CHEMISTRY (EEE,ECE & CSE)

UNIT-1

STRUCTURE AND BONDING MODELS

1. Write the equation for Schrodinger's wave equation?

The Schrodinger wave equation describes the wave characteristics of an electron in terms of its position, mass, total energy, and potential energy. The equation is based on a wave function that describes the motion of an electron wave through space.

Schrodinger wave equation can be written in many forms, one of which is written as,

$d^2 \Psi / dx^2 + d^2\Psi / dy^2 + d^2\Psi / dz^2 + 8\prod^2 m / h^2 (E - V) \Psi = 0$
or. $(d^2 / dx^2 + d^2/ dy^2 + d^2 / dz^2) \Psi + 8\prod^2 m / h^2 (E - V) \Psi = 0$
or, $\nabla^2 \Psi + 8\prod^2 m / h^2 (E - V) \Psi = 0$
Where, x, y, z = Space coordinates of the electron wave with respect to the nucleus.

∇^2 = Laplacian operator
m = mass of the electron

h = Planck's constant

E = Total energy of an electron

V = potential energy of an electron

E -V = kinetic energy of the electron

2. What is the significance of Schrodinger's wave equation?

- Ψ is a wave function that refers to the amplitude of an electron wave, i.e. the probability amplitude. It has no physical significance. The wave function could be positive, negative, or imaginary.
- Ψ^2 is known as probability density determines the possibility of finding an electron at a certain place within the atom. This means that if:
- Ψ^2 is zero, the chances of finding an electron at that position are negligible.
- Ψ^2 is high, the probability of discovering an electron is high, indicating that the electron has been there at that location for a long period.
- Ψ^2 is low, probability of finding an electron is minimal, indicating that the electron is only present for a short period of time.

3. What is Hund's rule?

i. Every orbital in a sublevel is singly occupied before any orbital is doubly occupied.

ii. All of the electrons in singly occupied orbitals have the same spin (to maximize total spin).

4. What is Pauli Exclusion Principle?

This principle states that no two electrons in an atom can have the same set of quantum numbers. This leads to the filling of electron orbitals in a specific order in the periodic table.

5. What is meant by Homo Nuclear Diatomic Molecules

a. Molecules formed upon the bonding of two same elements are known as homo nuclear diatomic molecules.

b. For example di hydrogen (H2), Di nitrogen (N2), etc. In this article, we will study the formation of these diatomic molecules, their stability, and other characteristics.

6. What is meant by Hetero Nuclear Diatomic Molecules

Diatomic molecules with two non-identical atoms are called hetero nuclear diatomic molecules.

When atoms are not identical, the molecule forms by combining atomic orbitals of unequal energies.

The result is a polar bond in which atomic orbitals contribute unevenly to each molecular orbital.

7. Write the electronic configuration of CO molecule?

Electronic configuration of C atom: 1s2 2s2 2p2 Electronic configuration of O atom: 1s2 2s2 2p4

Electronic configuration of CO molecule:

σ1s2, σ1s*2, σ2s2, σ2s*2, π2py2, π2pz2 σ2px2

8. Explain the term bond order and how it is calculated?

Bond order is the number of bonds between two atoms. Lewis structures, an important part of the valence-bond model, help calculate bond orders.

Bond Order = Bonding electrons−Antibonding electrons/2

9. Calculate the bond order of Nitrogen molecule?

$\sigma 1s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2$, $[\pi 2p_x^2 = \pi 2p_y^2] < \sigma 2p_z^2 < [\pi^* 2p_x = \pi^* 2p_y] < \sigma^* 2p_z$

Let's calculate the bond order of N_2:

$$Bond\ order = \frac{Bonding\ electrons - Anti\ bonding\ electrons}{2}$$

$$= \frac{10-4}{2} = 3$$

Therefore, the order of N_2 is 3.

$:N\equiv N:$

N_2 does not have unpaired electrons, hence it is diamagnetic.

10. What are the Limitations of MO Theory?

MO theory says that the electrons are delocalized. That means that they are spread out over the entire molecule. The main drawback to our discussion of MO theory is that we are limited to talking about diatomic molecules (molecules that have only two atoms bonded together), or the theory gets very complex.

UNIT-2

MODERN ENGINEERING MATERIALS

1.What is meant by semi conductivity?

Semiconductors are materials which have a conductivity between conductors (generally metals) and non-conductors or insulators (such as most ceramics). Semiconductors can be pure elements, such as silicon or germanium, or compounds such as gallium arsenide or cadmium salinity.

