Midterm Exam #1 Review of Topics

Chapter 1

We apply units to measurements and calculations to bring physical meaning to numbers.

In this course, we typically employ SI units, both fundamental and derived.

When converting between units, a process that requires multiplication(s), it is often useful to set up the units in a numerator and denominator before putting the numbers in.

For example, if you wish to convert a number from “apples” to “oranges”, write a fraction next to it, putting “apples” in the denominator and “oranges” in the numerator. Then you look up the conversion factor to see what numerical values go with each: i.e., if 3 apples = 1 orange, then write a “3” next to the “apples” and “1” next to the “orange”. Multiply this fraction with the original number of “apples” and the result will be the number of “oranges”.

When units that are raised to an exponent are converted, the conversion factor needs to be applied for each unit there.

For example, if you wish to convert a number from “cm$^3$” to “in$^3$”, you need to multiply by the in/cm conversion factor 3 times.

To use the significant figures rules, you need to be able to identify the significant figures in a problem statement. Note the number of significant figures in each value and find the number with the fewest. Usually, you are limited to an answer that has only as many significant figures as that number (since most calculations are multiplication/division).

You are not expected to have the exact number of significant figures in every calculation (unless they are specifically requested), but you should be within +1/-1 significant figures of the correct amount.

Chapter 2

The neutral atom contains one or more protons, one or more electrons and zero or more neutrons.

A proton has a charge of +1, an electron a charge of -1 and a neutron has no charge.
Protons and neutrons have similar mass and are found in the nucleus. Electrons have very little mass relative to the proton and neutron and are found in the vicinity the nucleus.

There are different stable combinations of protons and neutrons. Those combinations that contain the same number of protons are called isotopes. The makeup of a specific isotope is detailed using “Z” and “A”. Z is the atomic number, the number of protons, and A is the mass number.

For example, there are three isotopes of hydrogen: $^1\text{H}$, $^2\text{H}$, $^3\text{H}$. All are considered to be hydrogen, since they all have 1 proton. However, they have 0, 1 and 2 neutrons, as listed. In some places, you would also see them referred to as “hydrogen-1”, “hydrogen-2” and “hydrogen-3”, as listed.

The average atomic mass of an element that is shown on the periodic table is found by multiplying the mass of each stable isotope by its percent abundance.

The periodic table is arranged in order of the number of protons in an atom (not the mass). A row is called a “period” and a column is called a “group”. Atoms in the same group tend to have similar chemical properties.

Chapter 3

Both light (electromagnetic radiation or EMR) and matter have wave and particle aspects even though we observe in “normal” life experiences that energy is wave-like and matter is particulate.

This “wave-particle duality” results in phenomena on the microscopic scale that seems unintuitive or counter to our experience.

Properties of waves include: frequency ($\nu$), wavelength ($\lambda$), amplitude (A). Physical manifestations of wave behavior include diffraction and interference.

Waves can interfere with one another, either constructively or destructively. When they interfere constructively, they add to each other, and when they interfere destructively they subtract from one another.

Light waves follow this relationship: $\lambda \nu = c$. For light in a vacuum, $c = 2.998 \times 10^8$ m/s.

Planck is credited with quantifying the particulate nature of energy, the photon, with: $E_{\text{photon}} = \hbar \nu$. 
Einstein is credited with applying this concept to the phenomenon of the Photoelectric Effect (PE). In the PE, electrons are ejected from a metal surface by monochromatic light. The fact that not every wavelength causes this effect to be observed is at odds with the picture of light exhibiting only wave properties. Instead, the particles of light energy, “photons”, are being exchanged and must be of a minimum energy to eject the electrons from the metal.

The formula for the PE shows that the kinetic energy of an ejected electron is based on the energy of the photon and the work function, $\Phi$. The work function is the minimum energy required to eject an electron and varies with each metal. If a photon with insufficient energy strikes the surface, then the effect is not observed (rather than the electron having negative kinetic energy).

Experimentally, it is found that energy is quantized as well; atoms cannot have any arbitrary energy state, but there are “allowed” energy states. This was shown by the emission lines that are produced by excited elements; they could only be explained by the quantization of the atom’s energy states.

The first model to explain this, the Bohr model, postulated an electron circling a nucleus only at allowed distances (stationary states), hence specific energies. The Bohr model can only be applied to explain/predict the energy levels and position of the H-atom or any ion with just one electron.

De Broglie defined the wave nature of matter in terms of a wavelength: $h/(m v) = \lambda$.

Heisenberg showed that the more accurately you know the position of an object, the less accurately you can know it velocity (and vice versa). The Heisenberg Uncertainty Principle allows for a calculation of the least uncertainty you can have in one position, given an uncertainty in velocity (and vice versa).

To describe the behavior of the electron, Schrödinger applied a (3 dimensional) wave equation and solved for wave functions, $\psi$. There are many solutions for $\psi$, but each solution has a corresponding energy. In that way, the wave equations show distinct energy levels, in agreement with experiment.

