140A-Introduction to Solid State Physics--Study guide for first midterm:

Coverage:

Don't worry about memorizing complicated formulas, just try to understand their origin and how to use them. The exam will have a table of pertinent equations and constants on its first page. If needed, I will hand out a sheet with the 14 Bravais lattices.

•Reading-

- **Omar: All of Chapter 1, plus Sections 5.1-5.3 to p. 181, not Energy Bands, 5.8 through Eq. 5.28 only; 2.1-2.7**
- **For anyone in need of a review of basic quantum mechanics, Omar has a nice review in Appendices A.1-A.3, A.5, A.7, and A.8, which total only 10 pages**
- **Ibach and Luth: All of Chapter 1, 2.1-2.5 only, but lighter on 2.2 and 2.4, all lecture slides, through Slide 19 in Slide Set 3, all problems assigned to date**

Some concepts to understand or questions to be able to answer:

•Course introduction:

- **How is solid state physics/condensed matter physics important in fundamental science (e.g. Nobel Prizes in Physics, nanoscience) and modern technology (e.g. Moore's Law, magnetic data storage, energy production)?**
- **What is a field effect transistor? Why is it important?**
- **What is a nanostructure? Why are they important?**

•Review of some basic quantum mechanics and atomic physics: (Largely from Ibach and Luth, but see Appendices A.1-A.3, A.5 in Omar if needed)

- **Review of the hydrogen atom problem in quantum mechanics; separation into radial, polar, and azimuthal parts of wave function ψ; extension to many-electron atoms via a screened Coulomb interaction and Z_{eff}**
- **Conversion of imaginary atomic wave functions into real form for use in linear combination of atomic orbitals (LCAO) = tight-binding (TB) description of covalent bonding**
- **Many-electron wave functions for Fermions, anti-symmetry and the Pauli Principle**
- **Anti-symmetry and the Fermi hole for spin-parallel electrons, giving rise to the exchange interaction and lower energies if more electrons have parallel spin, thus also magnetism and Hund's First Rule.**
- **Filling of the periodic table, including reasoning for order of filling subshells: 1s, 2s, 2p, 3s, 3p, 4s, 3d,…, and special cases when outer d or f shells are half-, or totally-filled**

•Bonding in molecules and solids: (Largely Ibach and Luth, but see Omar, Appendices A.7, and A.8 if needed)

•Cohesive energy (lattice energy) of a crystal: meaning and calculation, including from individual bond energies in covalent solids

•Covalent bonding:

- **Simple quantum-mechanical description of bonding in a diatomic molecule via LCAO (tight-binding) description, minimization of energy, meaning of H_{AA}, H_{BB}, H_{AB}, H_{BA}, S_{AA}, S_{BB}, S_{AB}, S_{BA}, origin of secular equation for solution**
- **For simple molecules: bonding and anti-bonding wave functions, sigma and pi character**
- **Filling of molecular electronic levels**
- **Energy as a function of interatomic distance for molecules and solids: contributions from electron-nuclear attraction, nuclear-nuclear repulsion, and electron-electron repulsion**
- **Directed bonds: sp^3 tetrahedral bonding, sp^2+p bonding, other possibilities with d orbitals**
- **Broadening of electronic states into bands for solids, filling of bands and solid types based on filling: metallic, ferromagnetic metallic, insulator, semiconductor, ionic solid**

•Metallic bonding:

- **Some valence electrons acting essentially like free electrons, delocalize to reduce their energy and screen the core-core repulsions left behind**
- **Transition metals (3d, 4d, 5d and 4f, 5f series) have mixture of covalent and metallic bonding, example of Cu $3d^{10}$(covalent)$4s^1$(metallic, free-electron like)**

•Ionic bonding:

- **Ionization potential and electron affinity**
- **Electronegativity as measure of net electron attracting power**
- **Calculation of the net ionic attraction with 1/r variation and the Madelung constant**

- **Repulsive potential at short distance due to electron-electron repulsion with $1/r^n$ variation**
- **Calculation of binding energy (lattice energy) of crystal; derivation of pertinent parameters from form of overall interaction**

•Van der Waals attraction:

- **Oscillating dipoles due to electrons on atoms: $1/r^6$ variation**

•Hydrogen bonding:

- **H atom bound to very electronegative atom→weak bond to another electronegative atom**

•Relative strengths of five interaction types: covalent, metallic, ionic, van der Waals, hydrogen bonding

- **Bloch functions for electrons in periodic potential, general properties**

•Crystal structures: Primarily from Omar, Chapter 1

- **Translational periodicity and translation symmetry operations: meaning**
- **Basis vectors and the Bravais lattice**
- **Bravais lattice + basis = crystal**
- **Recognition of the bravais lattice and the basis in a real crystal**
- **Unit cells: primitive and non-primitive**
- **Primitive and non-primitive basis vectors for a given structure**
- **14 types of three dimensional Bravais lattices**
- **Planes in crystals and Miller indices: (hkl) and sets {hkl}**
- **Directions in crystals: [hkl] and sets <hkl>.**
- **Spacings between planes in crystals with orthogonal basis vectors**
- **Formulas of compounds from the crystal structure; counting atoms in the unit cell**
- **Packing of touching spheres in different crystals**
- **Other special crystal structures: sodium chloride, cesium chloride, diamond**
- **Calculation of ideal ionic radii ratios in different ionic crystals: cesium chloride, sodium chloride, zinc blende**
- **Point group symmetry operations:**
  - **Rotations by $2\pi/n$ = n-fold rotation**
  - **Reflection in a mirror plane**
  - **Inversion ($\vec{r} \rightarrow -\vec{r}$)**
- **Crystal group = Translation group + Point group**

•Diffraction and Crystal Structure Determinations-"Lite": Primarily Chapter 2 in Omar, but less quantitative for midterm, dealing only with problem types assigned in Problem Set 2 and simpler questions on scattering and diffraction

- **Types of scattering and diffracting de Broglie waves: photon, electron, neutron, helium atom,…**
- **Generation of x-rays: x-ray tube, synchrotron radiation**
- **Bragg's Law: two views via planar reflection and scattering from an array of individual atoms**
- **Derivation of the scattered intensity, basic formulas, division into atomic scattering factor f_a, geometric (unit cell or basis) structure factor F and lattice structure factor S**
- **The atomic scattering factor; general form and derivation**
- **The reciprocal lattice and its vectors $G_{hk\ell}$.**
- **The Ewald construction**
- **Forbidden reflections for some crystal structures (e.g., bcc and fcc) due to F**
- **Brillouin zones**