

## **AKSHAYA INSTITUTE OF TECHNOLOGY**

Lingapura, Tumkur-Koratagere Road, Tumkur-572106.



To provide transformational technical competence by synergizing professional ethics and spiritual values to meet the global challenges and societal needs



## DEPARTMENT OF CHEMISTRY "APPLIED CHEMISTRY FOR CSE STREAM" [BCHES102/202]



- To impart value-based quality technical education nurture the students to adopt themselves to the ever changing global needs
- To provide an experience the t inspires students to reach the highest level of accomplishment in their lives
- To provide an environment that enables students and faculty to make valuable contribution to the advancement of knowledge and creative practice of engineering

## **Prepared and verified by:**

Mrs. Ranjitha K M Assistant Professor Ms.Manasa.N. Assistant Professor

| Department of chemistry         |                                      |            |       |
|---------------------------------|--------------------------------------|------------|-------|
| Course Title:                   | Applied chemistry for CSE streams    |            |       |
| Course Code:                    | BCHES102/202                         | CIE Marks  | 50    |
| Course Type                     | Integrated                           | SEE Marks  | 50    |
| (Theory/Practical/Integrated)   |                                      |            |       |
| Teaching Hours/Week (L: T:P: S) | 2:2:2:0                              | Exam Hours | 03+02 |
| Total Hours of Pedagogy         | 40 hours Theory + 10-12 Lab<br>slots | Credits    | 04    |

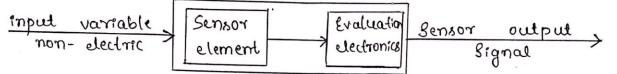
### **Department of Chemistry**

#### **Course outcomes**

| CO1 | Identify the terms processes involved in scientific and engineering and application.                  |  |
|-----|---|--|
| CO2 | 2 Explain the phenomena of chemistry to describe the methods of engineering processes                 |  |
| CO3 | Solve the problems in chemistry that are pertinent in engineering applications                        |  |
| CO4 | Apply the basic concepts of chemistry to explain the chemical properties and solution                 |  |
| CO5 | Analyze properties and multi processes associated with chemical substances in disciplinary situations |  |

## **MODULE 1: SENSORS AND ENERGY SYSTEM**

A sensor is a device that detects and responds to some type of input from the physical environment.



## **Components of Sensors:**

1. Receptor: it is a chemical element which is capable of interacting with analyte specifically and selectively. It produces signal corresponding to interaction in the form of change in potential, conductivity heat, pH etc.

2. Transducers: Transducers is used to convert the signal created by the receptor-analyte interaction into a readable value.

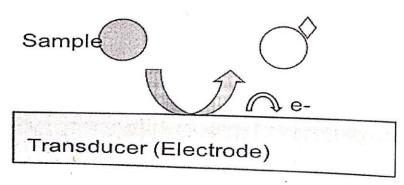
3. Electrical signals and Display.

4. The electronic system analyses the signal given by the transducer, converts the signal into digital form. These signals are then displayed.

### **Electrochemical Sensors:**

Electrochemical sensors are sensors in which an <u>electrode</u> is used as a transducer element in the presence of an analyte.

Electrochemical sensors are made up of three essential components: a **receptor** that binds the sample, the **sample or analyte**, and a **transducer** to convert the reaction into a measurable electrical signal. In the case of electrochemical sensors, the electrode acts as the transducer.



In electrochemical sensors, two electrodes are used. Anode: Zn, Pb or any other active metal Cathode: Working electrode-Ag Electrolyte: KOH, NaOH or any other inert electrolyte Membrane: Teflon

## Working:

The difference in potential between the anode and the cathode should be at least 0.5V.

When electrode is dipped in water to measure DO, anode undergoes oxidation liberating electrons

At cathode, DO undergo reduction. Ag cathode is inert, it only passes electrons to oxygen for reduction.

## **Applications:**

1. The oxygen sensors are used to determine dissolved oxygen in boiler water and to monitor dissolved oxygen concentrations in hydrogen fuel cell.

2. Used in security and defence applications like detection of toxic gases.

3. Used in water analysis and environmental monitoring.

4. Used in diagnostic and health care applications.

5. Used in soil parameter analysis and in agricultural applications.

## Conductometric Sensors

It involves the determination of the concentration of analyte based on the measurement of changes occur in electrolyte solution. Here electrodes are used to measure the conductance of the electrolyte. Conductance is depending on

- No. of ions
- Mobility of ions

Working:

Electrode used is conductivity cell. It is made up of two

platinum foils with unit cross sectional area and unit distance between them. Volume between the electrode is 1cm3. Conductance of unit volume of the solution is called specific conductance and it is given by

Here l/a is known as cell constant, R is resistance.

The conductivity is result of dissociation an electrolyte, into ions. The migration of the ions is induced by an electrical field. When a potential difference is applied to the electrode, there is an electrical field within the electrolyte, so the positively charged ions move towards cathode and negatively charged ions are move towards anode. Thus, the current in the electrolyte is caused by the ion movement towards the electrodes where the ions are neutralized and isolated as neutral atoms (or molecules). This chemical change is recognized by working electrode and transducers converts this chemical change into electrical signal.

