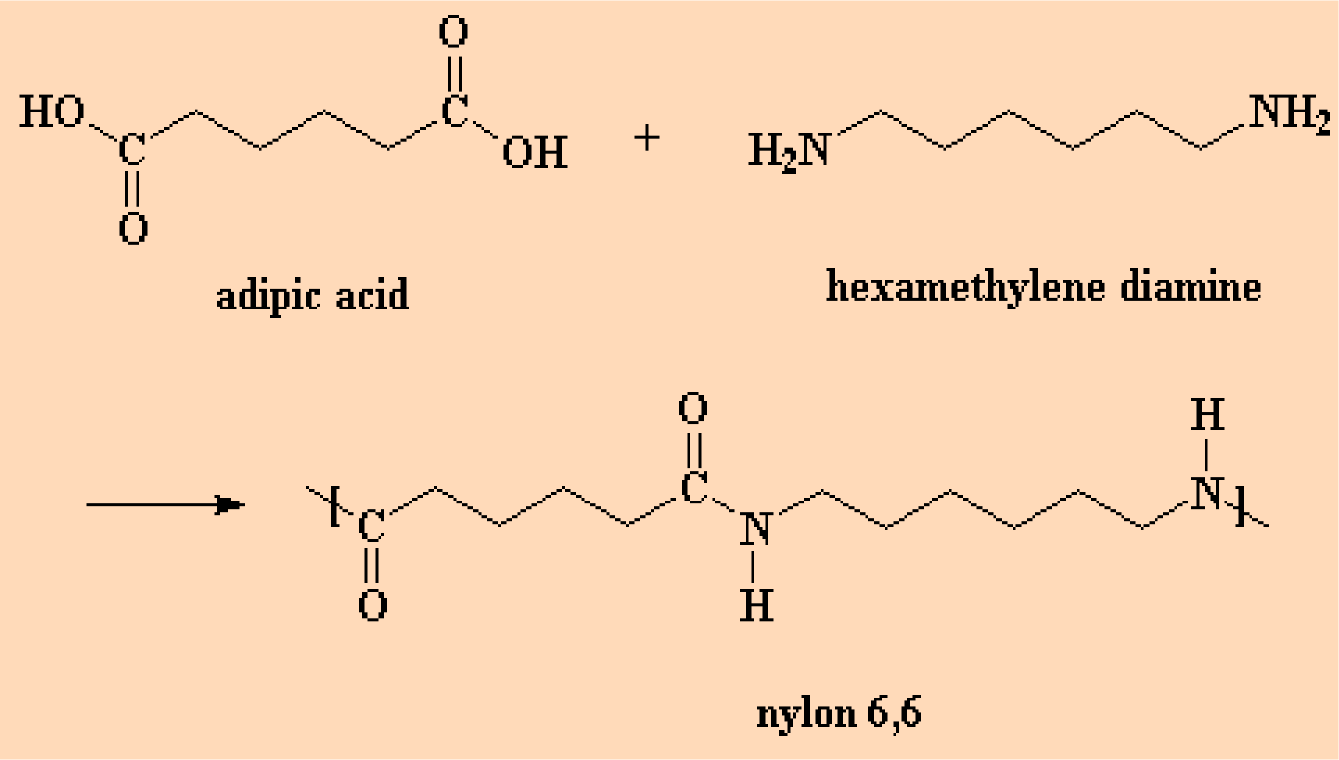
Module-2 Quantum Materials and Polymers

Quantum Dots: Introduction, size dependent properties-quantum confinement effect, surface-to-volume ratio & band gap. Synthesis of Cd-Se Quantum dots by wet chemical method and its applications. Construction, working principle and applications of quantum dot sensitized solar cells (QDSSCs).

Polymer: Introduction, number average and weight average molecular weight of the polymers and numerical problems. Structure-properties relationship of polymers (Crystallinity, Strength, Elasticity and chemical resistivity]. Synthesis and properties of nylon 6,6 and its advantages in 3D printing applications. Synthesis and properties of chlorinated polyvinyl chloride (CPVC), and polymethyl methacrylate (PMMA) and their uses in device applications.

Conducting polymers- Introduction, synthesis of polyaniline, conduction mechanism and its engineering applications.

Synthesis and properties of Nylon 6,6 and its advantages in 3D printing applications



Properties :

1.High tensile strength and stiffness.

2.Excellent wear and abrasion resistance.

3.High melting point and good thermal stability.

4.Low friction and good fatigue resistance.

5.Good chemical resistance but absorbs moisture.

Applications:

1.Used for making gears and bearings due to high wear resistance.

2.Ideal for mechanical housings and brackets in 3D-printed assemblies.

3.Applied in automotive components needing heat and strength.

4.Suitable for industrial tooling and jigs.

Synthesis and properties of chlorinated polyvinyl chloride (CPVC)

CPVC is produced by **chlorinating PVC**:

$$\mathbf{PVC + Cl_2 \rightarrow CPVC + HCl}$$

Chlorine atoms substitute hydrogen atoms on the PVC backbone, increasing chlorine content from ~56% (PVC) to 63–69% (CPVC).

Properties:

1.CPVC has higher heat resistance than PVC due to increased chlorine content.

2.It shows excellent chemical and corrosion resistance.

3.It has good mechanical strength and stiffness.

4.CPVC offers low thermal conductivity and good flame resistance.

5.It is durable, dimensionally stable, and suitable for hot-water piping.

Applications:

1.Used for hot and coldwater plumbing systems due to high heat resistance.

2.Applied in industrial chemical pipes and fittings.

3.Used in fire-sprinkler systems because of good flame resistance.

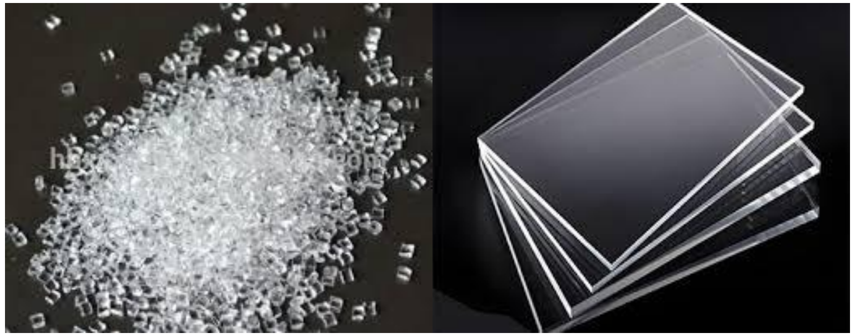
4.Suitable for ducting and ventilation components.

5.Used in industrial equipment liners for corrosion protection.

Polymethyl methacrylate (PMMA)

Methyl Methylacrylate

Polymethyl methylyacrylate



Properties of PMMA

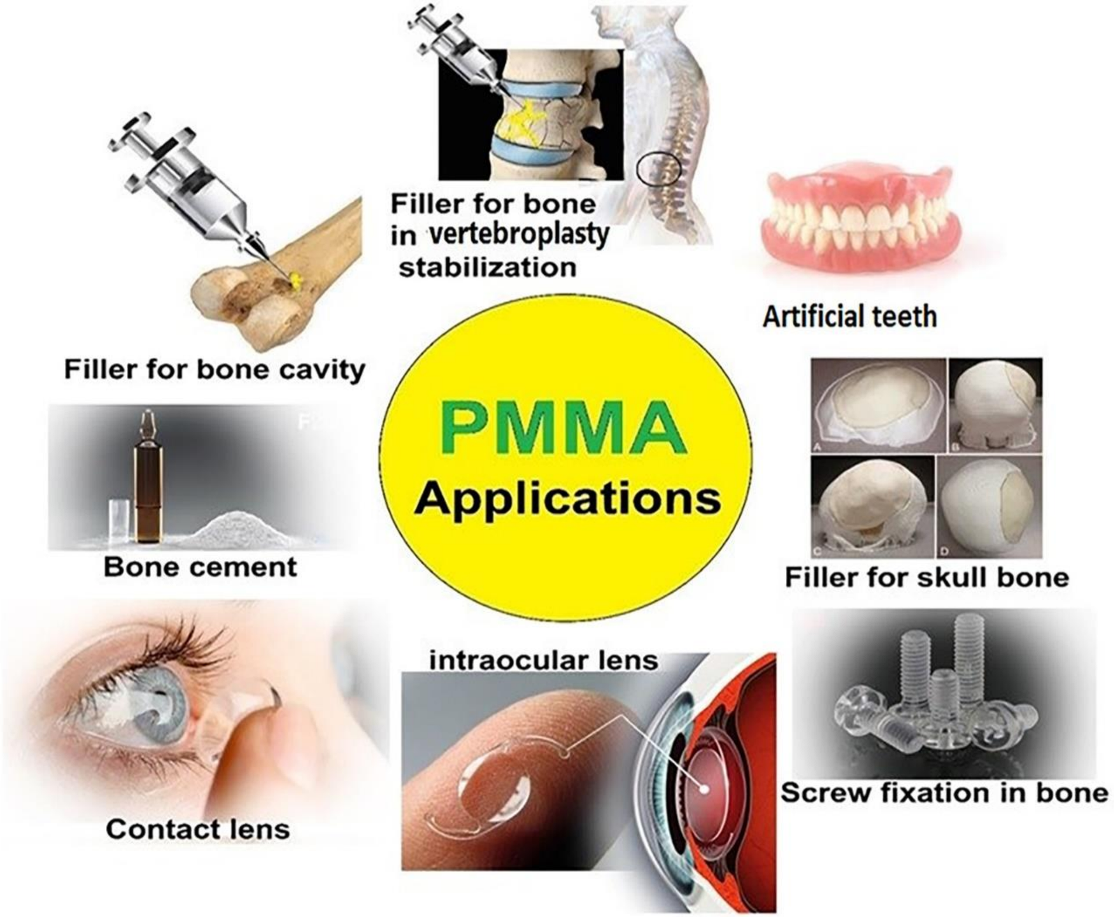
1.High optical transparency (92% light transmission)

2.Good UV resistance

3.High stiffness and hardness

5.Good weathering and scratch resistance

6.Lightweight compared to glass



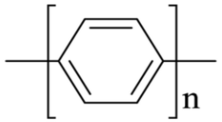
Uses of PMMA in Device Applications

1. Optical Devices Lenses, LED light guides, optical fibers, solar concentrators, Transparent protective covers for displays and sensors
2. Biomedical Devices Intraocular lenses (IOLs), Denture bases, bone cement (PMMA–based)Microfluidic device chips due to biocompatibility
3. Electronic Devices, Light diffusers in screens and LCD backlights, Encapsulation of LEDs, and Components for photonic devices
4. Automotive and Aerospace Headlight covers Aircraft windows and canopies Instrument panel covers
5. Micro fabrication & 3D Printing Photoresists (e.g., in e-beam lithography)Prototyping of transparent components MEMS device substrates.

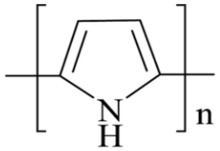
CONDUCTING POLYMERS

- Conducting polymers are organic polymers that conduct electricity like metals or semiconductors

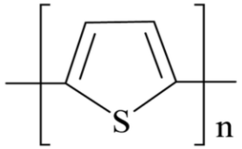
- They have conjugated backbones (alternating single/double bonds) allowing delocalized electrons, especially after doping (adding charges).



