0. The class website is located at
http://www.physics.oregonstate.edu/~tate/COURSES/ph575/
Read over the "Course Information" handout, noting the computational component and the associated poster and paper component. Note the statement that homework solutions need to have an interpretive component and be well-written. Browse the class website.

1. Write a ≈200-word summary of an article that discusses the band structure of a material of recent interest. Choose an article that has been published within the last two years in one of the journals listed under "online resources" on the class wiki. You can browse recent issues, or search the abstracts for "band structure".

2. Find an example of a solid in which (i) *s* (ii) *p* (iii) *d* orbitals are the most important for the material properties. Give a short explanation.

3. **Expressing *s, p, d* functions as linear combinations of Y_{lm} functions**
(based on Sutton, problem #5; Explore the Mathematica worksheet on the class webpage under "Online resources")
Goals: Visualize and manipulate complex and real wave functions. Express one orthogonal set (the *s, p, d* real spherical harmonics) in terms of another orthogonal set (the $Y_{\ell m_\ell}(\theta,\phi)$ complex spherical harmonics).

Sutton problem #5, p.239 lists the complex spherical harmonic functions $Y_{\ell m_\ell}(\theta,\phi)$.
Also see class webpage under "worksheets". These are the angular parts of the solutions to the Schrödinger eigenvalue equation
$H\underbrace{R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)}_{\varphi(\vec{r})} = E_n\underbrace{R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)}_{\varphi(\vec{r})}$ for the H-atom in the position representation.
Focus on the five $l = 2$ states. They form an orthogonal set.
Sutton Eq. 1.22 lists another orthogonal set of functions that describe the usual five *d*-orbitals for the H-atom. They are (excluding the $R_{n2}(r)$ part):

$$d_{z^2} = \sqrt{\frac{15}{4\pi}}\frac{\left(3z^2 - r^2\right)}{2\sqrt{3}r^2}$$

$$d_{x^2-y^2} = \sqrt{\frac{15}{4\pi}}\frac{\left(x^2 - y^2\right)}{2r^2}$$

$$d_{xy} = \sqrt{\frac{15}{4\pi}}\frac{xy}{r^2} \qquad d_{yz} = \sqrt{\frac{15}{4\pi}}\frac{yz}{r^2} \qquad d_{xz} = \sqrt{\frac{15}{4\pi}}\frac{xz}{r^2}$$

Your task, for each of the five d-states ….
(a) Make a 3-d plot of the shape of the *d*-orbital (angular part only; you may use the Mathematica template on the class website).
(b) Find which particular linear combination of the $Y_{\ell m_\ell}(\theta,\phi)$ makes up each *d* orbital.

For example, one d orbital is $d_{x^2-y^2}(x,y,z) = \sqrt{\frac{15}{4\pi}}\frac{x^2-y^2}{2r^2}$. You must write $d_{x^2-y^2} = a_{22}Y_{22} + a_{21}Y_{21} + a_{20}Y_{20} + a_{2,-1}Y_{2,-1} + a_{2,-2}Y_{2,-2}$ and evaluate the "a" constants.

4. **Expressing operators as matrices:**
In this course, you will come across operators expressed as matrices and you will have to manipulate matrix elements. The most common example is the Hamiltonian operator, but this problem will use angular momentum operators, L^2 and L_z. For this problem, all you need to know is that the $|Y_{2m_\ell}\rangle$ form an orthogonal set and are eigenstates of L^2 and L_z:

$$L^2|Y_{2m_\ell}\rangle = \ell(\ell+1)\hbar^2|Y_{2m_\ell}\rangle;\ L_z|Y_{2m_\ell}\rangle = m_\ell\hbar|Y_{2m_\ell}\rangle$$

(a) Find the 5x5 matrix representation for the L^2 and the L_z operators in the space described by the five complex basis vectors $|Y_{2m}\rangle$
(b) Do the same for the five real basis functions $|d_j\rangle$
(c) Show that the trace of the matrices is the same regardless of the basis.

Useful info: A matrix element for an operator O is defined as $O_{ij} = \langle i|O|j\rangle$ where the ket $|j\rangle$ represents the state of a system described by a set of quantum numbers j, and the bra $\langle j|$ is its complex conjugate. For example, in the case of the $l=2$ states of hydrogen where there are 5 basis states (10 if we include spin, but don't consider spin in this problem), the kets might be, in the $|Y_{\ell,m_\ell}\rangle$ basis:

$$|1\rangle = |\ell=2, m_\ell=-2\rangle = |Y_{2,-2}\rangle;\quad |2\rangle = |\ell=2, m_\ell=-1\rangle = |Y_{2,-1}\rangle;\quad |3\rangle = |\ell=2, m_\ell=0\rangle = |Y_{2,0}\rangle$$

$$|4\rangle = |\ell=2, m_\ell=+1\rangle = |Y_{2,+1}\rangle;\quad |5\rangle = |\ell=2, m_\ell=+2\rangle = |Y_{2,+2}\rangle$$

and in the $|d_j\rangle$ basis (where the primes remind us we're using a different basis)

$$|1'\rangle = |d_{x^2-y^2}\rangle;\quad |2'\rangle = |d_{yz}\rangle;\quad |3'\rangle = |d_{z^2}\rangle;\quad |4'\rangle = |d_{xz}\rangle;\quad |5'\rangle = |d_{xy}\rangle$$

EXTRA PROBLEMS for those who want more advanced formalism (physics majors, especially, I'm looking at you!):

6. Sutton, problems # 6, 7 &8
(They are the same, but one uses the language of vectors and the other the language of kets)
7. If you need extra practice getting used to the language of bras, kets, projections, and wave functions, repeat problems 1 and 2 for the p states. For those of you not used to this language, I can give extra sessions to help you. From long experience, I know that any confusion comes from notational issues, not from fundamental conceptual problems. Come and talk to me or to the TA. Also ask physics classmates to explain – it will be good for them – and you will be able to return the favor later in the course.