### **Applications:**

1. Used to estimate acid, base and mixture in the sample

2. Used to check ionic impurities in water sample

3. Used to measure acidity or alkalinity of sea water and fresh water

4.Conductometric biosensors are used in biomedicine, environment monitoring, biotechnology and agricultural related applications.

<u>Optical Sensors:</u>

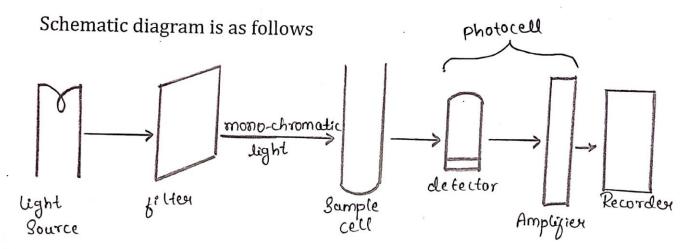
1. These sensors based on the interaction of electromagnetic radiation with the chemical species. Commonly UV-Visible-Infrared electromagnetic radiations are used. In an optical sensor, the optical signal arises from the interaction of the analyte with an incident radiation. This interaction could results in absorption, emission, scattering and reflection of light. The intensity of the radiation gives the information on the concentration of the analyte.

2. Optical sensors are used to determine the concentration of coloured solution. It is based on the measurement of absorbance of the coloured solution at particular wavelength. It is governed by Beer-Lambertz law.

3. The optical sensors components are light source, filters, photocell and display system.

## Working:

A monochromatic light is pass through analyte at particular wavelength. A part of light is absorbed by the analyte. The absorbance depends on the concentration of the solution and the path length of the light through the solution. The photocell converts emitted light into electrical signal These signals are recorded and displayed.



**Source**: tungsten bulb or lamp is used as a light source. **Filter**: It is a device to provide desired wavelength range **Sample cell**: sample is hold in glass cell. **Photocell**: Converts the emitted light into electrical signal.

### **Applications:**

- Used in the determination of any chemical species which can interact with electromagnetic radiations
- Can be used in environmental, pharmaceuticals, food related applications

## Thermometric Sensors:

It is based on the measurement of thermal changes during the interaction between analyte and receptor. Main component is a small tubular catalytic reactor fitted with a temperature transducer. Analyte is fed into the reactor. The wall of the reactor is coated with a catalyst which is capable of catalyzing the reaction, liberating the heat energy. Heat liberated is quantified by transducer and convert into voltage and fed to the data storage and processing unit.

The two main transducers which convert change in temperature into an electric signal are

**1. Resistive transducers**: Most commonly used resistive transducer is the thermistor. It is a semiconductor device made up of oxides of transition metals.

**2. Thermocouple:** It is a device which converts the temperature difference into an electrical voltage.

## **Applications:**

Used in determination of metabolites, bioprocess monitoring and environmental control and determination of combustible gases

## Electrochemical sensors for the pharmaceuticals

Electrochemical detection occurs at the interface between an analyte (diclofenac) of interest and the working electrode to which a potential is applied with respect to the reference electrode, while the corresponding current is measured.

Electrochemical sensors for detection of diclofenac

**Working electrode:** Carbon coated with MWCNT or Graphene **Counter Electrode:** Carbon coated with MWCNT or Graphene **Reference Electrode:** Ag/AgCl

When the sample containing diclofenac is put in the sensor, oxidation of diclofenac occurs on the surface of the sensing electrode. The change in potential of the reaction gives the concentration of diclofenac.

# Sensors for the measurement of dissolved oxygen (DO):

The oxygen present in the water in dissolved form is called as dissolved oxygen.

Two types of Sensors are used for measurement of dissolved oxygen (DO)

1. Optical Sensors

2. Electrochemical Sensors

<u>Optical Sensors:</u>

The main component of optical sensors is semi permeable membrane, sensing element, lightemitting diode (LED) and photo detector. The sensing element contains a luminescent dye.

### Working:

When the dye is exposed to light, it moves to excited state and return to ground state by emitting light with known intensity. When the DO crosses the semi permeable membrane and interacts with the dye, it reduces the intensity of the light emitted by dye. The intensity of the emitted light inversely proportional to the DO concentration. This intensity of light is measured using photo detector.

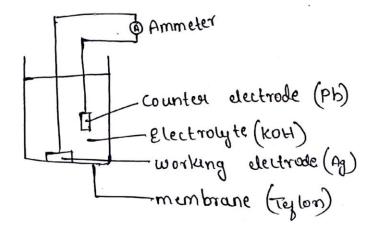
<u>Electrochemical Sensors:</u>

In electrochemical sensors, two electrodes are used.

Anode: Zn, Pb or any other active metal

**Cathode:** Working electrode-Ag

**Electrolyte:** KOH, NaOH or any other inert electrolyte **Membrane**: Teflon



## Working:

The difference in potential between the anode and the cathode should be at least 0.5V.

When electrode is dipped in water to measure DO, anode undergoes oxidation liberating electrons

 $2Zn \longrightarrow 2Zn^2 + 4e^-$ 

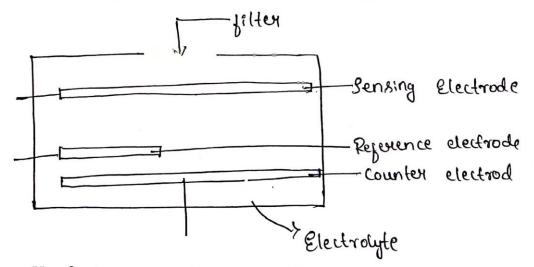
At cathode, DO undergo reduction. Ag cathode is inert, it only passes electrons to oxygen for reduction.