These wave functions ($\psi$) do not have a direct physical meaning alone, but the probability density (probability divided by volume) of finding the electron at a location is $\psi^2$. See the end of Chapter 3 (and the St. Olaf orbital simulator) for examples of probability density and probabilities for the 1s, 2s, and 3s orbitals.
The solutions to these wave equations provide three quantum numbers, the principal – n, the angular momentum – l, and the magnetic – m_l. They have integer values and different combinations of numbers result in different energy states as well as different regions in which the electron will likely be found. They are also interrelated; values of m_l depend on l and values of l depend on n.

The fourth quantum number is the spin QN, m_s, and it can have a value of +/−½.

The quantum numbers describe a size or level (n), type (l) and physical region (m_l), “spin” (m_s); shapes for l=0 subshell are spherical (s), for l =1 are dumbbell-like (p), for l =2 are clover-like (d), and for l =3 are more complex (f).

For species with only one electron, the energy state depends only on n. However, for all other species, the energy states depend on all 3 quantum numbers.

An orbital can only contain as many as two electrons, and they must have opposite spins. As a consequence, each electron in an atom will have a unique set of 4 QNs (the Pauli exclusion principle).

The electrons fill orbitals beginning with the lowest available energy state.

The positive charge of the nucleus attracts the atom/ion’s electrons, but the presence of multiple electrons causes the effective charge that an outer electron “sees” to be reduced, thus reducing the attraction and therefore increasing the energy state of the outer electron.

Because of greater penetration by certain types of orbitals (those with lower values of l), the order of the energy of subshells (or “sublevels”) in a given n, from low to high, is s < p < d < f (note that not every n can have all of these subshells).

As a result of this ordering (also called “splitting”), the energy of the 4s subshell is lower than the energy of the 3d subshell, so electrons fill the 4s subshell before the 3d; this pattern holds for the rest of the periodic table (5s before 4d, etc.). Also, the 6s subshell fills before the 4f.

Hund’s rule states that electrons filling degenerate energy levels (as in the three p-orbitals, or five d-orbitals, etc.) will form as few pairs as possible (and fill with parallel spins), which means that each orbital in the subshell is filled with one electron before they pair up.

Exceptions to the general pattern of filling orbitals exist in the transition metals. In the first row of transition metals (the 3d) the only two exceptions are chromium and copper.
Atoms in the same group tend to have the same valence electron configuration. Since the valence electrons are involved in chemical reactions, this explains why atoms in the same group tend to have similar chemical behavior.

When atoms become cations (positive ions) they lose their valence electrons first. The valence electrons are the outer electrons, and this is noted in the electron configuration by the largest value of \( n \). In some cases, the valence electrons are not the last electrons that have been written in the electron configuration.

In general, atomic radii decrease across the period and increase down the group.

In general, ionic radii decrease across the period and increase down the group (though there is a large jump at the transition of cations to anions).

A cation has a smaller radius than its parent while an anion has a larger radius than its parent.

In general, first ionization energy (\( \text{IE}_1 \)) increases across the period and decreases down the group.

Each successive IE requires more energy, and the largest jump occurs after all of the valence electrons have been removed.

In general, \( \text{EA}_1 \) increases across the period and decreases down the group.

Adding a second electron always requires energy (most \( \text{EA}_1 \)'s release energy).

An element with a small \( \text{IE}_1 \) and a small \( \text{EA}_1 \) will tend to be a cation in ionic bonds; these are typically metals.

An element with a large \( \text{IE}_1 \) and a large \( \text{EA}_1 \) will tend to be an anion in ionic bonds; these are typically non-metals. They also participate in covalent bonds.

An element with a large \( \text{IE}_1 \) and a small \( \text{EA}_1 \) will tend not to react; these are typically noble gases.

**Chapter 4**

Ionic bonds are described as the results of the transfer of electrons; they tend to form between metals and non-metals.
Covalent bonds are described as the sharing of electron pairs; they tend to form between non-metals and non-metals.

Metallic bonding is described as a pooling of the valence electrons of the metal that creates a mobile “sea” of electrons that can flow and keep the metal atoms together.

To name a binary ionic compound, we name the cation first and the anion second. If the cation is one that can have more than one charge, write the charge of the ion in the compound in parentheses after the cation. Add the “-ide” suffix to the anion.

In compounds with polyatomic ions (usually anions), use the name of the polyatomic ion in the appropriate place (first, if it is a cation, second if it is an anion).

The total charges of all the ions in an ionic compound must add up to an overall charge of zero.

You should be able to do this… but it will not be explicitly tested in midterm #1

Chapter 10

Transferring electrons to create ions is a net endothermic (it absorbs energy) process; what drives the formation of ionic substances is the large exothermic (it releases energy) lattice energy.