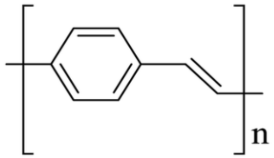
poly(p-phenylene)



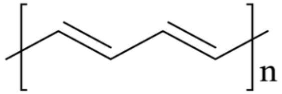
Polypyrrol



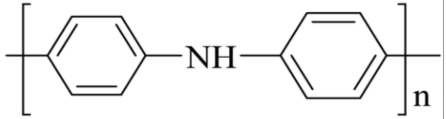
Polythiophene



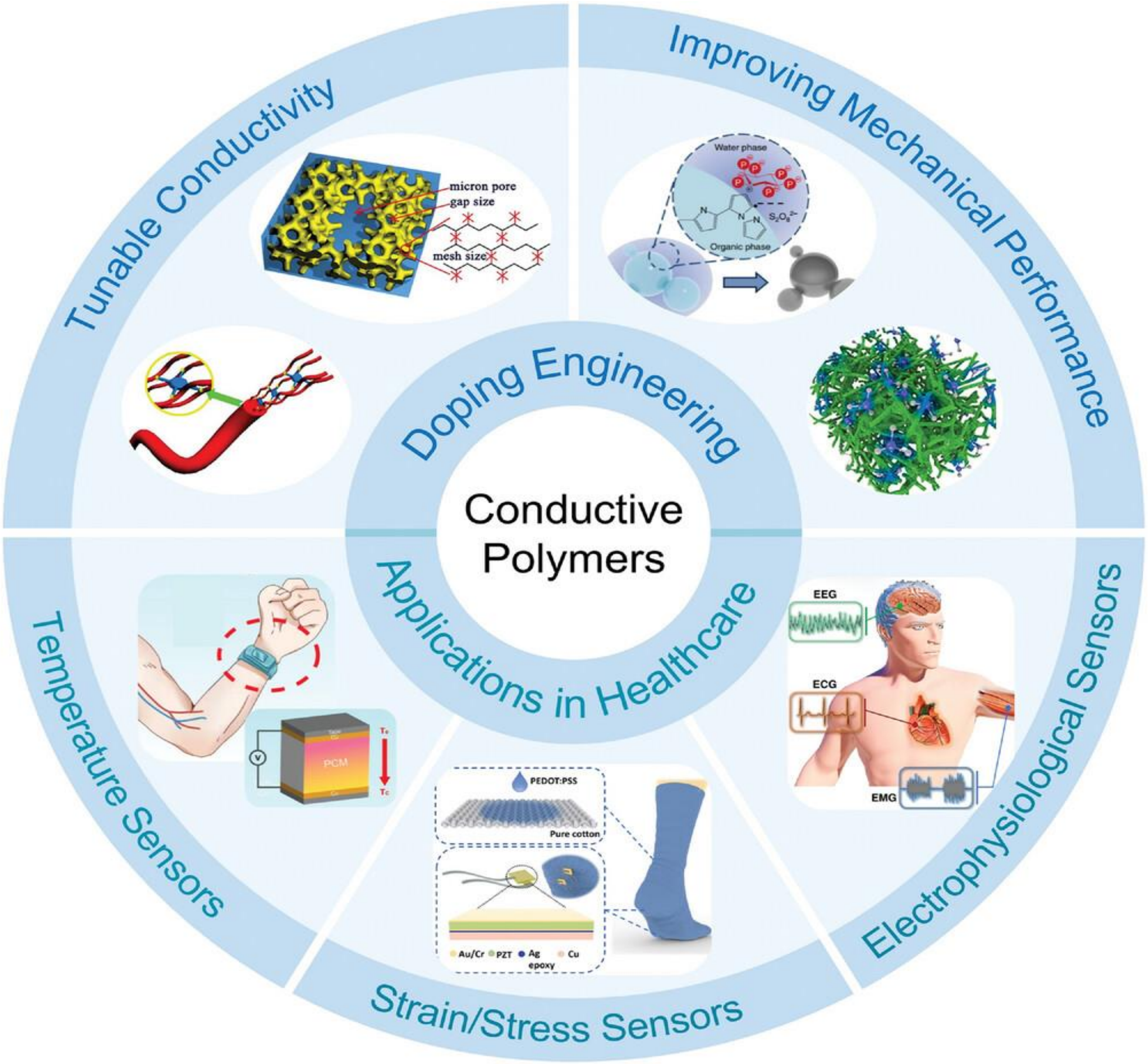
poly(p-phynylene vinylene)



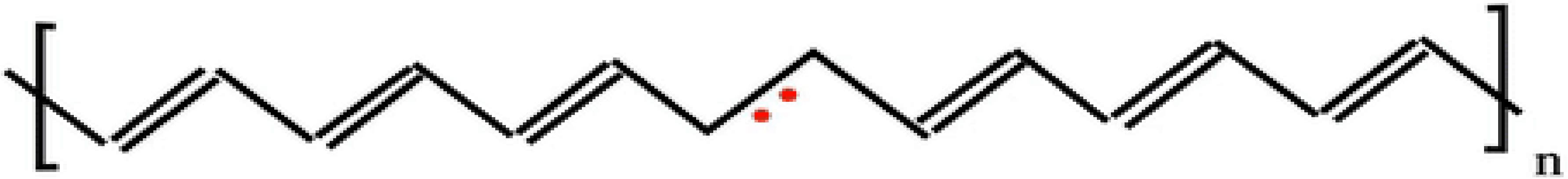
Polyacetylyne

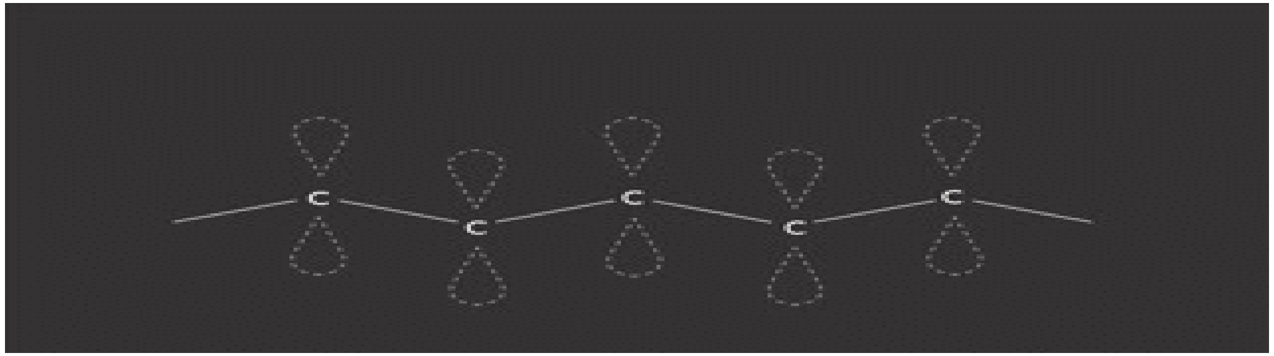


Polyaniline



Electrical conduction takes place in a positive bipolaron also.
Positive bipolaron is a



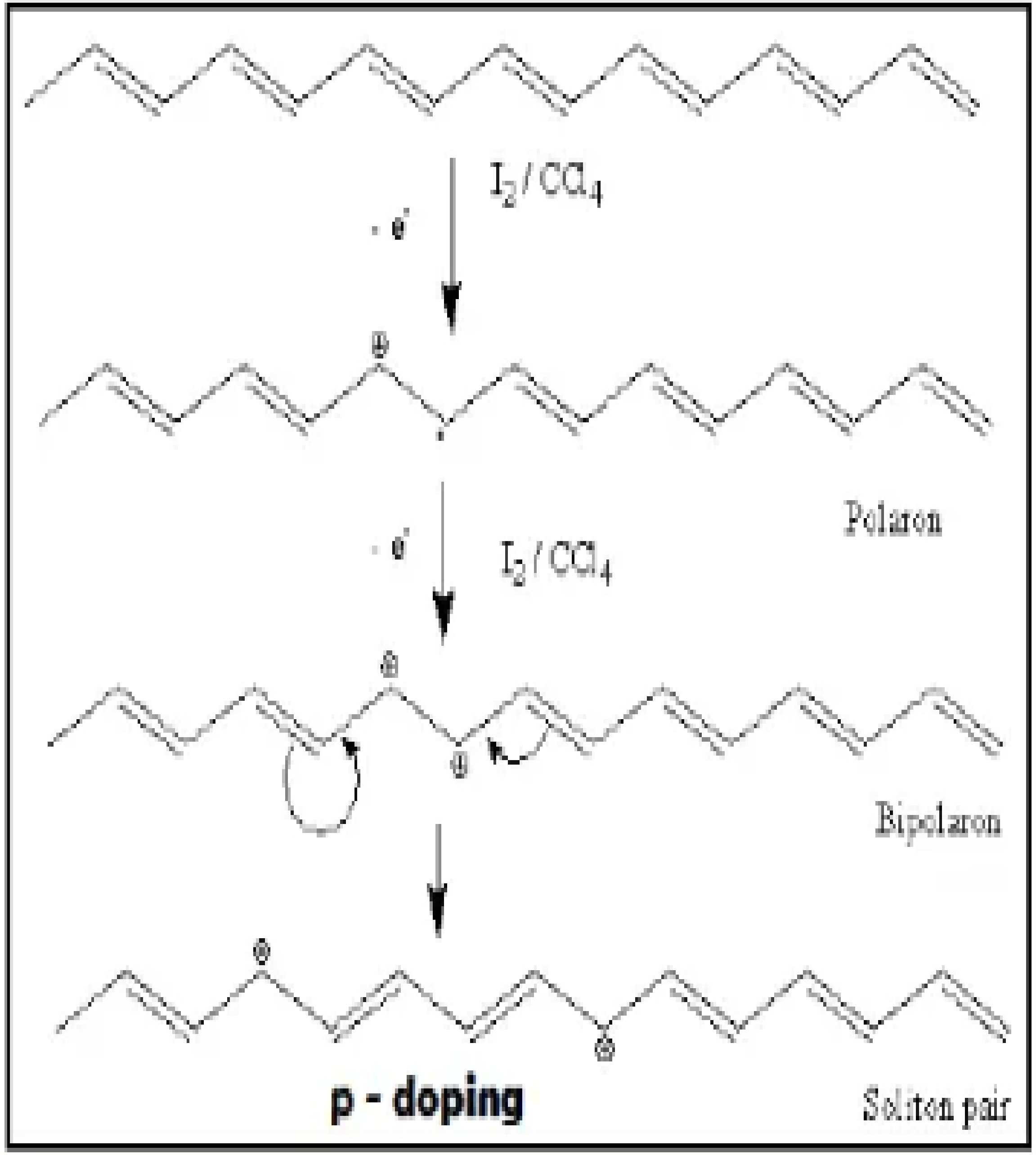


Types of Doping

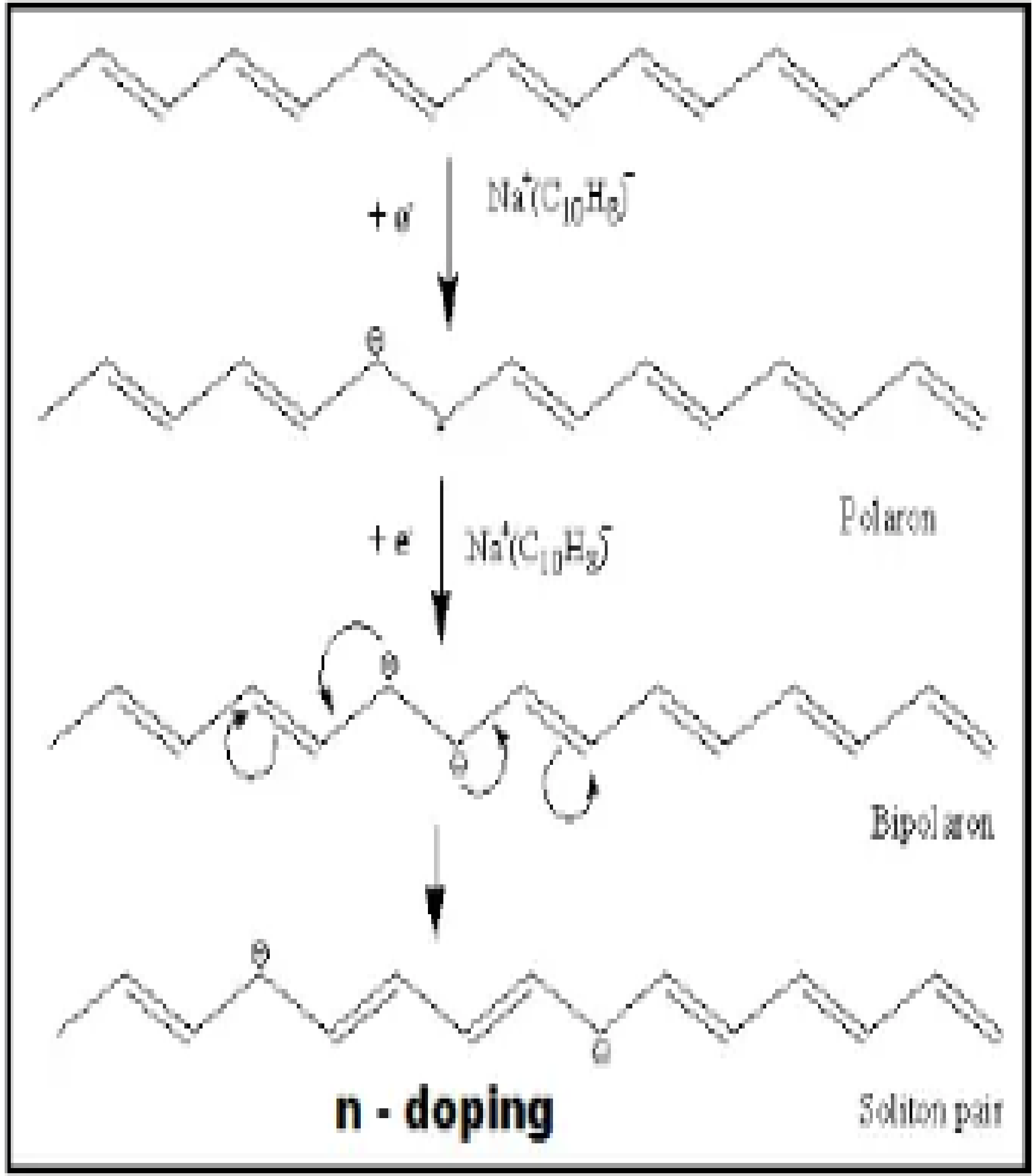
Oxidative doping (p-type doping): The polymer is treated with **an oxidizing agent** like iodine, aluminium chloride, perchloric acid etc. Oxidizing agent takes away electrons from p-back bone of the chain creating a hole. Thus, polymer becomes p-type conductor as it conducts by the movement of holes.