Overall reaction is

27n + 02 + 2H20 ----> 27n(0H)2

The current produced by the reduction of oxygen at cathode is proportional to the oxygen in the water sample.

Electrochemical gas sensors for SOx and NOx.



Filters: Used to prevent unwanted contaminants, mainly particulate matter

**Membrane:** A gas-permeable membrane is used to regulate the gas flow into the sensors. It allows only analyte gas to pass and prevent the leakage of the electrolyte.

**Electrodes:** two or three electrodes are used on the requirement. Working or sensing, counter and reference electrode.



**Electrolyte:** Electrolyte should be ionic conductor and chemically stable. Main role is , it transport charge within the sensor, contact all electrodes effectively and solubilise the reactant and product for efficient transport.

### Sensors for SOX:

The sensors contains two or three electrodes Sensing electrode: Au/Nafion Electrolyte: 0.5M H2SO4

#### Working:

The diffusion of gas analyte through filter, membrane and then finally through electrolyte on to the surface of sensing electrode.

Adsorption of analyte gas molecules on the surface of sensing electrode.

Oxidation of analyte on the surface of sensing electrode, liberating electrons.

Desorption of product from the electrode surface.

Diffusion of the products away from the reaction zone to bulk of

electrolyte.  $SO_2 + 2H_2O \longrightarrow SO_4^{2-} + 4H^+ + 2e^-$ 

#### **Sensors for NO2:**

The sensors contain two or three electrodes. Sensing electrode: Au, Pt/Nafion. Electrolyte: 10 M H2SO4

#### Working:

★ The diffusion of gas analyte through filter, membrane and then finally through electrolyte on to the surface of sensing electrode.

 $\star$  Adsorption of analyte gas molecules on the surface of sensing electrode.

\* Oxidation of analyte on the surface of sensing electrode, liberating electrons.

\* Desorption of product from the electrode surface.

\* Diffusion of the products away from the reaction zone to bulk of electrolyte.

 $NO + 2H^{\dagger} + 2e^{-} \rightarrow NO + 2H_2O$ 

## **Sensors for NO:**

The sensors contain two or three electrodes. Sensing electrode: Au/NASICON. Electrolyte: NaNO2

### Working:

★ The diffusion of gas analyte through filter, membrane and then finally through electrolyte on to the surface of sensing electrode.

\* Adsorption of analyte gas molecules on the surface of sensing electrode.

\* Oxidation of analyte on the surface of sensing electrode, liberating electrons.

\* Desorption of product from the electrode surface.

✗ Diffusion of the products away from the reaction zone to bulk of electrolyte.

 $NO + 2H_2O \longrightarrow NO_3^{2-} + 4H^+ + 3e^-$ 

Energy <u>Storage</u> <u>System</u>.

Energy storage is the capture of energy produced at one time for the use at a later time. Energy will comes from multiple form includes radiational, chemical, gravitational, potential and electrical.

## BATTERY.

A Battery 15 a device consisting of two or more galvanic cell connected in series or parallel or both. which convert chemical energy into electrical energy through redox reaction.

BASIC COMPONENTS OF BATTERY :

it ANODE: At anode oxidation reaction takes place with the liberation of electrons into external circuit. 21 CATHODE: At cathode reduction reaction takes place with the accept of electrons from external circuit. 32 ELECTROLYTE: It is a solution made up of salts of acid or alkali, which provide the medium for transfer of ions inside the cell between the anode and cathode.

ut <u>SEPARATOR</u>: It is used to separate the anode and cathode in a battery to prevent enternal short circuit.

s' MINOR COMPONENTS : Anode current collector, cathode current collector, rubber seal.

## CLASSIFICATION OF BATTERY :

Battory are classified ento three types. primary, secondary and Reserve battery.

It Primary Battery:

In primary Battery, the chemical energy is converted into electrical energy as long as the chemical components are active, the cell reaction is irreversible. These batteries are not be recharged. ez:- In-air battery, li-mnoz battery.

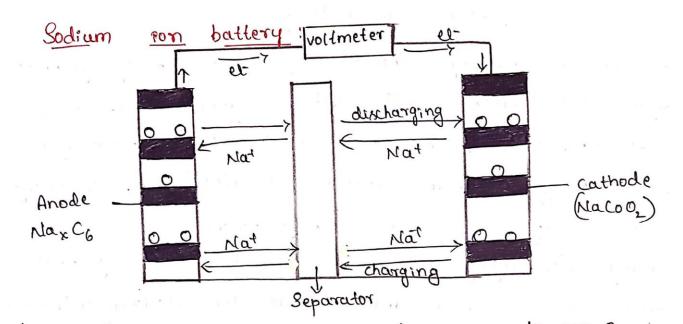
21 Secondary Battery :

In secondary battery cell reactions are reversible, The discharged battery can be rucharged by parsing current through it. these batteries are also called as storage cell.

ex: lead storage battery, lithium-ion battery.