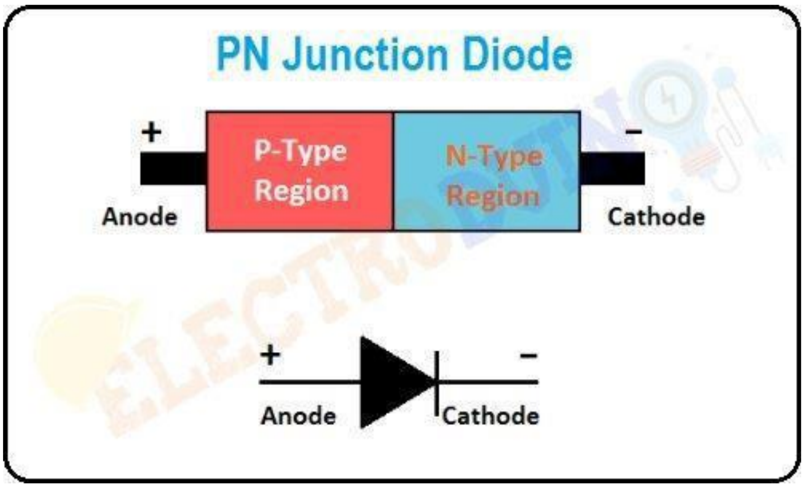
2. How are p-n junctions produced?

i. A p-n junction diode is a basic semiconductor device that controls the flow of electric current in a circuit.

ii. It has a positive (p) side and a negative (n) side created by adding impurities to each side of a silicon semiconductor.

iii. The symbol for a p-n junction diode is a triangle pointing to a line. Where the triangle is pointing is showing you which way the diode will let current flow.

iv. This one is allowing current to flow from right to left with the right side being the positive side.



3. Define super conductors?

A superconductor is defined as a substance that offers no resistance to the electric current when it becomes colder than a critical temperature.

Prominent examples of superconductors include aluminium, niobium, magnesium diboride, cuprates such as yttrium barium copper oxide and iron pnictides

4 Define Critical Temperature?

The critical temperature is the temperature below which the material changes from conductors to superconductors. The critical temperature is also called transition temperature. The transition from conductors to superconductors is sudden and complete.

5. What are the applications of SUPERCONDUCTORs

Superconductors are used in manufacturing high-speed connections in computer ICs, making superconducting coils, MRIs, etc.

Superconductors are used in particle accelerators, generators, transportation, computing, electric motors, medical, power transmission, etc.

Superconductors are primarily employed for creating powerful electromagnets in MRI scanners.

These conductors are used to transmit power for long distances.

They are used in memory or storage elements.

6. What are nanomaterials ?

Nanomaterial's can be defined as materials possessing, at minimum, one external dimension measuring 1-100nm.

Nanomaterial's can also be added to cement, cloth and other materials to make them stronger and yet lighter.

Their size makes them extremely useful in electronics, and they can also be used in environmental remediation or clean-up to bind with and neutralize toxins.

7. Write about Fullerenes

The fullerenes (allotropes of carbon) are graphene sheets rolled into tubes or spheres.

It is a cage like molecule composed of 60 carbon atoms (C60) joined together by single and double bonds to form a hollow sphere with 20 hexagonal and 12 pentagonal faces (a design that resembles a football).

It was named as buckminsterfullerene or buck ball after the name of American architect Buckminster Fuller.

The fullerene receives its name from the architect Buckminster Fuller, who designed homes in the shape of a geodesic dome based on pentagons and hexagons, sometimes even referred to as "buck ball". There are three important types of Fullerenes: C60, C70, and Fullerenes .

8. Write about Graphene?

Graphene is a crystalline allotrope of carbon with two-dimensional, atomic scale, hexagonal pattern. Here each carbon atom forms four bonds, three s bonds (sp2 hybridized) with its three neighbours and one p bond oriented out of plane. It is the basic structural element of other allotropes like graphite, fullerene, nanotubes, Nano cones, etc. hence called mother of all carbon nanomaterial‘s.

