

## 0.1 Semiconductor

Energy Gaps (eV):

- Conductor: 0
- Semiconductor  $0 \leq E_g \leq 3.4$
- Insulator:  $\geq 3.4$
- 
- Opaque:  $\leq 1.8$
- Transparent:  $\geq 3.1$
- Coloured  $1.8 < E_g < 3.4$

Note that when light is absorbed, we can see the complementary colour.

$$\Delta E \propto \left( \frac{1}{n_l^2} - \frac{1}{n_h^2} \right)$$

Gives the relative energy of energy levels.

**Intrinsic Semiconductors:** Si This may occur due to the random formation of holes from electrons moving. For pure semiconductors, there are  $2.2 \times 10^{12} e^- m^{-3}$

### 0.1.1 Extrinsic Semiconductors

If we dope the silicon with a group 15 element, we're adding more electrons. This adds a donor state, a little bit below the conduction band.

In this case, we have a n-type semiconductor, with equation  $\sigma = nq\mu_n$ .

n is the number of electrons in the conduction band, q is the charge of an electron, and  $\mu_n$  is the mobility of electrons.

If we dope it with a group 13 element, we're adding more holes. This forms an acceptor state slightly above the valence band.

This is a P-type semiconductor with equation  $\sigma = pq\mu_p$ .

p is the number of holes,  $\mu_p$  is the mobility of positive charges, and q is the charge of electrons.

Usually, we add about  $10^{20} \frac{\text{dopants}}{m^3}$ , which is orders of magnitude higher than the amount from the intrinsic semiconductor. (either in holes or electrons).

# Chapter 1

## Tetrahedral APF

Via trigonometric manipulation (figure 1), by which we can determine the relationship between  $a$  (lattice parameter) and  $r$  (atomic radius) as  $a = 8r \times \sin(35)$ ;

By this,

$$\frac{V_{atoms}}{V_{cell}} = \frac{4\frac{4}{3} \times \pi r^3}{(8r \times \sin(35))^3} = 0.34$$

## Chapter 2

# Thermodynamics

### 2.1 The Laws of Thermodynamics

1. For an isolated system

$$\Delta U = 0$$

For a closed system

$$\Delta U = q + W$$

q = heat in

W = work done on system

$$\Delta U = q - P\Delta V$$

can be rearranged to

$$q = \Delta H = \delta U + P\delta V$$

. This is how we introduce enthalpy.

2. The Entropy of the Universe is always increasing ( $\Delta S_{univ} = \Delta S_{system} + \Delta S_{surroundings} > 0$ )

$$\Delta S_{system} - \frac{q}{T} > 0$$

$$T\Delta S_{system} - q > 0$$

$$T\Delta S_{system} - \Delta H > 0$$

But we're comfortable with energy decreasing, so we can multiply by  $-1$  to get a quantity  $\Delta G = \Delta H - T\Delta S$

- 3.

Things occur on their own (*spontaneously*) without the input of extra energy occur due to an increase in the entropy of the universe.

- G = Gibbs energy =  $\Delta G = \Delta H - T\Delta S$

- H = Enthalpy

- J = Joules

- K = Boltzmann

- M = Molarity

- N = number of moles

- P = pressure

- q = Heat transfer

- R = gas constant

- S = entropy =  $\frac{q_{reversible}}{T}$

- T = temperature (thermodynamic, K)

- U = Internal energy

- V = Volume

- W = Work

There are three types of systems:

1. Open - Both energy and matter can be exchanged through the system and environment.
2. Closed - Only energy is exchangeable
3. Isolated - Neither energy nor matter can be exchanged.

In some special, useful cases (Constant P/1atm or Only expansion, PV work) gives  $\Delta H = \Delta U + P\Delta V$ .

An analogy for entropy - (q = sneezing) - In a crowded street, with high temperature vs. a quiet library (low temp)

At absolute zero, there is zero entropy. You can pick out a particle and know for sure that it's at the lowest energy. However, at infinite temperature, particles have equally distributed energies, and you'd have no idea what the energy of the particle is. Entropy then, is our level of certainty when blindly selecting a particle.

### 2.1.1 Internal Energy

We can have a lot of types of energy - translational/kinetic, rotational/angular, vibrational, electron translational, electronic spin, bond energy (eg. laser), nuclear ... etc

We don't really care or know all the energy sources, and thus we only consider changes in **Internal Energy**  $\Delta U$ .

For entropy, since we know that at 0K we have  $S = 0$ , we can also define an absolute entropy.

As we often have processes occur with open atmosphere, we have constant P. The only work is "PV" work. This is given by

$$W = P\Delta V$$

A useful defined quantity of enthalpy accounts for work pushing back the atmosphere.

$$\Delta H = \Delta U + P\Delta V$$

### 2.1.2 Spontaneity: Types of Processes

With given  $\Delta H, \Delta S_{sys}$  is it Spontaneous?

$\Delta H$	$\Delta S$	Spontaneity	Example
-	+	all temperatures	combustion of fuel
-	-	low temperatures	freezing of water
+	+	high temperatures	melting of ice
+	-	never	n/a

We can actually create a plot of  $G = -TS + H$  of G against T. If we take a random point on the G axis, that is the G-intercept, or H.

We position the solid phase at the bottom of the g axis, the liquid phase above it, and the gas phase far above that ( $\Delta H_{fusion} << \Delta H_{vaporization}$ ) We know that entropy is always positive so we have a negative slope for the "solid" line, a steeper decreasing line for the liquid line and a very steep slope for the gas line. These lines all happen to intersect.

We know that for low Gibbs energies and low temperatures, we get a region that belongs to ice. Then, there's a small region where the liquid phase is stable, (273K to 373K) and then a region where the gas phase is stable. This graph is for 1 atm.

However at low (vapour) pressures, the intersections are different, and the vapour phase has a steeper slope than before, which can cause us to go from solid to gas without going through liquid.

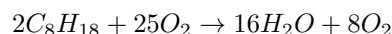
**Standard State** is the state of an element at 298.15K and 1 bar.

### 2.1.3 State vs Path Function

A state function does not involve how a value was attained, only the current value at the point.

A path function does. (Work, q(Heat))

### 2.1.4 Combustion of Octane



$$\Delta H^C = 16\Delta H_F(H_2O) + 8\Delta H_F(O_2) - (2\Delta H_F(C_8H_{18}) + 25\Delta H_F(O_2))$$

$$\Delta_F H^C = -10160J$$

per two mols of Octane.

PV work: Starting out with 25 mols of gas, we end up with 34 mols of gas, and we have gained 9 mols.

We can plug this into the ideal gas formula

$$\begin{aligned}P\Delta V &= \Delta nRT \\&= 9(8.31)(298K) \\&= 22kJ.\end{aligned}$$

### 2.1.5 Important Relationships

$$\Delta H_x = \Delta H_{f-Products} - \Delta H_{f-Reactants}$$

$$S_x = S_{Products} - S_{Reactants}$$

$$\Delta G_x = \Delta G_{f-Products} - \Delta G_{f-Reactants}$$