21 Reserve battery:

In Reserve battery one of the component of stored separately and incorporated into the battery when required usually electrolyte is stored separately. ex: Zn-Agro battery. Mg battery activated by water.



Sodium ion battery anode is made up g gn Hard carbon [C6] entercaladed with Nat atoms. and cathode 18 made up of sodium metal oxide (NaCOO2). Electrolyte consisting of NaPF6 dissolve in organic solvent like ethylene (carbonate). Separate is made of non-woven polypropylene. up At anode: NaxC6 <u>charging</u> XNat + Xet + C6 At cathode: Na1-x COO2 + XNat + Xe - cha > Nacoo2 <u>charging</u> Ma COO<sub>2</sub> + C<sub>6</sub> discharging Disadvantages Total qualtion: Nax C6 + Na, -x CO 02 Advantages \* lower operating voltage \* Easion to recycle \* Need high temp for \* low market prices optimal work Application of Sodium-ion-battery! used It 18 in

\* mobile phones

\* cameral, calculator, LCD TV,

\* laptop, computer etc.

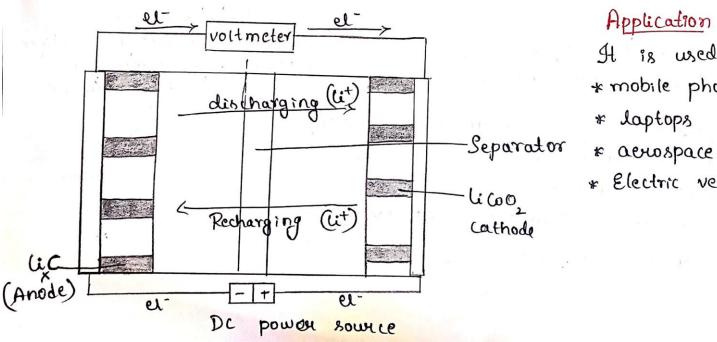
## Lithium - ion battery

In hi- ion battery anode is made up of graphite layer intercalated with lithium atoms, cathode is made up of lithium metal oxide (li Co Oz). Electrolyte is made up of lithium metal salt like (lipf6). Electrolyte is made up of non-moven polypropylene. During discharging li-atoms present in the graphite layer are oxidized and liberate the electron & li-rons. The electron flow from anode to cathode through external circuit. The lithium ions are more from anode to cathode through separator.

Cell supresentation :

Li/Lit, C/LiPF6 (ethylene carbonate)/LiCOO2.

Reaction : anode:  $lixC \xrightarrow{discharging} xli^+ + xe^- + C$ AŁ At cathode:  $\lim_{x \to \infty} \cos 0_2 + \chi (i^{\dagger} + \chi e^{-}) \longrightarrow \cos 0_2$ ====> (1600, + C Cell martion: LixC + Lirx COO2



## Application

- It is used in
- \* mobile phones
- \* laptops
- \* Electric vehicle

#### **MODULE 2 : MATERIALS FOR MEMORY AND DISPLAY SYSTEM**

*Memory Devices:* Introduction, Basic concepts of electronic memory, History of organic/polymer electronic memory devices, Classification of electronic memory devices, types of organic memory devices (organic molecules, polymeric materials, organic inorganic hybrid materials).

*Display system:* Photo active and electro active materials, Nanomaterials and organic materials used in optoelectronic devices. Liquid crystals (LC's) - Introduction, classification, properties and application in Liquid Crystal Displays (LCD's). Properties and application of Organic Light Emitting Diodes (OLED's) and Quantum Light Emitting Diodes (QLED's), Light emitting electrochemical cells

#### **MEMORY MATERIALS**

#### Definition of memory device:

A memory device is a piece of hardware used to store data. Most electronic devices such as computers, mobile phones, tablets, etc. All have a storage device that stores data and/or programs.

#### **Basic Concepts of Electronic Memory**

An electronic memory device is a form of semiconductors to rage which is fast in response and compact in size. A semiconductor storage system which can be read and written when coupled with a central processing unit (CPU, processor). The basic goal of a memory device is to provide a means for storing and accessing binary digital data sequences of "1's" and "0's".

Electronic memory device consists of

- 1. Two electrodes
- 2. Switching layer between two electrodes

The layer is operated from High Resistance State (HRS) to Low Resistance State (LRS) under an external electric voltage. The HRS can be regarded as "0" bit in data storage (OFF). The switching from HRS to the Low Resistance State (LRS) is equivalent to "0" to "1" binary conversion (ON). If a single material (used in making memory device) provides more than two resistance states (bistable), the storage capacity of a single memory increases exponentially.

*Classification of Electrical (electronic) Memory Devices:* Electronic memory devices can be divided into 4 types depending the type of material it is made of.

- 1. Transistor-Type Electronic Memory Devices
- 2. Capacitor-Type Electronic Memory Devices
- 3. Resistor-Type Electronic Memory Devices
- 4. Charge Transfer Type Electronic Memory Devices

#### Transistor-Type Electronic Memory

Transistors are made from silicon, a semiconductor. It is converted to p-type and ntype semiconductor by doping trivalent and pentavalent impurities. Transistors are made using

p-type and n type semiconductor. A transistor is a miniature electronic component

that can work either as an amplifier or a switch. A computer memory chip consists of billions of transistors; each transistor is working as a switch, which can be switched ON or OFF. Each transistor can be in two different states and store two different numbers, ZERO and ONE. Since chip is made of billions of such transistors and can store billions of Zeros and ones, and almost every number and letter can be stored.