9. Differentiate between single-walled carbon Nano-tube and multi-walled carbon Nano- tube?

Single-walled carbon Nano-tube	**Multi-walled carbon Nano-tube**
SWNT is made up by rolling a graphene sheet into a seamless cylinder.	MWNT is made up by the concentration of carbon nanotubes.
SWNT require optimization of experimental parameters for synthesis.	MWNT are synthesized easily. The may be found in the emission of LPG or propane based fuels.
The internal diameter is comparatively smaller (approximately 5-10nm).	They have well-ordered graphite structures.
SWNT bare used in electronics, water filtration, hydrogen storage, oil spill removal etc.	MWNT have comparatively fewer applications.

10. What are the Applicationsof fullerenes?

Fullerenes (C60) and their derivatives have potential antiviral activity, and may be used for the treatment of HIV-infection.

They have potential medicinal applications as they can bind specific antibiotics and target certain types of cancer cells such as melanoma.

They are used as biological antioxidants.

They are also used as potential photosensitizers in photodynamic therapy and catalysts for hydrogenation.

WATER TECHNOLOGY

1. What is hard ness of water due to?

The hardness of water is due to the presence of soluble bicarbonates, chlorides and sulfates of calcium and magnesium. Water which does not give lather with soap is hard water.

2. How temporary hardness differs from permanent hardness?
temporary hardness:

The presence of magnesium and calcium carbonates in water makes it temporarily hard. In this case, the hardness in water can be removed by boiling the water. When we boil water, the soluble salts of $Mg(HCO_3)_2$ are converted to $Mg(OH)_2$, which is insoluble, and hence gets precipitated and is removed. After filtration, the water we get is soft water.

permanent hardness:

When the soluble salts of magnesium and calcium are present in the form of chlorides and sulphides in water, we call it permanent hardness because this hardness cannot be removed by boiling.

3. What is reverse osmosis?

reverse osmosis, separation technique in which pressure applied to a solution forces the solvent through a semipermeable membrane from a region of low concentration to one of high concentration, leaving behind the solutes. The membrane allows passage of small solution components, such as fresh water, while preventing passage of larger molecules, like salts and other impurities.

4. What is break point of chlorination?

Breakpoint chlorination is defined as the point where enough chlorine has been added to a quantity of water to satisfy its disinfecting demand. In other words, it is the point where all undesirable contaminants have been removed from the water. At breakpoint chlorination, all chlorine added to the solution is consumed by chemical reactions with the contaminants, resulting in no free available chlorine (FAC) in the water

5. **Define priming and foaming?**

Foaming is the formation of thick layer of steam bubbles on the top of the water surface inside the boiler.

Priming is the condition in which large amount of water are carried along with the steam into the steam line because of,

> Excessive foaming

> Improper amount of steam space

> By a sudden rush of steam

6. What is electrodialysis?

Electrodialysis (**ED**) is used to transport salt ions from one solution through ion-exchange membranes to another solution under the influence of an applied electric potential difference. This is done in a configuration called an electrodialysis cell.

7 What is caustic embrittlement?

As water evaporates in the boiler, the concentration of sodium carbonate increases in the boiler. In high pressure boilers, sodium carbonate is used in softening of water by lime soda process, due to this some sodium carbonate maybe left behind in the water. As the concentration of sodium carbonate increases, it undergoes hydrolysis to form sodium hydroxide.

The presence of sodium hydroxide makes the water alkaline in nature. Inside the cracks, the water evaporates and the amount of hydroxide keeps increasing progressively. The concentrated area with high stress works as anode and diluted area works as cathode. At anode, sodium hydroxide attacks the surrounding material and then dissolves the iron of the boiler as sodium ferrate forming rust. This causes embrittlement of boiler parts like rivets, bends and joints, which are under stress.

8. What is sedimentation?

Sedimentation is one of the methods that municipalities use for treating water. It is a physicalwater treatment process. Gravity is used to remove suspended solids from water.

The effectiveness depends on the size and weight of the particles. Suspended solids that have a specific gravity similar to water remain suspended while heavier particles settle. The sedimentation process in wastewater treatment usually occurs in tanks of various shapes.

9. Explain why CaCO3 is selected for expression of hardness of water?

The hardness of water is generally expressed as $CaCO_3$ equivalent because calcium carbonate ($CaCO_3$) is the most common mineral that causes hardness in water. When water is considered "hard," it typically contains high levels of calcium and magnesium ions, which can form insoluble compounds with soap and other cleaning agents, leading to scale buildup in pipes and appliances.

By expressing the hardness of water in terms of $CaCO_3$ equivalent, it allows for a standardized and easily understandable way to measure and compare the hardness of different water sources. This is important for determining the appropriate treatment methods to reduce hardness and prevent potential issues associated with hard water.