The lattice energy is a result of the attraction between the oppositely charged ions as the form the repeating/alternating cation-anion structure.

The Born-Haber cycle represents the steps required for the formation of an ionic solid; it also allows for the calculation of the lattice energy. You do not need to do the actual calculation! However, it may provide some context for lattice energy.

When comparing the lattice energies of two ionic compounds: if the ions’ charges remain fixed, the lattice energy decreases as one or more ions’ radii increase. If the ions’ charges change, the lattice energy increases as the charge of one or more of the ions increase (this overwhelms whatever change may occur in the radii).

We focus on solid materials defined as crystalline; that is, they have a well-defined shape and structure and long-ranged order, as opposed to materials that are amorphous (and have, at best, only short-ranged order).
The smallest repeating structure in a crystal that still represents the overall structure is called the unit cell.

The Simple Cubic (sc) unit cell has one (net) atom per cell, a coordination number of 6, and an edge length of $2r$ and a packing efficiency of 52%.

The Body-Centered Cubic (bcc) unit cell has two (net) atoms per cell, a coordination number of 8, and an edge length of $4r/\sqrt{3}$ and a packing efficiency of 68%.

The Face-Centered Cubic (fcc) unit cell has four (net) atoms per cell, a coordination number of 12, and an edge length of $2r\sqrt{2}$ and a packing efficiency of 74%.

The fcc is a “close-packed” cell, meaning that it represents the highest packing efficiency possible for equal sized spheres.

We often split up 3D unit cells into z-diagrams, which take horizontal slices at every height (value of $z$) that corresponds to a particle center.

Atoms on different locations of the z-diagram contribute different net amounts to the number of atoms per unit cell. For unit cells containing different atoms, the z-diagram allows us to determine the empirical formula.

We also use information about the unit cell type to determine the density of a substance, given a radius, or vice versa.

**Band Theory**

While single atoms have individual energy levels (as we saw with atomic spectra), in a solid where there are $N$ atoms whose many orbitals overlap, there exist bands of allowed electron energies.

These energy bands have some defined energy range and within them, have many energy levels, each separated by only a small amount of energy ~$10^{-23}$ eV.

Between these energy bands are energy values that are not allowed, since energy is quantized, and these spaces between energy bands are called band gaps.

The electron-containing band with the highest energy is called the valence band, and the empty band above is the conduction band.
Materials with no band gaps or with overlapping valence and conduction bands are called conductors (note that this is equivalent to having a partially full valence band).

Materials with a small band gap (~<3 eV) are generally called semiconductors and those with larger band gaps (>3 eV) are called insulators.

Band gaps vary with the material; within a group, the band gap of a pure material will decrease as you move from the top to the bottom of the periodic table (as the metallic character of the element increases).

Band gaps in compound semiconductors are related to the size and the $\Delta E_N$ of the unit cell. The smaller the unit cell, the better the overlap of the atomic orbitals, the better the overlap, the larger the band gap is. The greater the $\Delta E_N$, the higher the ionic character of the bonds are, the more “localized” an electron is, the harder it is to conduct, the larger the band gap.

We can excite electrons in one of three ways: electrically, thermally and optically. In order to conduct (electricity, heat, etc) the electrons need to change their energy state. Photons can excite electrons; often, visible light has sufficient energy to promote electrons to the conduction band (over the band gap) in semiconductor.

The conductivity of metals decreases with increasing temperature and with increasing impurities.

The conductivity of semiconductors, in general, increases with increasing temperature and increasing impurities. The effect of promoting electrons to open “electron holes” or from donor levels by increased temperatures and of adding additional electrons or “electron holes” by impurities tends to overwhelm the effects that are seen in metals.

Semiconductors where impurity atoms have been added (often called “extrinsic” or “doped” semiconductors) possess more or less electrons than the atoms that make up the crystal structure and are called n-type and p-type, respectively.

In n-type semiconductors, extra electrons have been added to the lattice (a “donor” level) and the extra charge carriers that improve the conductivity are electrons.

In p-type semiconductors, extra “electron holes” have been added to the lattice (an “acceptor” level) and the extra charge carriers that improve the conductivity are the electron holes.
Experimental

We saw how the absorption of different wavelengths of light from white light leads to objects being observed to have color particular colors, and that if a solution absorbs a color of light, that is not the color that is observed.

We utilized Beer’s law, $A = \epsilon bc$, in order to relate concentration to absorbance (or vice versa) utilizing the molar absorptivity, $\epsilon$.

We used calibration curves in multiple experiments to relate one quantity, as measured on an instrument, to another.

We observed the line spectra emitted by a number of elements and in particular, the visible series of hydrogen.

We used our knowledge of the form of an equation to plot data in a way that made the relationship linear (we “linearized” it). We can, in principle, be given a mathematical equation and determine a way to plot it as a straight line.