#### Capacitor-Type Electronic Memory

A capacitor consists of two metal plates which are capable of storing an electric charge. It is used to store data. It is like a battery that holds data based on energy. If the capacitor is charged, it holds the binary numeral, "1" and holds "0" when the cell is discharged.

If the parallel plates of a capacitor are separated by dielectric layer, charges dissipate slowly and memory would be volatile. On the other hand, if the medium between the electrodes is ferroelectric in nature, can maintain permanent electric polarization that can be repeatedly switched between two stable states (bistable) by an external electric field. Thus, memory based on ferroelectric capacitors (FeRAM) is non- volatile memory.

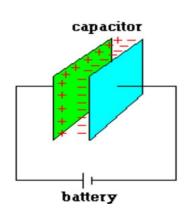
#### **Resistor-Type Electronic Memory**

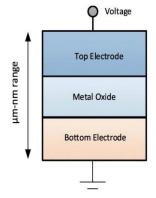
Memory devices containing switchable resistive materials are classified as resistor

-type memory, or resistive random access memory (RRAM). Resistor-type electronic memory usually has a simple structure, having a metal-insulator-metal structure generally referred to as MIM structure. The structure comprises of an insulating layer (I) sandwiched between the two metal (M) electrodes and supported on a substrate (glass, silicon wafer, plastic or metal foil). Initially, the device is under high resistance state or "OFF" and logically "0"state, when resistance changed or under external applied field changes to low resistance state or "ON" logical value "1".

#### Charge Transfer Effects Type Electronic Memory

A charge transfer (CT) complex is defined as an electron donor- acceptor (D-A) complex, characterized by an electronic transition to an excited state in which a partial transfer of charge occurs from the donor moiety to the acceptor moiety. The conductivity of a CT complex is dependent on the ionic binding between the D-A components.





#### Classification of electronic memory based on storage type of the device:

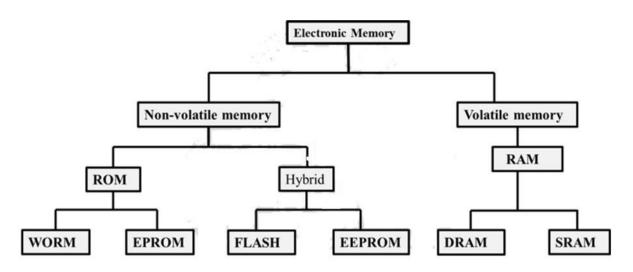
Electronic memory can be divided into two primary categories: volatile and non-volatile memory.

Non-volatile memory: Non-volatile memory (NVM) or non-volatile storage is a type of memory that can retain stored information even after power is removed. Volatile Memory: Volatile memory is a type of memory that maintains its data only while the device is powered. If the power is interrupted for any reason, the data is lost.

#### Further it is divided as shown below:

#### **ROM: Read Only Memory**

- $\checkmark$  ROM is a non-volatile memory.
- ✓ Information stored in ROM is permanent.
- $\checkmark$  Information and programs stored on it, we can only read.
- ✓ Information and programs are stored on ROM in binary format.
- $\checkmark$  It is used in the start-up process of the computer.



#### WORM (Write Once Read Many times)

Describes a data storage device in which information once written, cannot be modified. This write protection affords the assurance that the data cannot be tampered with once it is written to the device, excluding the possibility of data loss from human error, computer bugs, or malware.

#### **EPROM** (Erasable programmable read-only memory)

EPROM also called EROM is a type of PROM but it can be reprogrammed. The data stored in EPROM can be erased and reprogrammed again by ultraviolet light. Reprogrammed of it is limited. Before the era of EEPROM and flash memory, EPROM was used in micro controllers.

#### **HYBRID MEMORIES**

These can be read and written as desired, like RAM, but maintain their contents without electrical power, just like ROM. It is a Non-Volatile memory.

#### FLASH

It is an electronic non-volatile computer memory storage medium that can be electrically erased and reprogrammed. Flash memory is a non-volatile memory chip used for storage and for transferring data between a personal computer (PC) and digital devices.

#### **EEPROM (Electrically Erasable Programmable Read-Only Memory)**

Electronically erasable programmable read only memory, is a standalone memory storage device such as a USB drive. It is a type of data memory device using an electronic device to erase or write digital data.

#### **RAM: (Random Access Memory)**

It is a computer's short-term memory. It can be read and changed in any order, typically used to store working data and machine code.

RAMs consist of ferromagnetic particles embedded in a polymer matrix having a high dielectric constant. One of the most common RAMs is called iron ball paint, which contains tiny metal- coated spheres suspended in an epoxy-based paint. The spheres are coated with ferrite or carbonyl iron.

#### **DRAM (Dynamic Random Access Memory)**

It is a type of semiconductor memory that is typically used for the data or program code needed by a computer processor to function. All DRAM chips manufactured to date use capacitors containing electrodes made of doped silicon or polysilicon and dielectric films of silicon dioxide and/or silicon nitride.