Reductive doping (n-type doping): The polymer is treated with a **reducing agent** like sodium or lithium naphthalides. Reducing agents supplies electrons to p- back bone of the chain.

The polymer becomes n-type conductor as it conducts by free mobile electrons.



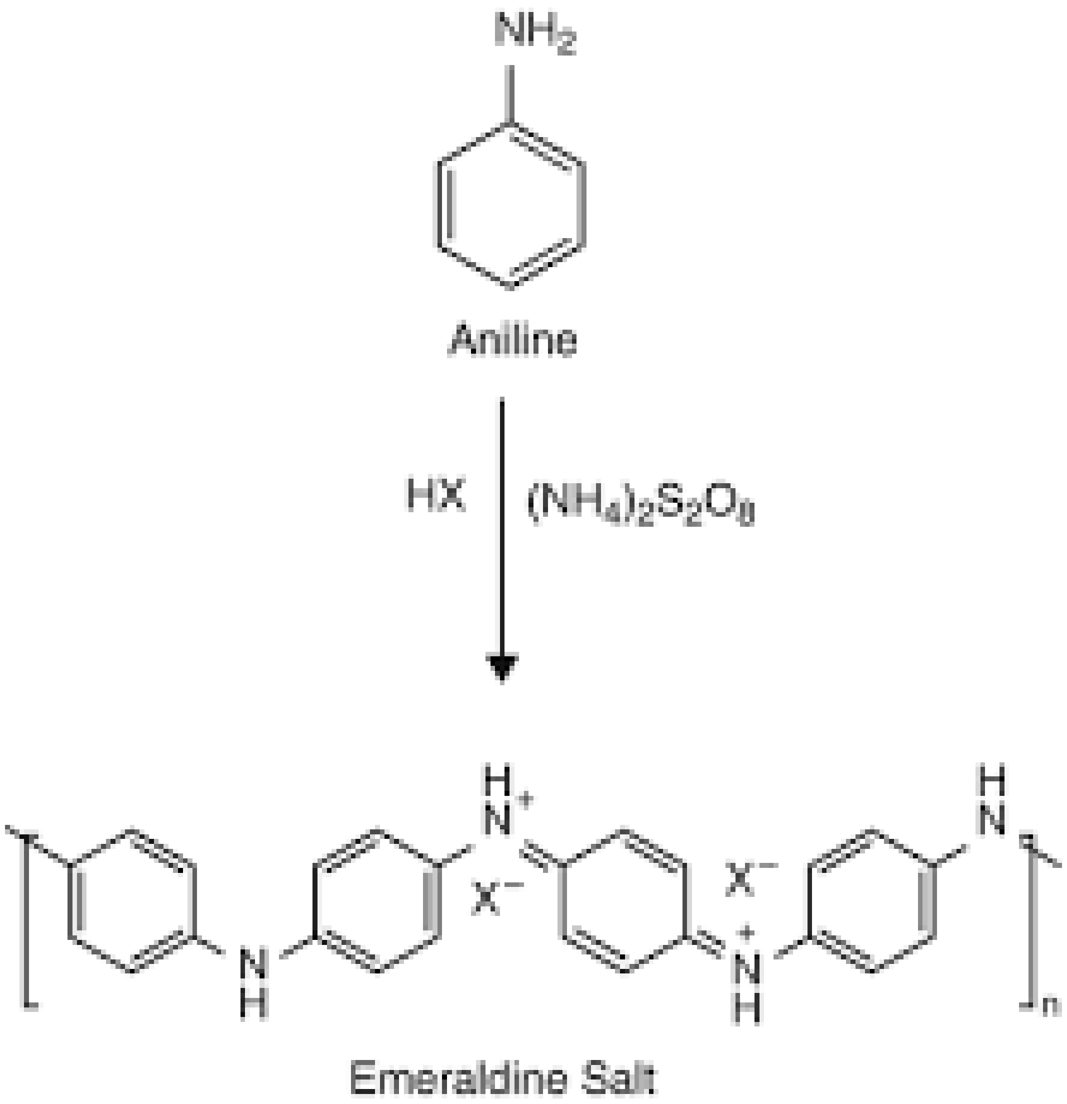
I_2 / CCl_4
- e⁻
Polaron
- e⁻
I_2 / CCl_4
Bipolaron
Soliton pair
p - doping



+ e⁻
$Na^+(C_{10}H_8)^-$
Polaron
+ e⁻
$Na^+(C_{10}H_8)^-$
Bipolaron
Soliton pair
n - doping

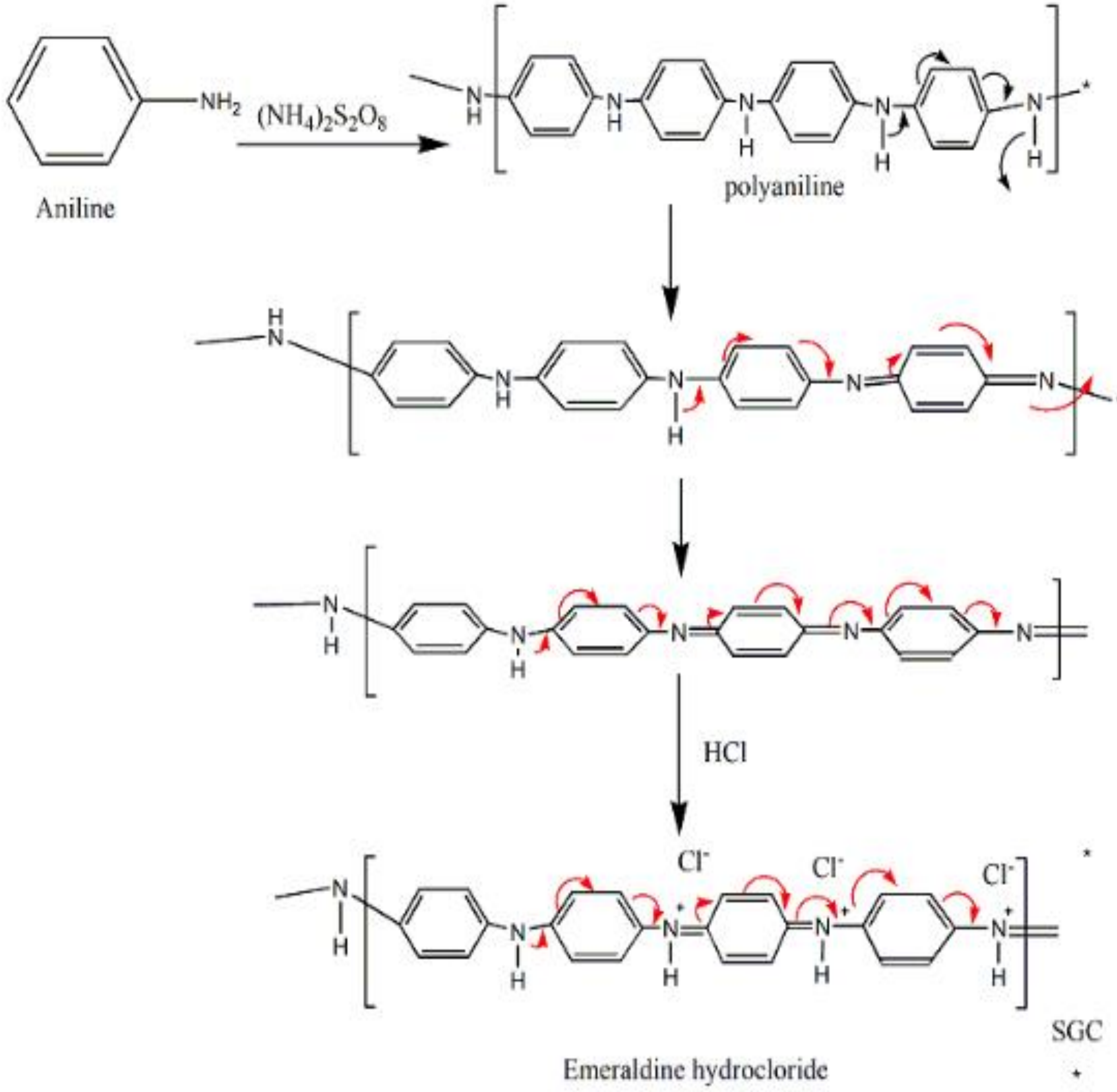
Polyaniline

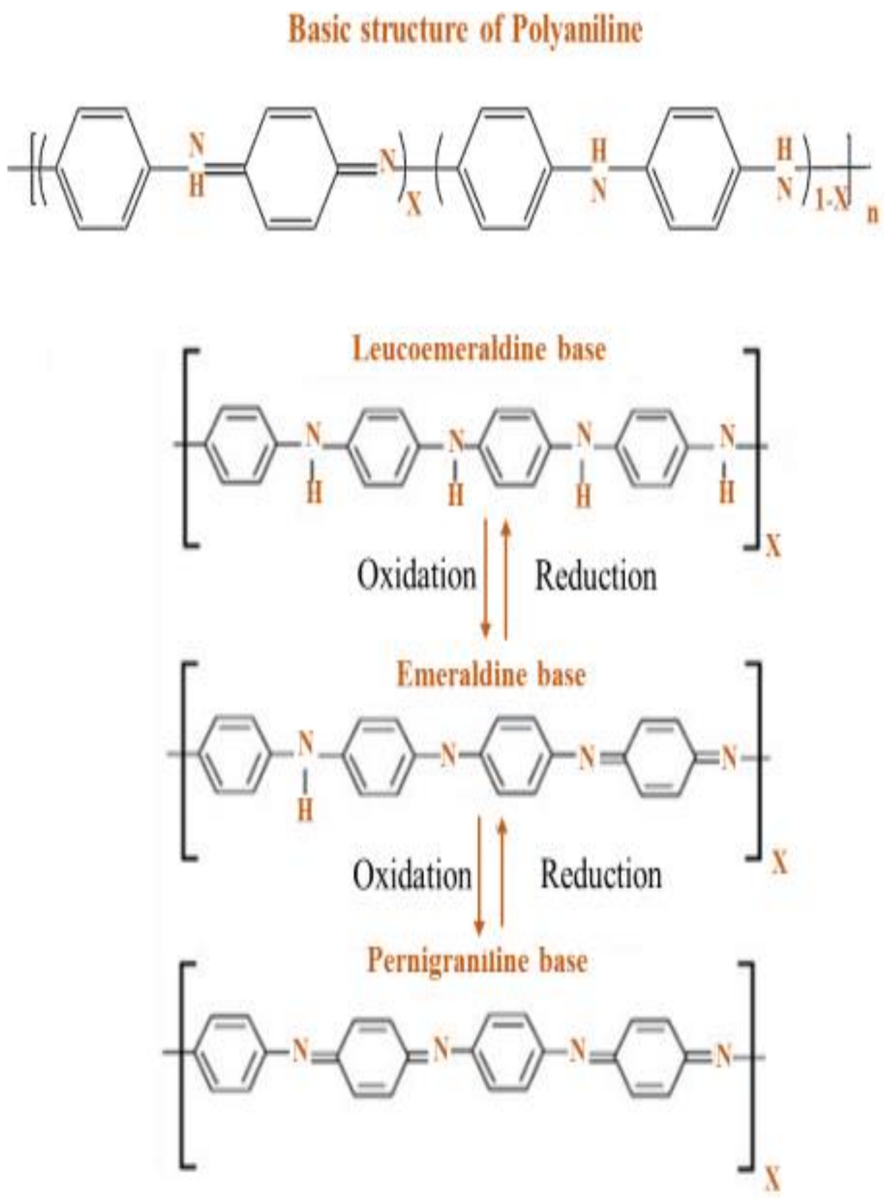
- Polyaniline (PANI) is a highly versatile, conducting polymer made from aniline, known for its tunable conductivity
- It exists in different oxidation states such as Leucoemeraldine, Emeraldine, Pernigraniline and can change color with doping, transitioning from colorless to blue/violet.

