

Lecture 9, Jan 31, 2022

Atomic Bonding Continued

- Bonding depends on a balance of attractive and repulsive terms: $E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n}$
 - First term is the Coulomb force, second is the core shell repulsion
 - e.g. In ionic bonding $A = q_1 q_2$ (Coulomb potential)
 - At infinity there is zero potential; as we move closer the energy goes more negative as there is lower energy due to the attractive force
 - When we get too close the potential energy shoots up again as the two atoms begin to repel, due to the electrons getting too close and the electron densities start overlapping
 - * The atoms are virtually incompressible so as we start to push them into each other the energy shoots up
 - The combined Coulomb potential and the core shell repulsion leads to a minimum in the energy curve where the atoms will settle
- For elements with similar electronegativity, electrons are shared to make covalent bonds
 - e.g. CH_4 – C has 4 valence electrons, needs 4 more for the outer shell; H has 1 valence electron and needs 1 more; electronegativities of the two elements are comparable
- If electrons can be readily removed from the atoms, they become delocalized in an electron cloud and we get metallic bonding
- Ionic and covalent bonds can be mixed; in this case the *percentage ionic character* can be calculated as $1 - e^{-\frac{\Delta X_{AB}^2}{4}}$ where ΔX_{AB} is the difference in electronegativity between the two elements
 - e.g. MgO: $1 - e^{-\frac{(3.5-1.2)^2}{4}} = 73.4\%$ ionic
- Characters of bonds:
 - Ionic bonds: Large bond energy, nondirectional
 - Covalent bonds: Variable bond energy, directional
 - * The other bonds are nondirectional because the s subshell is symmetric; if we have covalent bonding we're likely to have p subshells involved which can be directional
 - * Also in ionic bonding the outer shell is completely filled
 - Metallic: Variable bond energy, nondirectional
- The shape of the potential curve for bonding gives the quantum harmonic oscillator when we're looking at a small section near the equilibrium, so we get energy levels that are evenly spaced (as opposed to proportional to n^2 for the infinite well)
- Bond properties:
 - Bond length r between two atoms
 - Bond energy E_0 (depth of the equilibrium energy from zero)
 - * Energy is $-E_0$ at unstretched bond length r_0
 - Melting temperature T_m
 - * Larger E_0 (deeper potential curve) means more work is required to rip the bonds apart, therefore higher melting temperature
 - Coefficient of thermal expansion α : $\frac{\Delta L}{L_0} = \alpha(T_2 - T_1)$
 - * Deeper potential curve gives a smaller α since more energy is required to stretch or compress the atoms together
 - * For small energy the energy curve is symmetric so heating it does not have much effect, but as we introduce more energy the curve goes to the right more than it does to the left, so there is a net elongation
- The local parabolic approximation also enables Hooke's law