#### SRAM (Static Random Access Memory)

It is a type of RAM that holds data in a static form, that is, as long as the memory has power. SRAM: It is made up of metal-oxide-semiconductor field-effect transistors (MOSFETs).

#### **Types of organic memory devices**

Organic memory device stores data based on different electrical conductivity states (ON and OFF states) in response to an applied electric field.

#### There are three types of organic memory devices

- 1. Organic molecular memory devices
- 2. Polymeric molecules
- 3. Organic-Inorganic hybrid materials

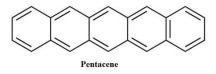
**Molecular memory devices:** If organic molecular material used to store the data is called organic-based memory device. Organic electronic memory devices based on organic molecules were first reported in several acene derivatives including naphthalene, anthracene, tetracene, pentacene, perylene, p-quarterphenyl and p-quinquephenyl.

#### **Organic molecules**

#### The p-Type Organic Semiconductor Material "Pentacene"

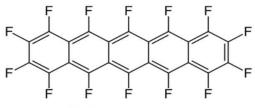
An Organic molecule with  $\pi$  conjugated system and possesses holes as major charge carrier is called p-type semiconductor. Ex: Pentacene These molecules show bistable states when external field is applied i.e. ON and OFF state. It is linearly fused aromatic compound with five benzene rings. It can be obtained in crystal and thin film form.

It shows good hole mobility, hence it behaves as a p-type semiconductor.



The n-type organic semiconducting material Perfluoropentacene

When all the hydrogen atom of pentacene is replaced by Fluorine atoms, it formed Perfluoropentacene. Basically Fluorine is electron withdrawing nature. Hence it convers this molecules into n-type semiconductor.

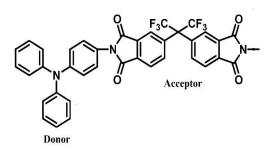


Perfluoropentacene

#### **Polymeric Molecules**

Polymer used for organic memory device is Polyimide (PI) with Donor-Triphenylamine and Acceptorphthalimide.

This polymer has high thermal stability and mechanical strength. The donors and acceptors of PIs contribute to the electronic transition based on an induced charge transfer (CT) effect under an applied electric field.



#### **DISPLAY SYSTEM**

A system through which information is conveyed to people through visual means.

Photoactive and electro active organic materials

Organic semiconductors used in electronic and optoelectronic devices are called as electroactive and Photoactive materials. Photoactive and electroactive organic materials are the semiconductors composed of  $\pi$ -electron systems.

#### Advantages

- 1. Light weight and flexible
- 2. Easily synthesized by chemical method.
- 3. Production cost is less
- 4. Used in thin-film flexible devices
- 5. Properties can be fine-tuned by structure modification

#### **Photoactive Process:**

- 1. Absorption and emission of light radiation in the wavelength region from ultraviolet to near infrared.
- 2. Photogeneration of charge carriers (photons of light creates electron-hole pair in the semiconductor)
- 3. Transport of charge carriers (Charge carriers are particles or holes that freely move within a material and carry an electric charge)

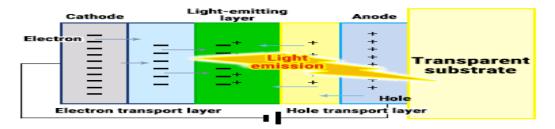
#### **Electroactive Process**

Injection of charge carriers from the electrode (The process whereby light is emitted at the junction of N- and P-type semiconductors when an external electric source is applied to drive the electrons and the holes into the junction) Transport of Charge carriers

Photoactive and electro active organic materials are the semiconductors composed of of  $\pi$ -electron systems which are used in electronic and optoelectronic devices.

#### Working Principle

Photoactive and electroactive material absorb and emit light in the UV to IR region. Display system (OLED) consisting of photoactive and electroactive material absorb light and allows an electron to jump from HOMO of a Donor to LUMO of an Acceptor. This phenomenon generate and transport charge carriers.



When electrons move from cathode, anode allows movement of holes towards light emitting layer under an applied field. Electron-hole pairs are created at the Light-

Emitting-Layer and energy is released due to recombination. This energy is sufficient to excite an electron from HOMO to LUMO in the light emitting layer

made of photoactive and electroactive materials. There is a re-emission of light while electron is returning to HOMO level. This light is extracted by a transparent substrate placed adjacent to either of the electrode.

#### **Optoelectronic Process**

1. Absorption and emission of light radiation in the wavelength region from

ultraviolet to near infrared.

- 2. Photogeneration of charge carriers (photons of light creates electron-hole pair in the semiconductor).
- 3. Transport of Charge carriers (Charge carriers are particles or holes that freely move within a material and carry an electric charge).
- 4. Injection of charge carriers from the electrode (The process whereby light is emitted at the junction of N- and P-type semiconductors when an external electric source is applied to drive the electrons and the holes into the junction).
- 5. Exhibit excellent non-linear optical properties (originate from the interactions between the electrons in the molecule and the electric fields in light (electromagnetic radiation).

#### Organic materials used in optoelectronic devices

The organic compounds with conjugation and  $\pi$  – electron are capable of exhibiting the optoelectronic properties. Organic materials are broadly classified as 3 categories.