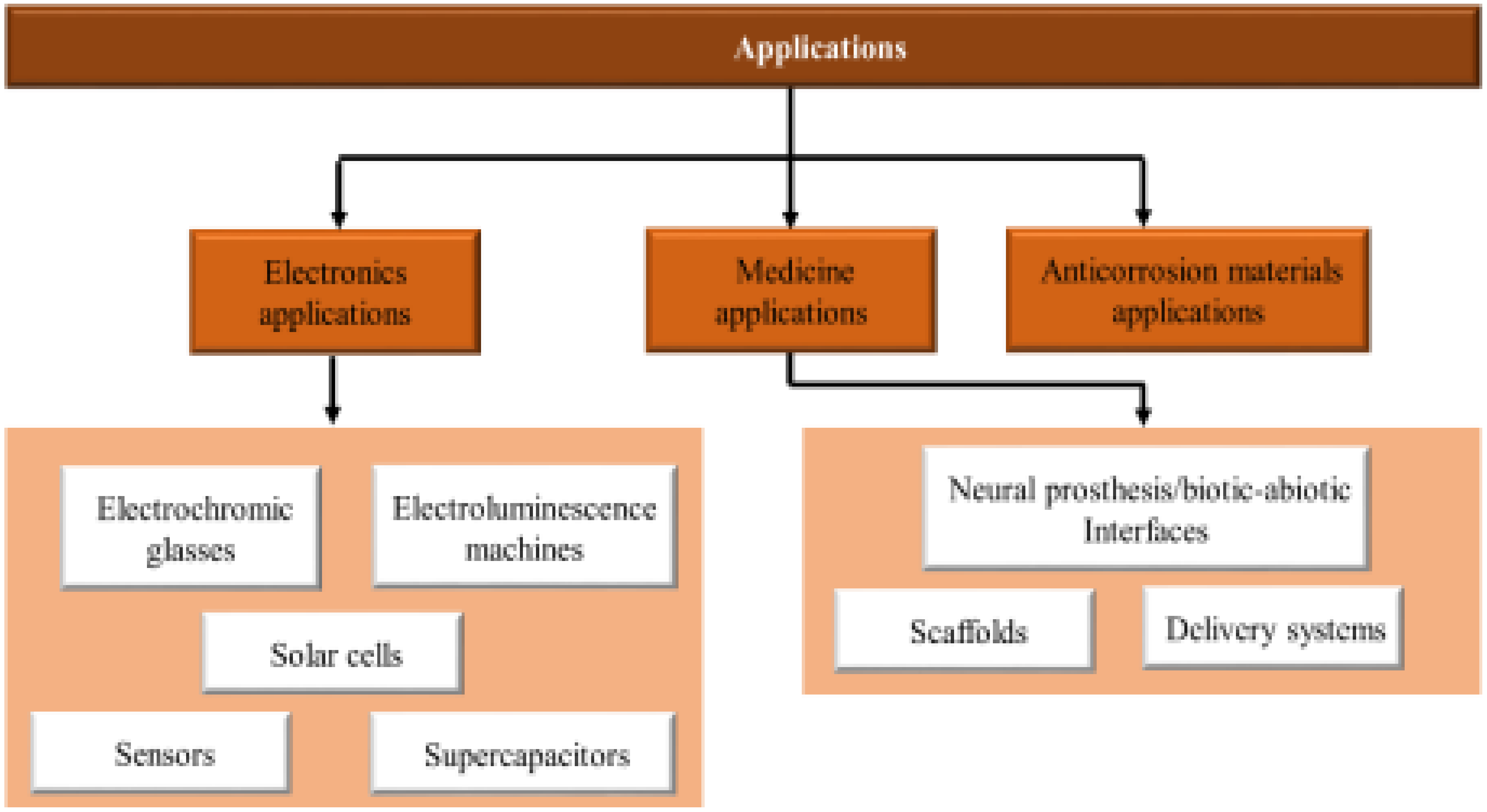


Synthesis of Polyaniline

Mechanism of conduction in Polyaniline (PANI)



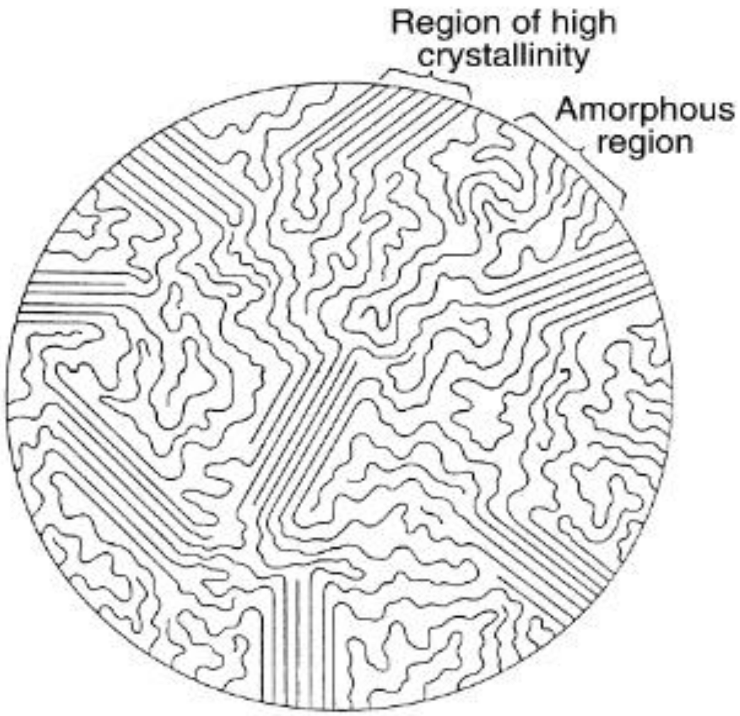



Applications
Electronics applications
Medicine applications
Anticorrosion materials applications
Electrochromic glasses
Electroluminescence machines
Solar cells
Sensors
Supercapacitors
Neural prosthesis/biotic-abiotic Interfaces
Scaffolds
Delivery systems

Polymers: Structure-property relationship of polymers (Crystallinity, Strength, Elasticity and chemical resistivity]

1.Crystallinity: The degree of ordered molecular arrangement and extent of close packing within a polymer is called crystallinity. **Higher crystallinity leads** to greater strength, stiffness, chemical resistance as well as Tg value because the ordered structure is more rigid and harder to break apart or dissolve.

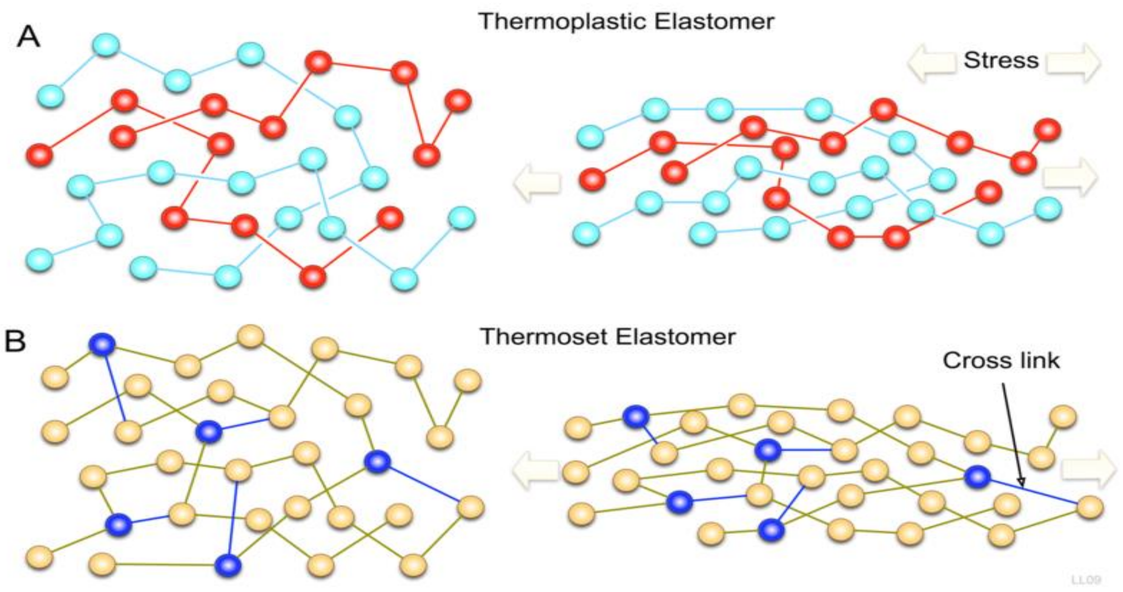
For example, high-density polyethylene (HDPE) is more crystalline than LDPE, making it stronger, harder, and more chemically resistant but less flexible and less transparent.



2.Strength

The strength mainly depends upon the rigidity of the polymeric chains and the bond strength within a molecule.

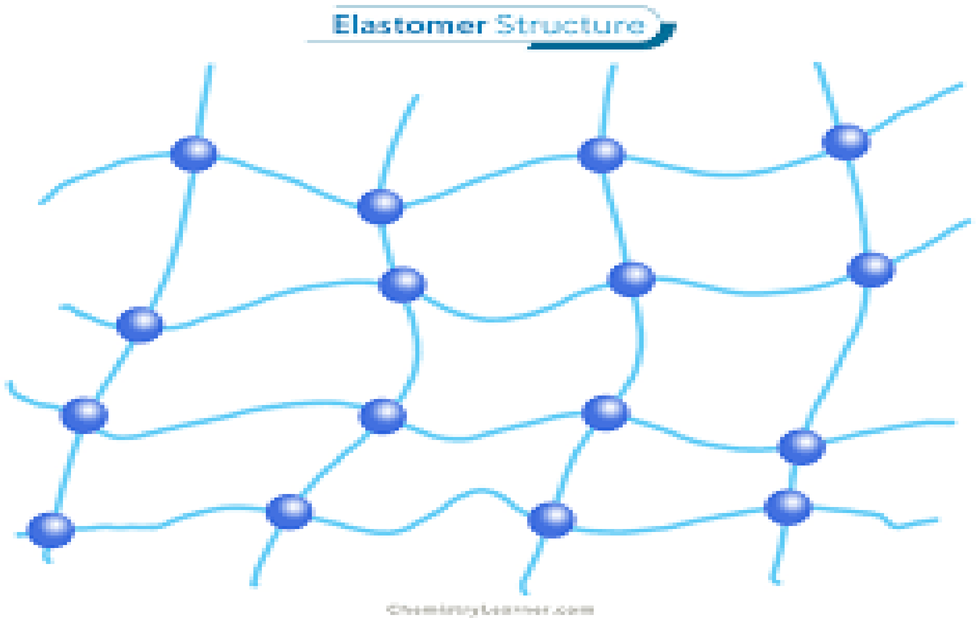
Apart from this strength of a polymer increases with increase in molecular weight and nature of intermolecular forces.



3.Elasticity

The deformation of polymer takes place under stress and it regains its original form when stress is removed.

It is mainly because of uncoiling and recoiling of molecular chains.



Chemical resistivity

Chemical resistivity of polymers refers to its ability to resist swelling, softening, dissolving, and loss of strength when exposed to solvents or chemicals.

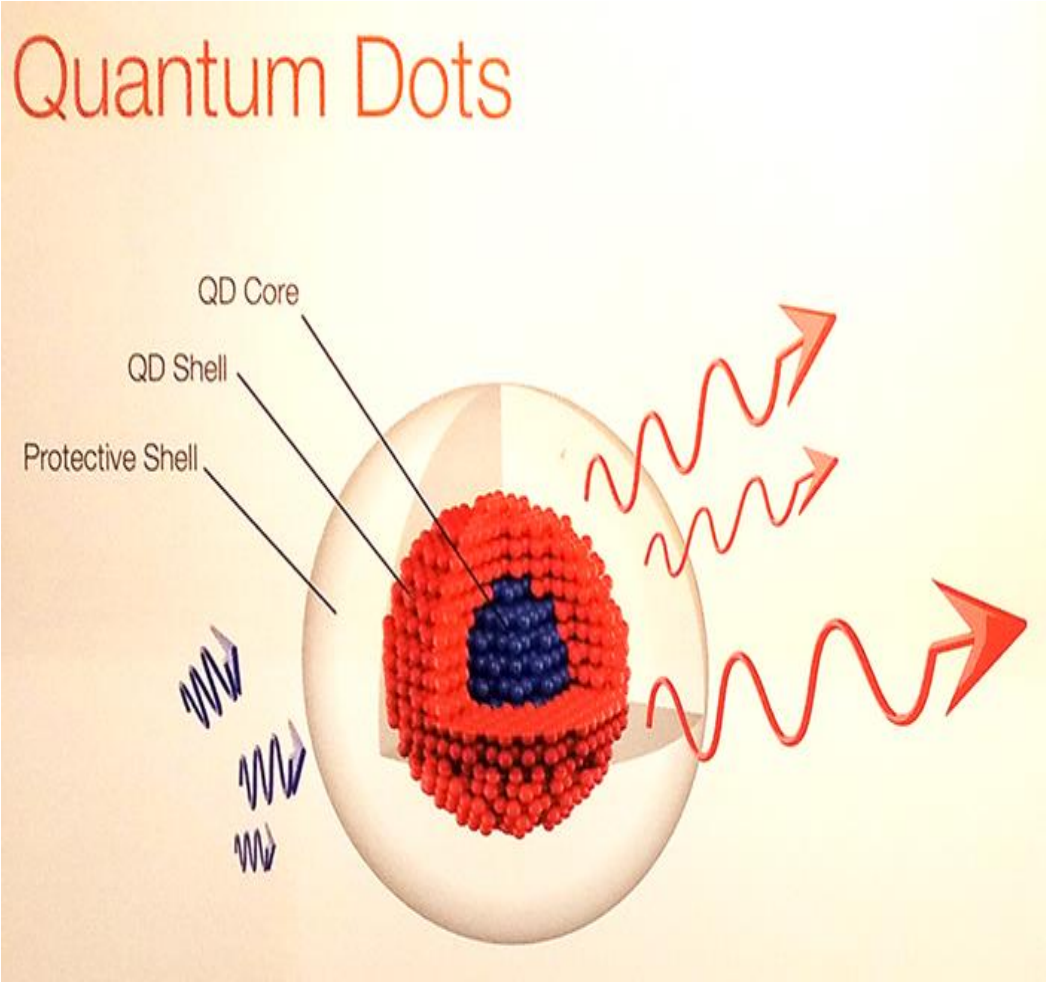
Factors affecting chemical resistivity:

- Polar groups: Polymers containing polar groups such as –OH or –COOH are dissolved by solvents like water or alcohols
- Polymers with higher degree of crystallinity exhibit greater chemical resistance than their counterparts
- Chemical resistivity increases as the degree of cross linking in the polymer structure increases.

