compare your band structure with a DFT calculation on $La_2CuO_4$, the parent compound of all High-$T_C$ superconductors. Focus on the striped band. The 0 on the energy axis is the Fermi energy:




[1] Think of the filling of electrons into $d$ orbitals in a square-planar crystal field. Highly disperse bands are considered to be very important for High-$T_C$

4. The Cyrot-Lackmann theorem:

   Sometimes, it is convenient to be able to guess the form of the density of states at some *local* site in a structure. Françoise Cyrot-Lackmann [*J. Phys. Chem. Solids* **29** (1968) 1235] has suggested a theorem (the Moments Theorem) that allows one to do this.

   The theorem states:

   > The $n^{th}$ moment of the local density of states on an atom $i$ is the sum of all paths of length $n$ hops starting and ending on site $i$.

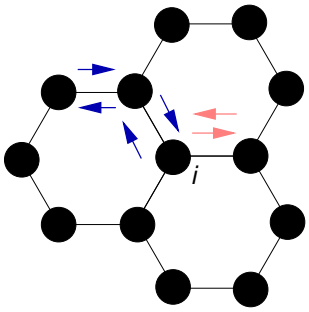
   The $n^{th}$ moment $\mu_i^{(n)}$ of the local DOS at site $i$ is defined:

   $$\mu_i^{(n)} = \int_{\text{whole band}} (E-\alpha)^n D_i(E)\, \mathrm{d}E$$

   where $\alpha$ is the center of gravity of the local DOS, and $D_i(E)$ is the local DOS at site $i$.

   As for any normalized distribution, the zeroth moment is 1 (the area under the DOS curve), the first moment is the mean or the center of gravity $\alpha$, the second moment is the width (like the standard deviation) of the DOS, and the higher moments describe the shape (skewness, kurtosis *etc.*).

   How are the hops calculated ? This is illustrated for the graphite lattice for the atom at site $i$:

   The pink arrows indicate hops of length 2. There are three such hops possible.[2] Each of these hops contributes $\beta^2$ to $\mu^{(2)}$. $\beta$ is the strength of the interaction between ions, and is related to covalency (more covalent $\Rightarrow$ larger $\beta$). There are no hops of length 3, so $\mu^{(3)} = 0$.[3]

   The blue arrows indicate hops of length 4. Each of these contributes $\beta^4$ to $\mu^{(4)}$ and there are 6 such hops. In addition, one can hop from site $i$ to a neighbor and back *twice*. This provides an additional $3 \times \beta^4$ (since there are three neighbors).

   So we have:

   $$\mu^{(0)} = 1;\ \mu^{(1)} = \alpha;\ \mu^{(2)} = 3\beta^2;\ \mu^{(3)} = 0;\ \mu^{(4)} = 9\beta^4$$

   It is known that for the moments of a distribution, the dimensionless quantity $s$ given by:

   $$s = \frac{\mu^{(4)}\mu^{(2)} - (\mu^{(2)})^3 - (\mu^{(3)})^2}{(\mu^{(2)})^3}$$

   is indicative of whether the distribution is unimodal ($s \geq 1$) or bimodal ($s < 1$).

   (a) Calculate $s$ for the site $i$ in the graphite lattice and use this to describe the nature of the local DOS at site $i$.

   (b) Calculate $s$ for an atom in the middle of a 1D chain and for an atom at the end of the chain. Are the DOS unimodal or bimodal at these sites ?

5. Effects of dimensionality:

   (a) Show from considerations of $\mu^{(2)}$ that on going from 2D to 3D, (a square lattice to a simple cubic lattice) the DOS broaden significantly ($\mu^{(2)}$ is larger).

   (b) Is the DOS skewed or symmetric in the above two cases ?

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[2] One can only hop along a bond.

[3] $\mu^{(3)} = 0$ means the DOS is symmetric about its center of gravity. In other words, it is not skewed. $\mu^{(3)} < 0$ means the distribution is skewed towards higher energies with a long tail at lower energies. $\mu^{(3)} > 0$ means the opposite.