- 1. Small Molecules
- 2. Oligomers with well-defined structures
- 3. Polymers

#### Nanomaterials (Silicon Nanocrystals) for Optoelectronic devices

#### Any substance in which at least one dimensions is less than 100nm is called nanomaterials. The properties of nanomaterials are different from bulk materials due to:

- 1. Quantum Confinement effect
- 2. Increased surface area to volume ratio

#### The improved electronic properties yielded for nanostructured silicon in comparison to its bulk, which led the use of Silicon Nanocrystals in electronics and optoelectronics fields.

#### Special properties of Silicon Nanocrystals for optoelectronics

- 1. Silicon Nanocrystal has wider band gap energy due to quantum confinement.
- 2. SiNCs shows higher light emission property (Photoluminescence)
- 3. SiNCs exhibit quantum yield of more than 60%.
- 4. Si-NCsexhibittunableelectronicstructure

#### **Applications:**

- 1. SiNCs are used in neuromorphic computing and down-shifting in photovoltaics
- 2. SiNCs are used in the construction of novel solar cells, photo detectors and optoelectronic synaptic devices.

Organic materials for Optoelectronic devices [Light absorbing materials – Polythiophenes] (P3HT)

Polythiophenes are an important class of conjugated polymers, environmentally and thermally stable

material. Chemical structure of P3HT Poly (3-hexylthiophene) is a polymer with chemical formula  $(C_{10}H_{14}S)n$ . It is a Polythiophenes with a short alkyl group on each repeat unit.

Highly ordered (P3HT) are composed of closely packed, p–p stacked (p–p distance of 0.33nm) fully extended chains which are oriented perpendicular to the substrate.

#### Structure of P3HT

#### **Properties:**

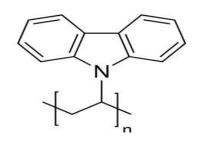
- 1. P3HT is a semiconducting polymer with high stability and exhibits conductivity due to holes therefore considered as p-type semiconductor.
- 2. Poly-3-hexylthiophene (P3HT) has great capability as light-absorbing materials in organic electronic devices.
- 3. P3HT has a crystalline structure and good charge-transport properties required for Optoelectronics.
- 4. P3HT has a direct-allowed optical transition with a fundamental energy gap of 2.14eV.
- 5. Fundamental band gap of P3HT is 490nm visible region, corresponding to  $\pi \rightarrow \pi^*$  transition, giving electron-hole pair.
- 6. P3HT indicates that an increase in the conductivity is associated with an increase in the degree of crystallinity.

#### **Applications:**

- 1. P3HT-ITO forms a p-n junction permits the charge carriers to move in opposite direction and hence, used in Photovoltaic devices.
- 2. It can be used as a positive electrode in Lithium batteries.
- 3. Used in the construction of Organic Solar Cells.
- 4. Manufacture of smart windows.
- 5. Used in the fabrication new types of memory devices.

#### Light emitting material-Poly [9-vinylcarbazole] (PVK)]

Poly(N-vinyl carbazole) (PVK)is one of the highly process able polymers as hole conducting material and therefore used as an efficient hole transport material to prepare highly efficient and stable planar heterojunction perovskite solar cells.



# Structure of poly (9-vinylcarbazole)

#### **Applications:**

- 1. PVK has been commonly used in OLEDs, light harvesting applications. Photorefractive polymer composites and memory devices.
- 2. Used in the fabrication of light-emitting diodes and laser printers.
- 3. Used in the fabrication of organic solar cells when combined with TIO on glass substrate.
- 4. Used in the fabrication of solar cells when combined with Perovskite materials.

#### LIQUID CRYSTALS

A distinct state of a matter in which degree of molecular ordering is intermediate between the ordered crystalline state and completely disordered liquid state.



#### **<u>Classification</u>**:

Liquid crystals are classified into two types Thermotropic liquid crystals

Lyotropic liquid crystals

1) <u>Thermotropic liquid crystals</u> (TLC): The compounds which exhibit liquid crystal behavior with variation of temperature are called thermotropic liquid crystals.

Ex: 1) Cholesteryl Benzoate: (145.5°C & 178.5°C)

2) P-Azoxy Anisole: (118°C & 135°C)

**<u>2) Lyotropic Liquid Crystals</u>:** Some of the compounds transformed into liquid crystal phase when mixed with another substance or solvent by the variation of concentration of the compound are called lyotropic liquid crystals

Ex: 1) Soap water mixture

2) Phospholipid water mixture

#### **Types of Thermotropic liquid crystals:**

There are four types of liquid crystals

- 1. Nematic Liquid Crystals (NLC)
- 2. Chiral Liquid Crystals or Cholesteric Liquid Crystals (CLC)
- 3. Smectic Liquid Crystals (SLC)
- 4. Columnar Liquid Crystals or Discotic Liquid Crystals (DLC)

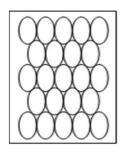
#### Nematic Liquid Crystals (NLC)

- 1. These are formed by the compounds that are optically inactive.
- 2. The molecules have elongated shape and are oriented parallel to the director.
- 3. These molecules possess intermolecular force of the attraction such that they stay parallel to one another to form nematic liquid crystals.