Quantum Dots:

Introduction to QDs:

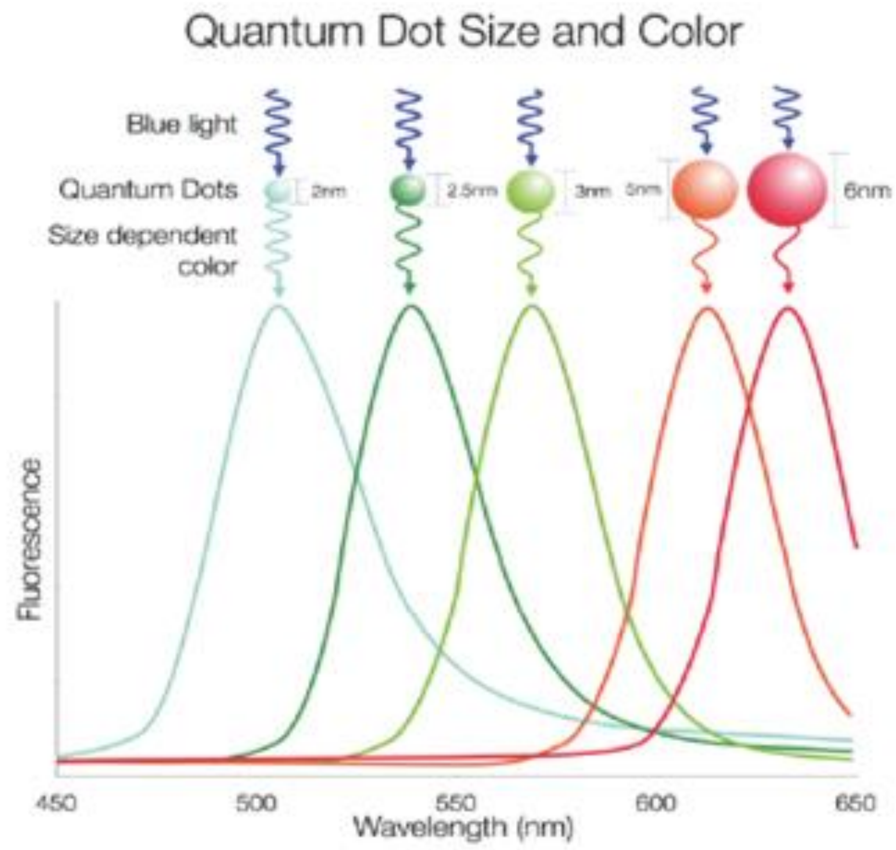
- Quantum dots (QDs) are semiconductor particles having size in the range of 2 to 10 nanometers with optical and electronic properties that differ from those of larger particles.
- These "artificial atoms" emit different colors of light depending on their size, with smaller dots emitting high energy blue light and larger dots emitting lower energy red light.



Smaller QDs (e.g., radius of 2~3 nm) emit shorter wavelengths generating colors such as violet, blue or green. While bigger QDs (e.g., radius of 5~6 nm) emit longer wavelengths generating colors like yellow, orange or red.

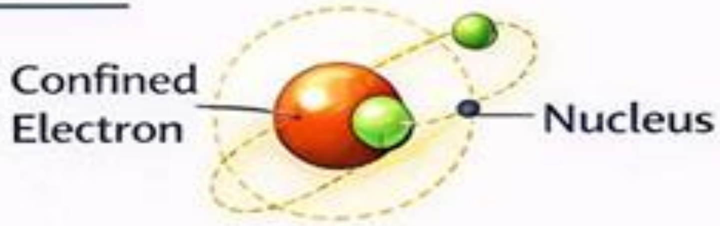
Applications of CdSe Quantum Dots (QDs):

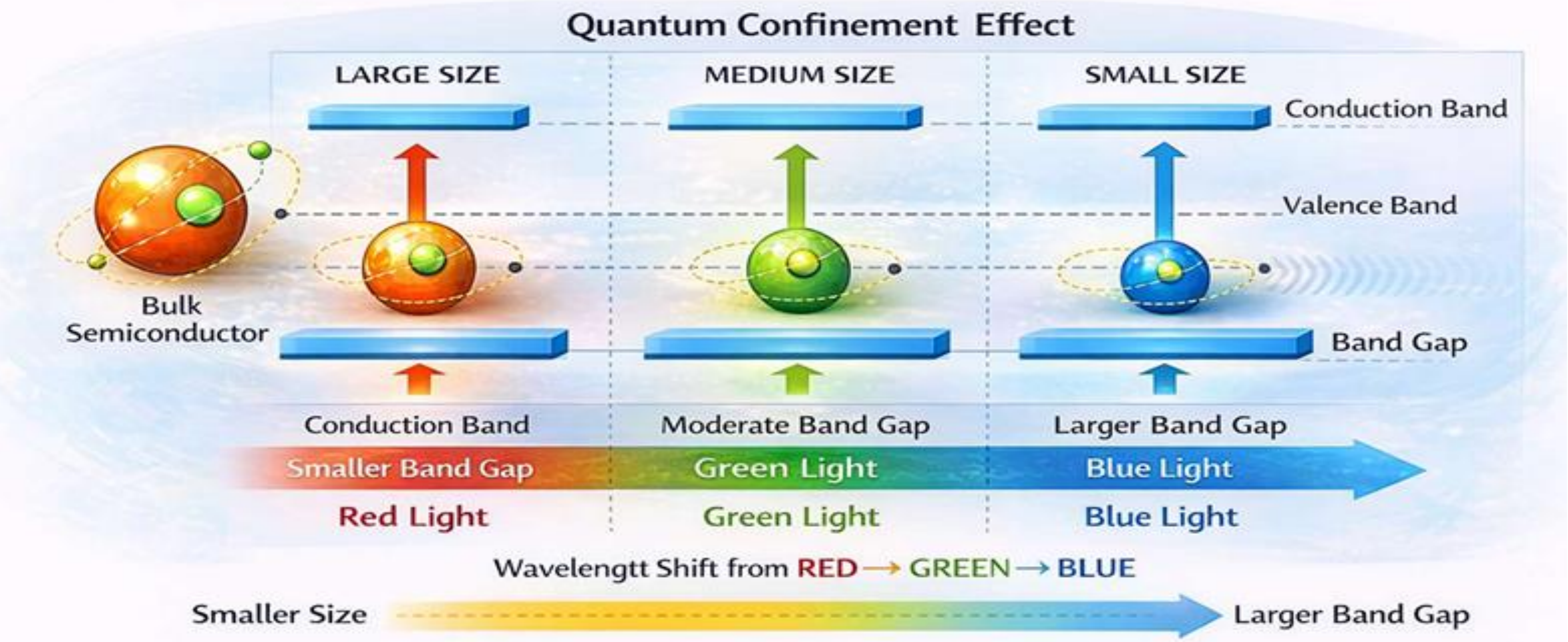
1. Optoelectronics
2. Energy / Photovoltaics
3. Biomedical / Healthcare
4. Displays and Lighting
5. Fluorescence tagging



Quantum Confinement Effect

Electrons are confined in extremely small semiconductor particles (quantum dots), leading to size-dependent energy levels and tunable optical properties.





Characteristic Properties of Quantum Dots

1.Band Gap Energy

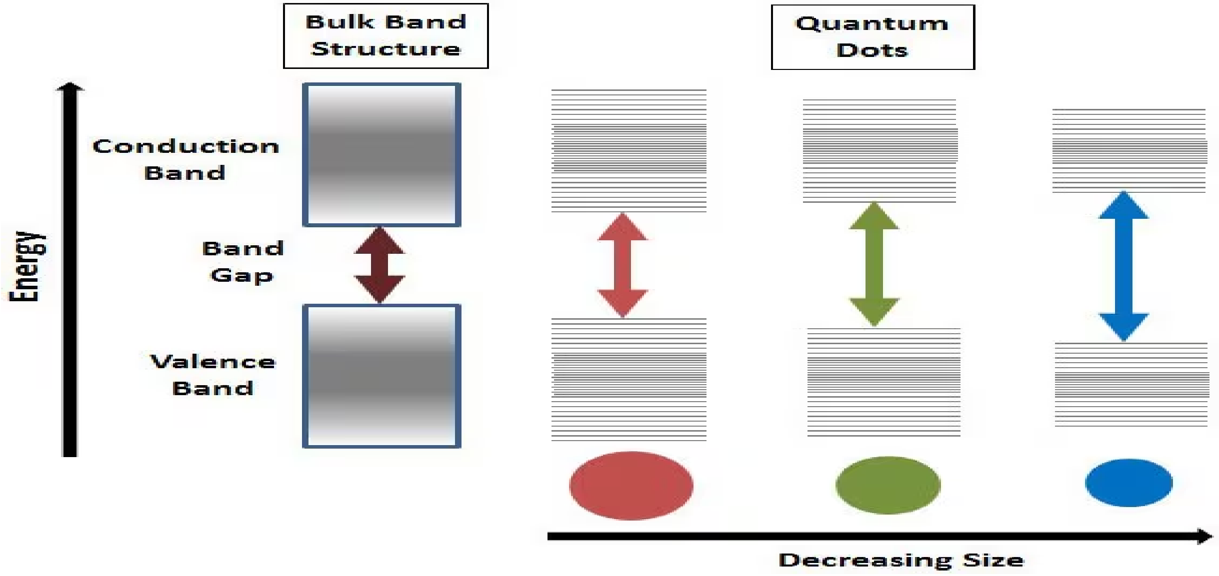
Bulk Semiconductor: Continuous band structure with fixed band gap.

Quantum Dot: Band gap increases as size decreases.

Small QD → strong confinement → higher energy transitions → blue-shifted emission.

Large QD → weaker confinement → lower energy transitions → red-shifted emission.

Example: CdSe QDs ~2 nm → emit blue, ~4 nm → emit green. ~6 nm → emit red



2. Surface-to-Volume Ratio

Smaller QDs: Large fraction of atoms at the surface → more surface defects and higher reactivity.

Larger QDs: Closer to bulk, fewer surface effects.

3. Optical Properties

Absorption: Smaller dots absorb at higher energies (blue-shift).

Emission: Color is tunable (blue → green → yellow → red) by varying size.

Sharp/narrow emission peaks → pure, bright colors (useful in displays, LEDs).

