Review Topics for Midterm

1. **Bonding ~40% test**
   1. Hybridization in covalent structures
   2. Trends in periodic table – EN, size, mass, valence
   3. Pauling’s ionicity fraction
   4. Shape (nature) of bonding force/energy vs. interatomic separation curves. How force and energy curves influence material properties. Know where $E_o, r_o, \sigma, \epsilon$ are on the curves and what they mean.
   5. Bonding models: simple and more advanced. Do not memorize formulas but know what each term, or group of terms, means in relation to the bond force/energy and interatomic distance; cohesive energy/atom(U’); lattice energy (V), etc.
   6. Appropriate pair potentials for ionic materials must obviously contain an electrostatic component, a short-range repulsion and an attractive VDW component.

2. **Crystal structures (“so far”) ~60% test**
   1. Definition of crystal structure. Metallic, ionic and covalent crystal structures – where do you expect to find them on periodic table.
   2. Centering operations. Count lattice points (ions or atoms) per unit cell. Determine chemical formula (stoichiometry) and number of formula units per unit cell.
   3. Close packed sites and interstitial sites in metallic and ionic crystal structures.
   4. Calculate linear, planar, volume (bulk) densities (know your Miller indices!).
   5. Classifying crystal structures: packing, compositional ordering, and filling of interstitial sites.
   6. 3 site selection rules for ceramic (majority ionic bonding) crystal structures. Shannon radii table.
   7. Be familiar with all crystal structures we went over in class (applying the above concepts).
   8. Interstitial compounds – where to find them.
   9. Periodic Trends in Bonding and Structure
10. Four 2-D (primitive) crystal systems $\rightarrow$ Seven 3-D (primitive) crystal systems \((\text{know their lattice parameters})\)

11. Types of lattices; Number of lattice points: tells you number of atoms needed to define your basis.

12. Lattice points are categorized based on the 3 possible centering operations (base, face and body) + primitive (simple) arrangements.

13. Can we add additional lattice points to the primitive lattices (or nets), in such a way that we still have a lattice (net) belonging to the same crystal system? \textit{Answer}: in 2-D we can only add one more lattice point to rectangular to get centered rectangular lattice $\rightarrow$ (Five 2-D Bravais lattices).
   1. Since the surroundings of every lattice point must be identical, we can only add new lattice points at centered positions.

14. By repeating this procedure in 3-D, where there are now 3 possible ways to add lattice points at the center between existing lattice points, we have base (A,B and/or C), face (F) or body (I),

15. We can now apply these 5 forms of centering (I,F,A,B,C) to all seven 3-D (primitive) crystal systems: 5x7=35 possibilities.
   1. In several cases we do generate a new lattice, in other cases we can redefine the unit cell and reduce the cell to another type. Also, must maintain minimum symmetry requirements for that crystal system \((\text{know the minimum symmetry requirements for the 7 crystal systems})\).
   2. Reducing from 35 to \textbf{Fourteen} 3-D (7 primitive and 7 non-primitive) Bravais lattices means either the unit cell is not unique (choose one that is easier to work with) or crystal system symmetry is lost.
   3. Repeating this exercise for all types of lattice centering, we end up with 7 additional \textbf{non-primitive} lattice types that cannot be reduced to primitive ones of the same crystal system: \(\text{mC,oC,oI,oF,tI,cI,cF}\). \textit{(know these)}:
16. One of the 14 Bravais lattices + basis positions (vectors) = crystal structure (we went over many examples so far).

<table>
<thead>
<tr>
<th>System</th>
<th>Axial lengths and angles</th>
<th>Bravais Lattice</th>
<th>Lattice Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>Three equal axes at right angles ( a = b = c; \alpha = \beta = \gamma = 90^\circ )</td>
<td>Simple Face-centered</td>
<td>P I F</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>Three axes at right angles, two equal ( a = b \neq c; \alpha = \beta = \gamma = 90^\circ )</td>
<td>Simple Body-centered</td>
<td>P I</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>Three unequal axes at right angles ( a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ )</td>
<td>Simple Body-centered Base-centered Face-centered</td>
<td>P I C F</td>
</tr>
<tr>
<td>Rhombohedral (trigonal)</td>
<td>Three equal axes, equally inclined ( a = b = c; \alpha = \beta = \gamma \neq 90^\circ )</td>
<td>Simple</td>
<td>R</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>Three equal coplanar axes at 120°, third axis at right angles ( a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ )</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>Three unequal axes, one pair not at right angles ( a \neq b \neq c; \alpha = \gamma = 90^\circ \neq \beta )</td>
<td>Simple Base-centered</td>
<td>P C</td>
</tr>
<tr>
<td>Triclinic</td>
<td>Three unequal axes, unequally inclined and none at right angles ( a \neq b \neq c; \alpha \neq \beta \neq \gamma \neq 90^\circ )</td>
<td>Simple</td>
<td>P</td>
</tr>
</tbody>
</table>
Pages to Review in DeGraef book
(based on order we went over in class)

1\textsuperscript{st} edition

All of Chapter 2

Chapter 17 (pp. 459-493). Note that some of these structure we did not cover in class but concepts we went over still apply.

Chapter 22 (pp. 654-681)

All of Chapter 3

Chapter 10 (pp. 230-237)

2\textsuperscript{nd} edition

All of Chapter 2

Chapter 17 (pp. 425-454). Note that some of these structure we did not cover in class but concepts we went over still apply.

Chapter 21 (pp. 561-585)

All of Chapter 3

Chapter 10 (pp. 230-236)