10 How does boiler corrosion occur?

Boiler corrosion is degradation of boiler and it’s metal by electrochemical reaction or by pitting action of dissolved oxygen in boiler water.

boiler corrosion causes

1. Dissolved oxygen in boiler water.
2. Presence of corrosive gases such as Oxygen (O_2), Carbon Dioxide (CO_2), Hydrogen Sulphide (H_2S) in the boiler water
3. Sludges of bicarbonate and carbonate
4. Low PH
5. Low feed water temperature
6. Acidity imparted to water due to decomposition of Carbon Dioxide (CO_2) or Hydrogen Sulphide (H_2S)

7.Dissolved solids

UNIT-2

ELECTRO CHEMISTRY AND APPLICATIONS

1. **What is Dry corrosion?**

Dry corrosion, also known as oxidation, is a type of corrosion that occurs when material chemically reacts with gases in a dry environment. There's no liquid involvement, and the reaction results in the formation of an oxide layer on the surface of the metal.

2. **What is Piling-Bedworth rule?**

The Pilling-Bedworth ratio (P-B ratio), in terms of metal corrosion, is the ratio of elementary cell volume of metal oxide to the elementary cell volume of the equivalent metal where the oxide has been created.

By using the P-B ratio, it can be determined if it is possible for the metal to undergo passivation in the presence of dry air by building a protective oxide film.

3. **What is differential aeration corrosion?**

Differential aeration corrosion is a type of corrosion that occurs when oxygen concentrations vary across a metal's surface. The varying concentration of oxygen creates an anode and a cathode on the metal's surface. Oxidation then occurs because an anode and a cathode have been established on the surface.

4. **What is meant by the term passivity?**

Passivity refers to a corrosion preventative mechanism whereby an oxidation layer forms a continuous film on a metal's surface that prevents further corrosion. Passivity is the loss of electrochemical reactivity, thereby decreasing the corrosion rate of the metal. Passivation is used on many different engineering alloys, such as stainless steel, nickel-based alloys, and aluminum-based alloys.

5. **What is electrode potential?**

Electrode potential appears at the interface between an electrode and electrolyte due to the transfer of charged species across the interface, specific adsorption of ions at the interface, and specific adsorption/orientation of polar molecules, including those of the solvent.

6. What is fuel cell?

A fuel cell can be defined as an electrochemical cell that generates electrical energy from fuel via an electrochemical reaction.

Fuel cells require a continuous input of fuel and an oxidizing agent (generally oxygen) in order to sustain the reactions that generate the electricity. Therefore, these cells can constantly generate electricity until the supply of fuel and oxygen is cut off.

7. How are fuel cell useful?

Fuel cell electric vehicles, or FCEVs, use clean fuels and are therefore more eco-friendly than internal combustion engine-based vehicles.

They have been used to power many space expeditions including the Appolo space program.

Generally, the byproducts produced from these cells are heat and water.

The portability of some fuel cells is extremely useful in some military applications.

These electrochemical cells can also be used to power several electronic devices.

8. Define reduction potential?

Reduction involves gain of electrons, so the tendency of an electrode to gain electrons is called its reduction potential.

The equilibrium potential difference between the metal electrode and the solution surrounding it is called the electrode potential. It is also defined as the tendency of an electrode to lose or gain electrons

9. Write the Nernst equation for the calculation of electrode reaction?

$E_{cell} = E^0 – [RT/nF] \ln Q$

Where,

- E_{cell} = cell potential of the cell
- E^0 = cell potential under standard conditions
- R = universal gas constant
- T = temperature
- n = number of electrons transferred in the redox reaction
- F = Faraday constant
- Q = reaction quotient

10.What are irreversible cells?

Reversible cell

A cell is said to be reversible if it satisfies the following three conditions:

If an emf exactly equal to that of a cell is applied from an external source, the chemical reaction taking place in the cell will stop i.e no current flows.

If the external emf is slightly greater than the actual emf of the cell applied, the current will begin to flow In the opposite direction and the cell reaction gets reversed.

If the external emf is slightly lower than that of the actual emf of the cell applied to it, a very small amount of current will flow corresponding to a very small amount of chemical changes taking place in the cell.

Irreversible cell
A cell is said to be irreversible if it does not satisfy the above criteria of reversibility, called as irreversible cells.