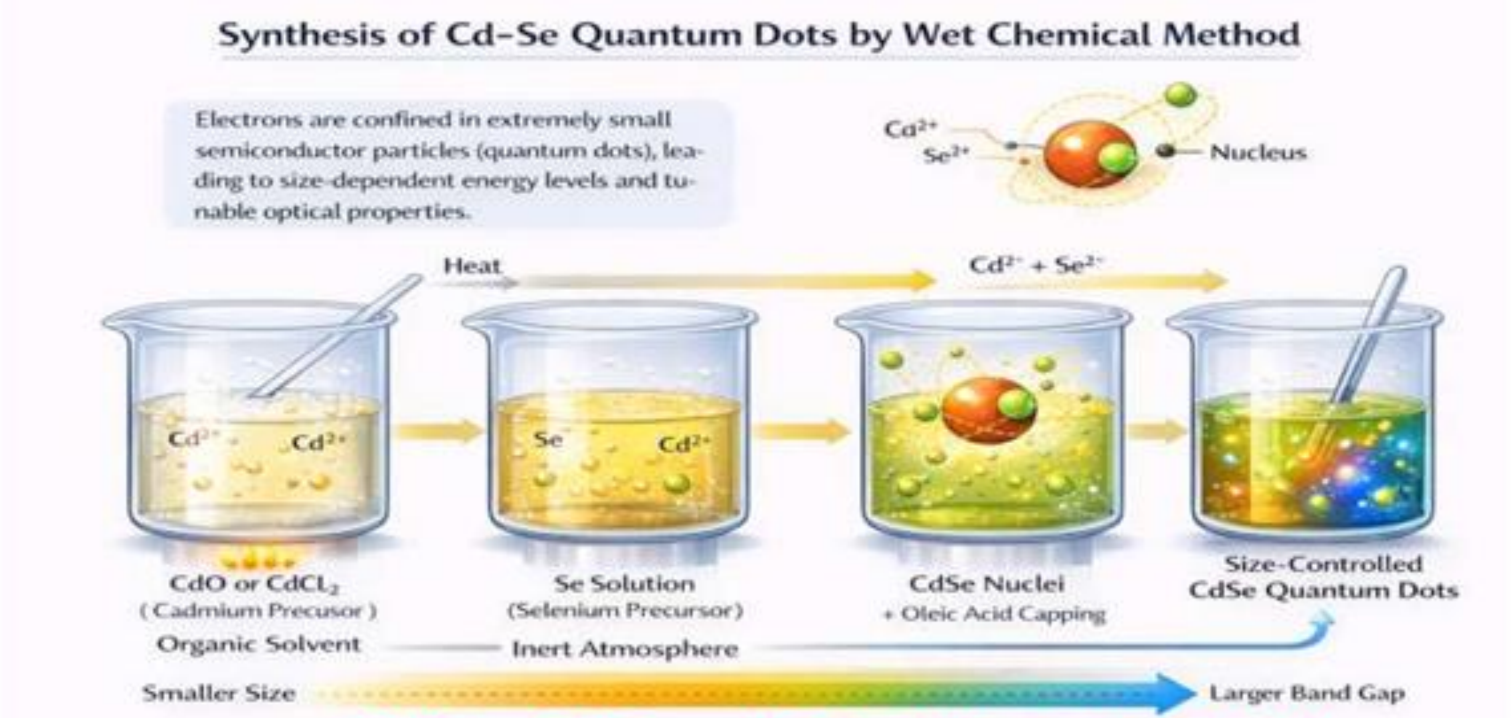
4. Electronic Properties: **In bulk:** continuous energy bands.

In QDs: discrete, atom-like energy levels.

Smaller dots → widely spaced energy levels.

Larger dots → more closely spaced levels, approaching bulk

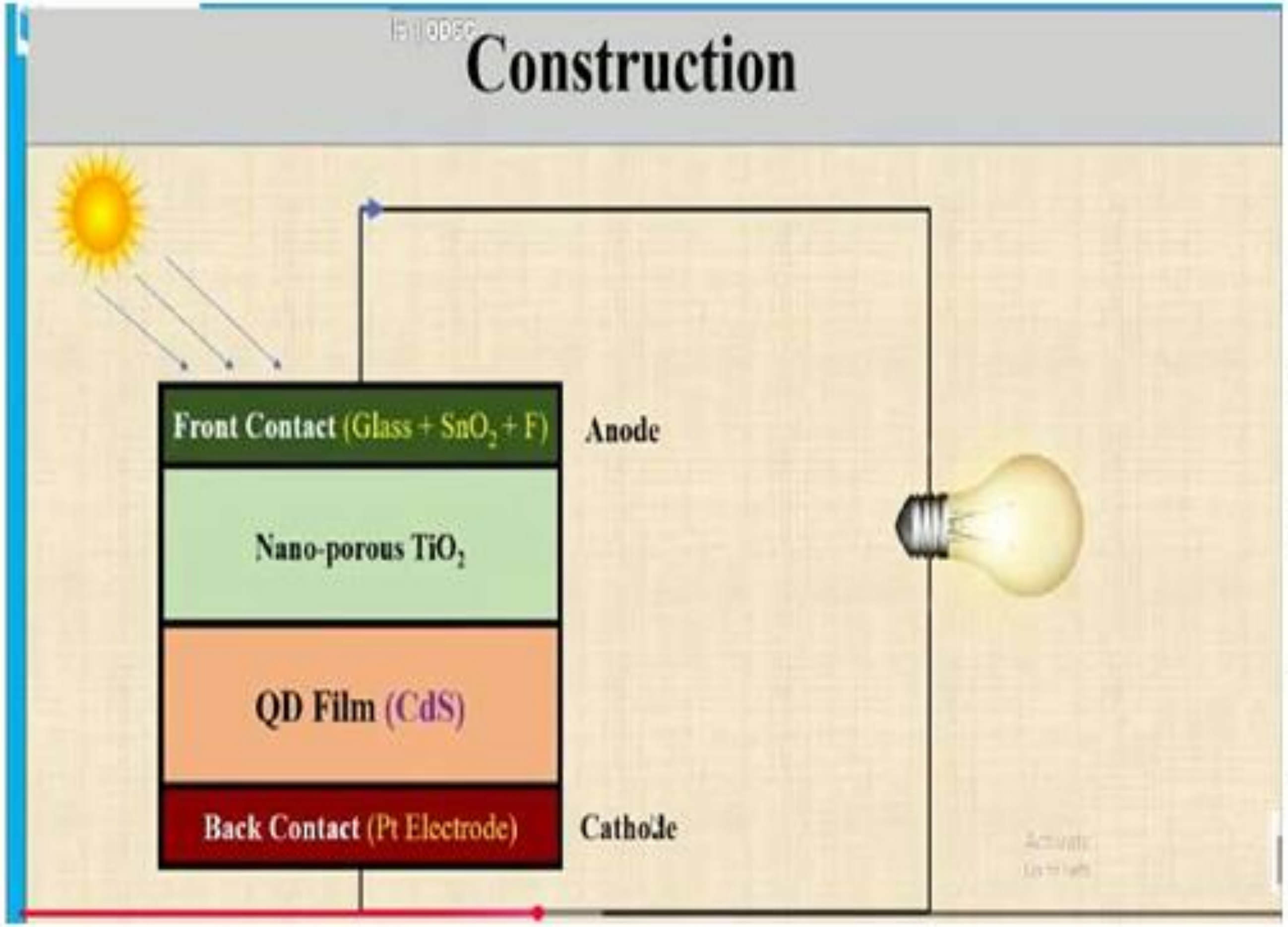
Synthesis of Cd-Se Quantum dots by wet chemical method and its applications.



$$Cd^{2+} + Se^{2+} \longrightarrow CdSe \text{ (Quantum Dots)}$$

First, a cadmium precursor (CdO or $CdCl_2$) is dissolved in an organic solvent with a capping agent (oleic acid). Separately, selenium powder is dissolved to form a selenium precursor solution. The cadmium solution is heated under an inert atmosphere. The selenium solution is then quickly injected into the hot cadmium solution. Cadmium and selenium ions react to form CdSe nuclei. Controlled heating allows particle growth, determining size. Finally, the solution is cooled, and the quantum dots are purified by centrifugation and washing.

Construction, working principle and applications of quantum dot sensitized solar cells (QDSSCs).

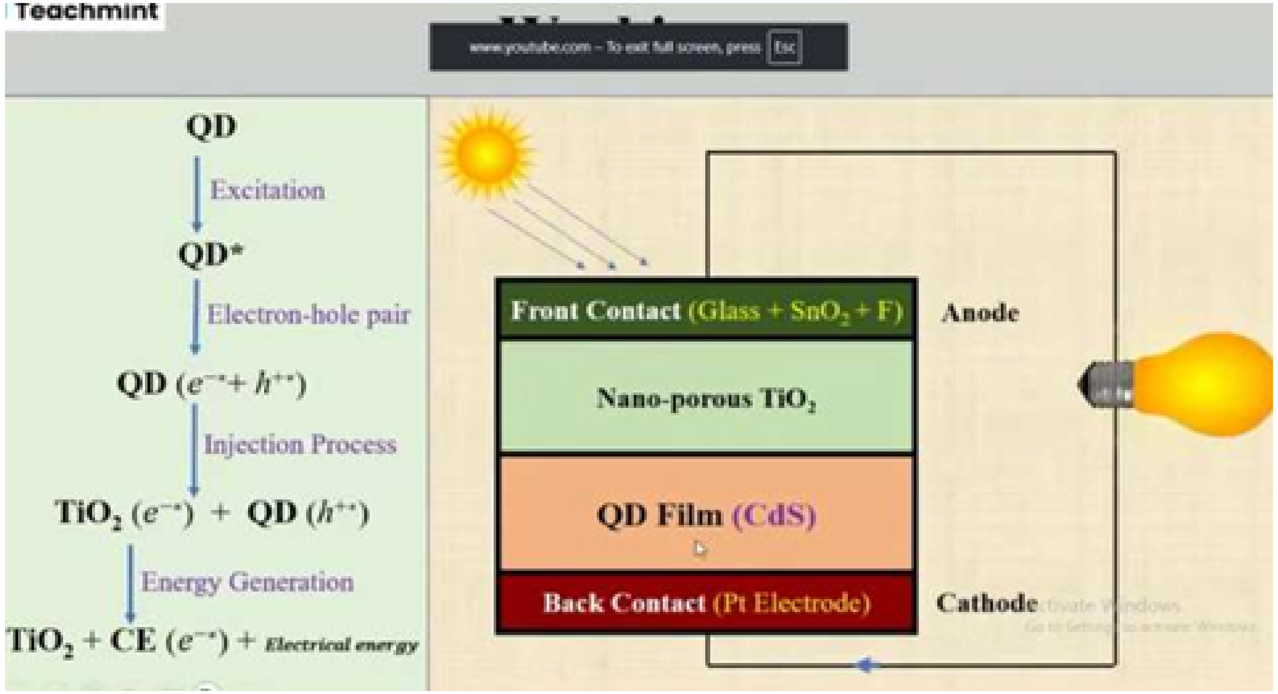


1. Anode: Glass coated with **ITO** (Allows light to enter and collects electrons)

2. Semiconductor Photoanode: Nanoporous TiO_2 (Provides large surface area)

3. **Quantum Dot Sensitizer** Layer: CdS QDs , Absorb sunlight and generate charge carriers

4. Counter Electrode (Cathode): Pt or carbon-coated electrode: it helps to complete the circuit.



Applications of QDSSCs

1.Low-cost photovoltaic devices

2.Flexible and lightweight solar panels

3.Indoor and low-light energy harvesting

4.Wearable and portable electronics

5. Used in solar cells

Working Principle of QDSSCs:

1. Incident sunlight is absorbed by quantum dots, generate electron–hole pairs.
2. Excited electrons are injected into the conduction band of TiO_2. Then, electrons flows into Pt electrode.
3. The electrolyte transports holes back to the quantum dots.
4. The cycle repeats, producing continuous electrical power.

MODULE 3: Sustainable Energy Systems (Syllabus)

Sl.No	Details	Duration	Remarks
2.1	**Energy Systems:** Introduction, basic overview of Nernst equation, construction and working of concentration cell (copper concentration cell)	1 hr	
2.2	Numerical problems on concentration cell	1 hr	Numerical
2.3	Construction, working and applications of Li-Ion battery. Introduction to **Next-Generation Energy Devices.**	1 hr	
2.4	Construction and working of sodium ion battery and redox flow battery for EV applications.	1 hr	
2.5	Construction and working of ultra-small asymmetric super capacitor and its applications in IoT/wearable devices.	1hr	
2.6	**Sustainable Energy Devices:** Introduction, fuel cells, difference between fuel cell and battery, construction, working principle, applications and limitations of solid-oxide fuel cell (SOFCs).	1 hr	
2.7	Introduction to solar energy, construction, working principle, applications and limitations of solar photovoltaic cell (PV cell).	1 hr	
2.8	Production of green hydrogen by photocatalytic water splitting by TiO_2 method and its advantages. Important questions discussions	1 hr	

MODULE 3: Sustainable Energy Systems (Syllabus)

Energy Systems: Introduction, basic overview of Nernst equation, construction and working of concentration cell and numerical problems. Batteries-Classification of batteries, construction, working and applications of Li-Ion battery.

Next-Generation Energy Devices: Introduction, construction and working of sodium ion battery and redox flow battery for EV applications. Construction and working of ultra-small asymmetric super capacitor and its applications in IoT/wearable devices.

Sustainable Energy Devices: Introduction, fuel cells, difference between fuel cell and battery, construction, working principle, applications and limitations of solid-oxide fuel cell (SOFCs) and solar photovoltaic cell (PV cell). Production of green hydrogen by photocatalytic water splitting by TiO2 catalyst and its advantages.