Ex: a) P-Azoxy Anisole (PAA) b) P-Azoxy Phenetole

#### **Chiral Liquid Crystals or Cholesteric Liquid Crystals**

1. These are formed by optically active compounds having





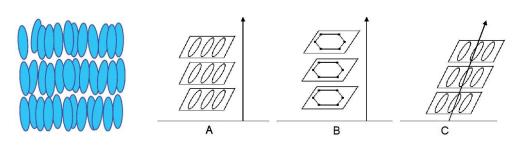
chiral center.

- 2. Hence molecules acquire spontaneous twist about an axis normal to molecular direction.
- 3. The twist may be right or left depending on molecular conformation.
- 4. Molecules are arranged themselves in such a way that group of molecules alike at different angles with respect to their adjacent groups.

#### Ex: a) Cholesteryl benzoate b) Cholesteryl formate etc.

#### Smectic Liquid Crystals (SLC):

- 1. These liquid crystals have small amount of positional order and orientational order.
- 2. If the director is perpendicular to the plane, it is called *smectic A*. These are least ordered of the orthogonal smectic phases. The molecules are arranged in columns.
- 3. If the director is perpendicular to the plane and molecules are arranged in hexagonal order, it is called *smectic B*.
- 4. If the director makes an angle other than 90°, it is called *smectic C*.



#### Columnar Liquid Crystals or Discotic Liquid Crystals (DLC)

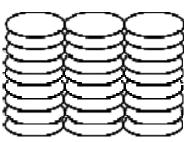
- 1. In these liquid crystals, there is an orientation order but no positional order.
- 2. There is a random motion of the molecules perpendicular to the plane.
- 3. The molecules orient themselves along the director.
- 4. The molecules tend to position themselves in columns.
- 5. The columns are arranged in hexagonal lattice.

#### **Properties**

- > Liquid crystal can flow like a liquid, due to loss of positional order
- > These are elongated and have some degree of rigidity
- > They have less orientational order
- Transition from crystalline solids to liquid crystals caused by a change of temperature.

#### Applications of liquid crystals:

- 1) Liquid crystals are used in watches, calculators, mobile telephones, laptops, computers etc.
- 2) These are used in blood pressure instrument, digital thermometers and TV Chanel indicators.



3) These are used in potentiometer, conductometer, Colorimeter etc.

#### Application of Liquid Crystal in Display System (LCD): Principle:

- 1) The display panel is composed of two polarizers and a mirrored surface.
- 2) A thin film of the liquid crystal is placed between two glass sheets. One of the glass sheet on one side is coated with electrically conducting material such as SnO<sub>2</sub>.
- 3) In the absence of applied voltage, the liquid crystal molecules are precisely aligned.
- 4) The entire panel appears silvery because light passes through both the polarizers, reflects off the mirrored surface and then passes through both the polarizers.
- 5) When the voltage is applied the alignment of the LC molecules changes.
- 6) This results in the polarized light from the first polarizer not being rotated by 90° completely to align with second polarizer.
- 7) The second polarizer blocks the passing of light and causes the segment of the panel to appear black.

#### **Organic Light Emitting Diodes (OLED's)**

OLEDs are thin film devices consisting of a stack of organic layers sandwiched between two electrodes. OLEDs operate by converting electrical current in to light via an organic emitter.

OLED is an electroluminescent device that uses organic molecules as a source of light emission. Light is emitted by organic material when an external field is applied across it.

# **<u>Properties</u>**: Some of the key properties of Organic Light Emitting Diodes (OLEDs) include:

- 1. **Thinness and flexibility:** OLEDs are very thin and flexible, which makes them suitable for use in curved or flexible displays.
- 2. **High contrast:** OLEDs have a high contrast ratio, which means that they can produce deep blacks and bright whites, resulting in images with vivid and rich colours.
- 3. **Fast response time:** OLEDs have a fast response time, which means that they can switch on and off quickly, resulting in smooth and seamless motion in video content.
- 4. **Wide viewing angle:** OLEDs have a wide viewing angle, which means that the image quality is maintained even when viewed from different angles.
- 5. **Energy efficiency:** OLEDs are energy efficient as they do not require a back light like traditional LCD displays, resulting in lower power consumption.

#### **Applications**

- 1. Flat-panel TV screen
- 2. Digital cameras
- 3. Mobile phones

#### **Quantum Light Emitting Diodes (QLED's)**

QLED is an electroluminescent device that uses quantum dots (QD's) as a source of light emission.

#### **Properties:**

1. Accurate and vibrant colours: QLEDs are capable of producing highly accurate and vibrant colours due to their use of quantum dots, which emit light of a specific colour

when they are excited by a light source or an electrical current.

- 2. **Energy-efficient**: QLEDs are more energy-efficient than traditional LCD displays because they do not require as much back lighting.
- 3. **High contrast**: QLED displays have high contrast ratios, which means that the difference between the darkest and brightest areas of the display is greater, resulting in more detailed and life like images.
- 4. **Long life span**: QLEDs have a longer life span than traditional LCD displays because they do not suffer from the same issue soft back light burnout or colour fading over time.
- 5. **Fast response times**: QLED displays have fast response times, which mean that they can display fast-moving images without motion blur or ghosting.
- 6. **Flexibility**: QLEDs can be made on flexible substrates, which allows for the creation of flexible displays that can be bent or curved.

#### **Applications**

- 1. Flat-panel TV screen
- 2. Digital cameras
- 3. Mobile phone