MODULE 3: Sustainable Energy Systems

Energy systems – Introduction:

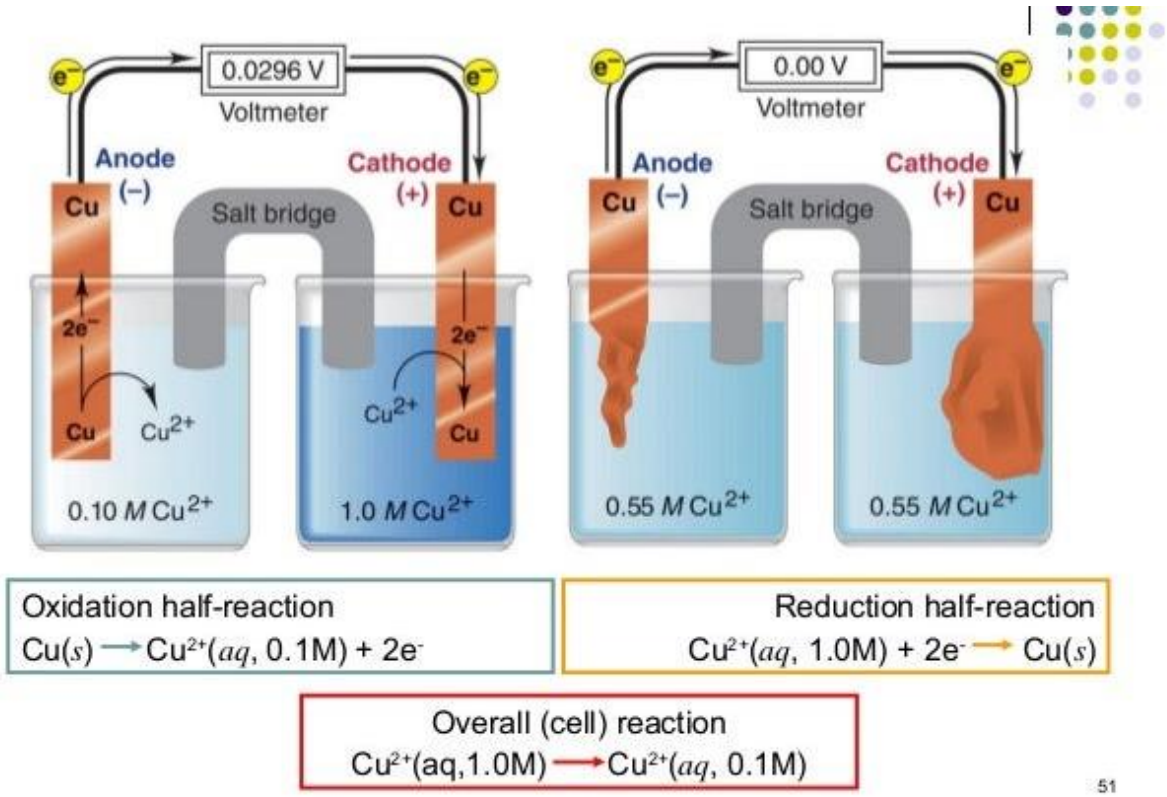
Energy systems encompass the ways energy is produced, converted, stored, and utilized across technological domains to sustain activities, power devices, or generate electricity.

Electrochemistry – Introduction, definition of electrochemistry, redox reaction, electrodes (anode and cathode), electrode potential, EMF, cell representation, electrolytic cell, galvanic cell, concentration cell, electrode systems.

Classification of electrode system:

- **Working (Indicator) Electrode**: platinum, gold, or glassy carbon electrodes.
- **Reference Electrode**: Standard Hydrogen Electrode (SHE), Silver/Silver Chloride (Ag/AgCl), and Sat., Calomel Electrode (SCE).
- **Auxiliary (Counter) Electrode**: Inert materials like platinum or graphite.
- **Metal Electrodes**: Platinum, gold, mercury, silver.
- **Metal-metal ion electrode:** Zn/ Zn2+
- **Metal-Sparingly soluble salt:** Hg/HgCl
- **Ion selective Electrodes (ISEs)**: Glass pH electrode, fluoride ion electrode.
- **Gas Electrodes**: Measure gases dissolved in solution; e.g., oxygen or CO2 electrodes.

Concentration cell: Introduction, working, cell reaction and cell equation.



Concentration cell: cell equation and numerical.

$$^{\ominus}M_{(s)} \mid M^{n+}[C_1M] \parallel M^{n+}[C_2M] \mid M_{(s)}{}^{\oplus}$$

Now, EMF of the cell is calculated using the equation;

$$E_{cell} = E_{cathode} - E_{anode}$$

$$= \left\{E^0 + \frac{0.0591}{n}\log C_2\right\} - \left\{E^0 + \frac{0.0591}{n}\log C_1\right\}$$

$$E_{cell} = \frac{0.0591}{n}\log\frac{C_2}{C_1} \quad \text{at } 298K$$

In general, $\boxed{E_{cell} = \frac{2.303RT}{nF}\log\frac{C_2}{C_1}}$

Batteries – Introduction:

Battery is an electrochemical cell; it consists of one or more galvanic cells connected in series or parallel connection. It converts chemical energy into electrical energy during discharging and electrical energy into chemical energy during charging.

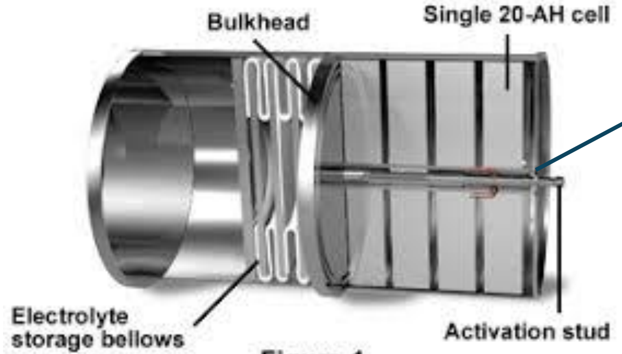


Figure 1

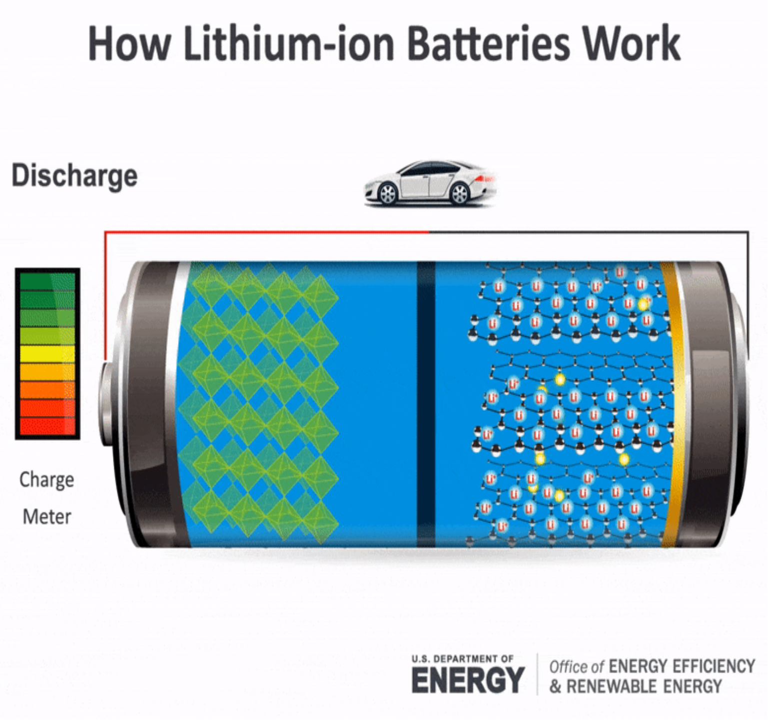
Reserve Battery

Classification of Batteries:

Batteries are classified into three types viz.,

1) Primary batteries (non-rechargeable) – eg: Zn-air battery, Lithium battery.
2) Secondary batteries (rechargeable) - eg: Li ion, sodium ion battery
3) Reserve batteries - eg: Magnesium- water activated batteries, zinc-silver oxide batteries, etc.

Lithium ion Battery-Introduction, construction and working



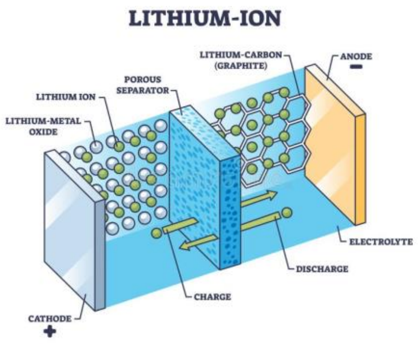
Lithium Based Batteries

Lithium is the lightest and highly reactive metal. The electrochemical properties of lithium are excellent. The outstanding electrochemical properties of lithium make it a key component in high-energy-density batteries for applications like electric vehicles and portable devices.

Lithium-ion battery (LIB)

Composition of the battery

Reactive species at anode : Li/Graphite
Reactive species at cathode : $LiCoO_2$
Electrolyte : Lithium salt
Separator : Polypropylene
Output Voltage : 3.6 V



Construction:

In lithium- ion battery, the Li ions (electrons) move from the negative electrode (anode) to the positive electrode (cathode) during discharge and back when charging.

Li ion Battery-Introduction, construction and working

Anode is made of carbon material (graphite) with a high energy density and large doping capacity of lithium ion. Cathodes are metal oxide material containing lithium with capable of dedoping lithium ion during charging and undergo lithium doping during discharging.

Electrolyte is made of lithium salts ($LiPF6$, $LiBF4$ or $LiClO4$) dissolved in organic solvents such as ethylene carbonate/ methylene carbonate/ ether . Lithium ions migrate between the two electrodes through an electrolyte.

Separator used is polypropylene.

The output voltage of this battery is 3.6V.

Working:

During charging lithium ions in cathodic side (positive electrode) move towards anodic side (negative electrode)

$Cathodic\ Reaction: LiCoO_2 \rightarrow Li(1-x)CoO_2 + xLi+ + xe-$

$Anodic\ Reaction: x\ Li+ + xe- + 6C \rightarrow xLiC6$

$Overall\ Reaction: L\ iCoO2 + 6C \leftrightarrow Li(1-x)CoO2 + xLiC6$

During discharging lithium ions move from anode to cathode.

$Anodic\ Reaction: xLiC6 \rightarrow xLi+ + xe- + 6C$

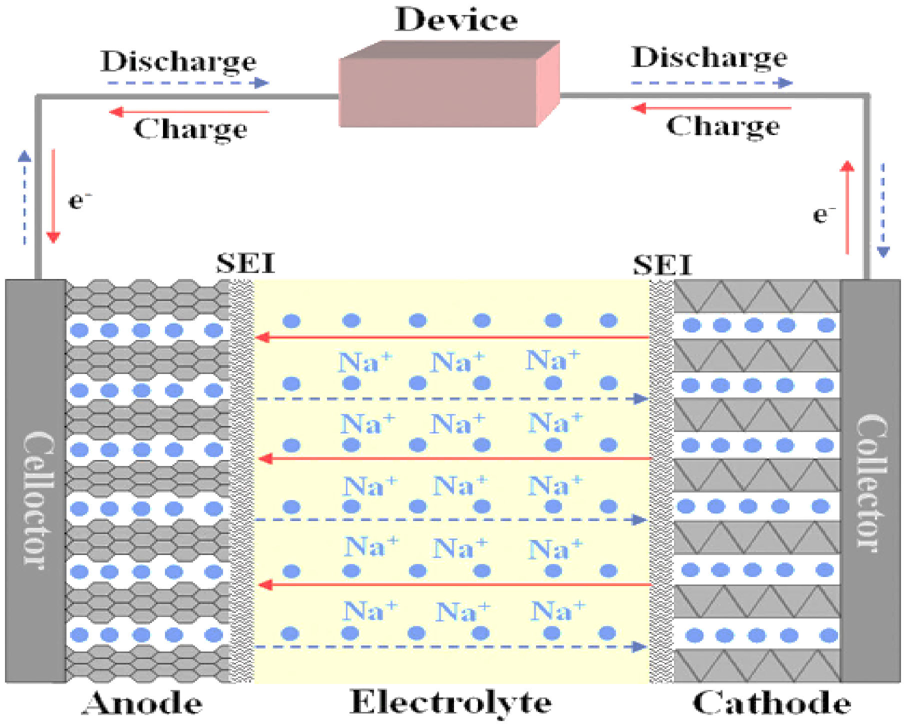
$Cathodic\ Reaction: Li(1-x)CoO_2 + xLi+ + xe- \rightarrow LiCoO_2$

$Overall\ Reaction: L\ i(1-x)CoO_2 + xLiC6 \leftrightarrow LiCoO_2 + 6C$

Applications

The Li- ion batteries are used in mobile phones,

Next generation Energy Devices – Introduction to sodium ion battery, construction and working with diagram. Advantages and disadvantages of sodium ion battery over lithium ion battery.



Charge

Cathode: $NaMnO_2 \rightarrow Na_{1-x}MnO_2 + xNa^+ + xe^-$

Anode: $C + xNa^+ + xe^- \rightarrow Na_xC$

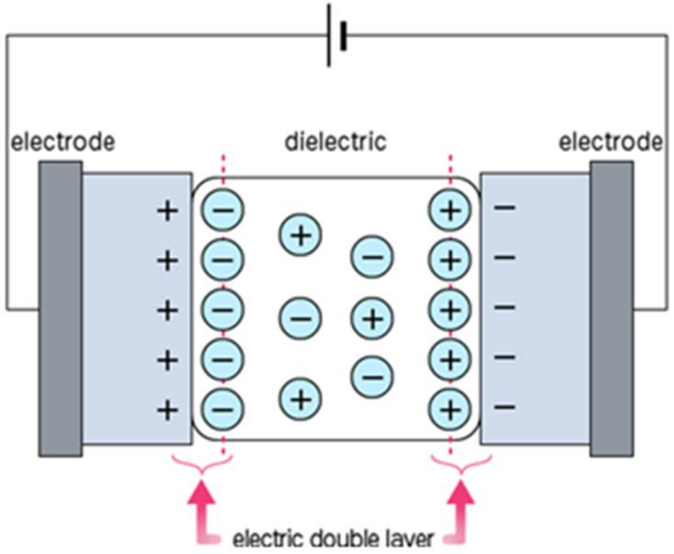
Overall: $C + NaMnO_2 \rightarrow Na_{1-x}MnO_2 + Na_xC$

Discharge

Cathode: $Na_{1-x}MnO_2 + xNa^+ + xe^- \rightarrow NaMnO_2$

Anode: $Na_xC \rightarrow C + xNa^+ + xe^-$

Overall: $Na_{1-x}MnO_2 + Na_xC \rightarrow NaMnO_2 + C$



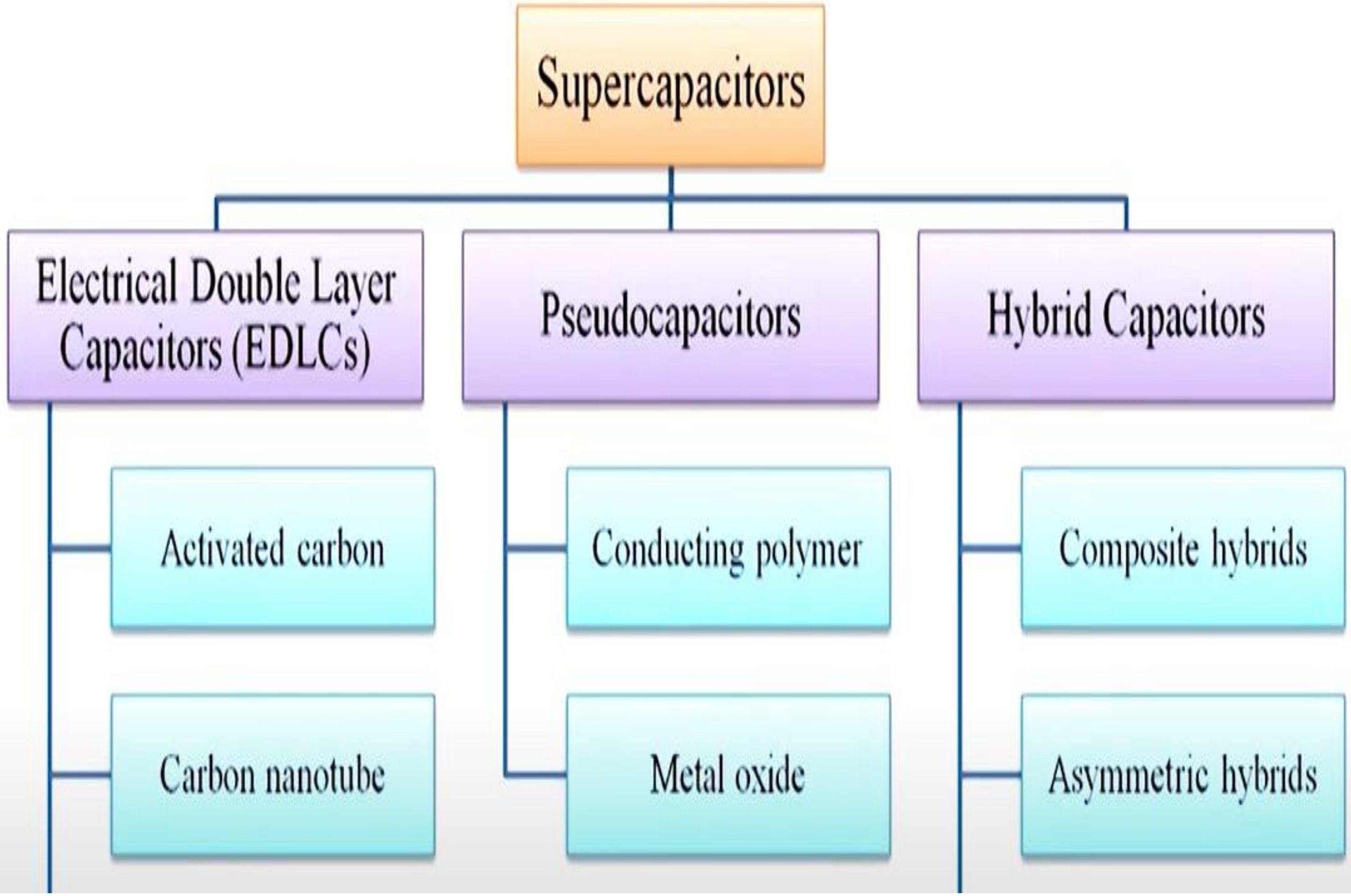
double-layer capacitor

What is a Super capacitor?

- Super capacitors are specially designed capacitors with much higher capacitance value and energy density.

Energy storage in super capacitors occurs either by:

- Pure charge storage at the electrode/electrolyte interface by Electrochemical double layer (EDLC).
- Charge transfer to a layer of redox molecules on the electrode surface.
- They bridge the gap between capacitors and batteries, offering high power density and compact design


Supercapacitors
Electrical Double Layer Capacitors (EDLCs)
Pseudocapacitors
Hybrid Capacitors
Activated carbon
Carbon nanotube
Conducting polymer
Metal oxide
Composite hybrids
Asymmetric hybrids

Construction and working of ultra-small asymmetric super capacitor and its applications in IoT/wearable devices.

Definition: A super capacitor is an energy storage device that bridges the gap between batteries (high energy) and conventional capacitors (high power).

Construction: An ultra-small ASC typically consists of:

Electrodes:

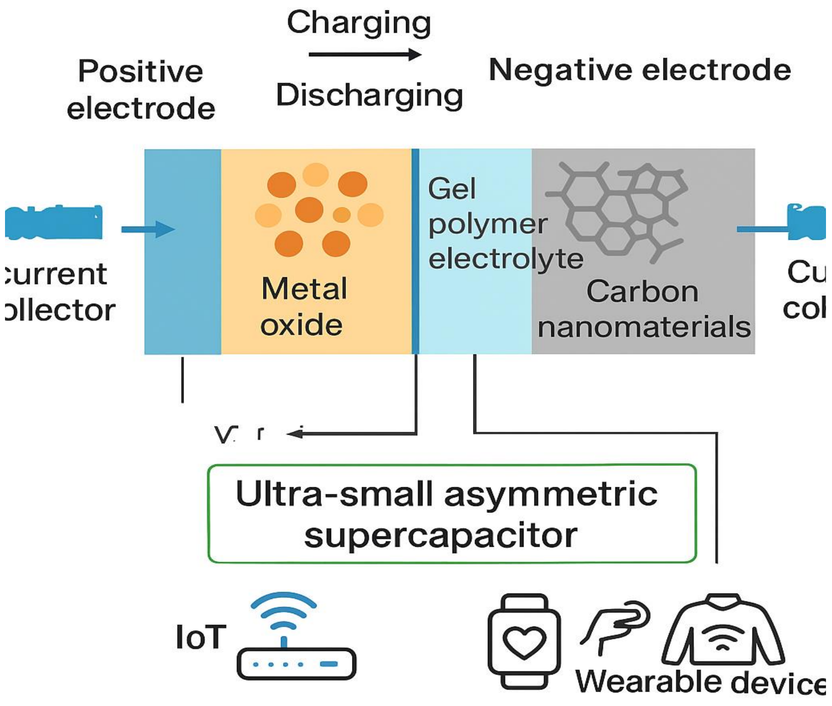
Positive electrode: Transition metal oxides/hydroxides (e.g., MnO_2)

Negative electrode: Carbon-based nanomaterials (e.g., graphene),

Electrolyte: Solid-state gel polymer electrolyte (e.g., PVA/H_2SO_4)

Separator: Ultra thin porous membrane

Current collectors / Substrate: PET, PDMS, cellulose paper or metal foils.

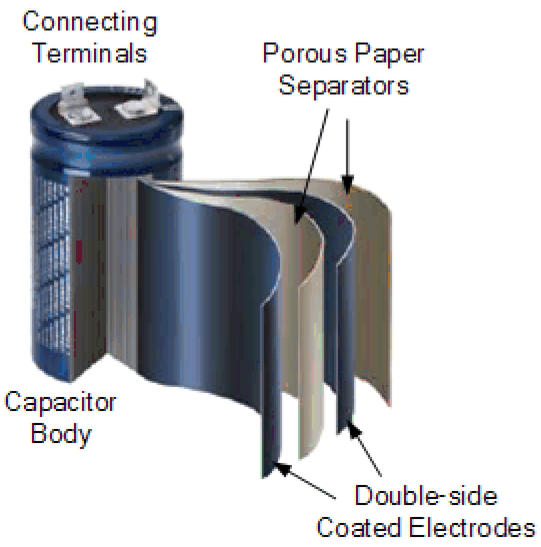


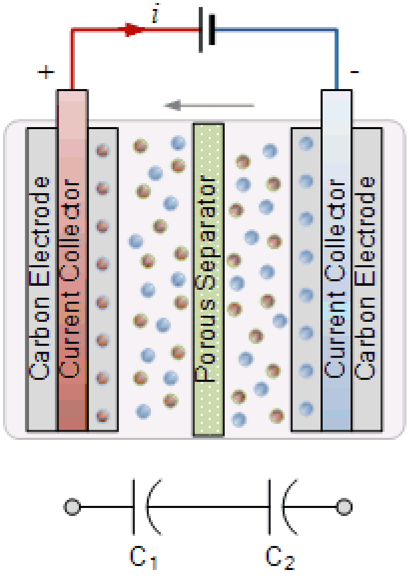
Working:

An ultra-small asymmetric supercapacitor operates by combining two different electrode materials-one storing charge through fast surface reactions (pseudocapacitance) and the other through electrostatic charge accumulation (electric double-layer capacitance). When voltage is applied, ions from the electrolyte move rapidly toward each electrode, creating distinct charge-storage mechanisms on each side. This asymmetry increases the operating voltage window and enhances energy density compared to symmetric designs. During discharge, the stored ions and electrons flow back through the external circuit, delivering power efficiently.

Applications:

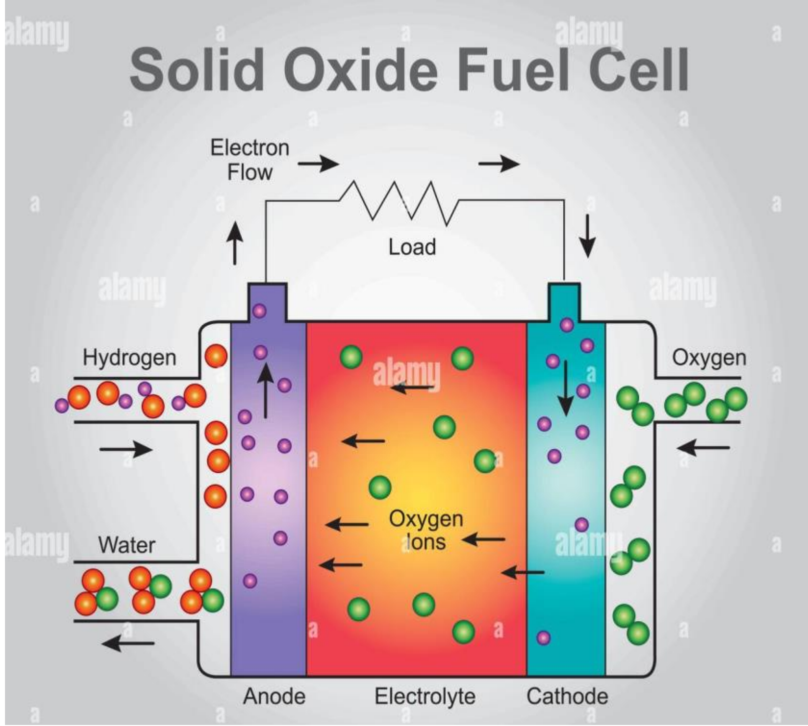
- **IoT Devices: Providing quick energy bursts for micro-sensors and wireless communication modules.**
- **Biomedical Implants: Supporting low-power implants requiring reliable, biocompatible energy storage.**
- **Nanoscale Robotics: Supplying compact, lightweight energy for micro-robots and actuators.**
- **Energy Harvesting Systems: Used in self-powered micro devices.**
- **Wearable Electronics: Powering flexible, skin-mounted sensors and health-monitoring devices with high stability.**



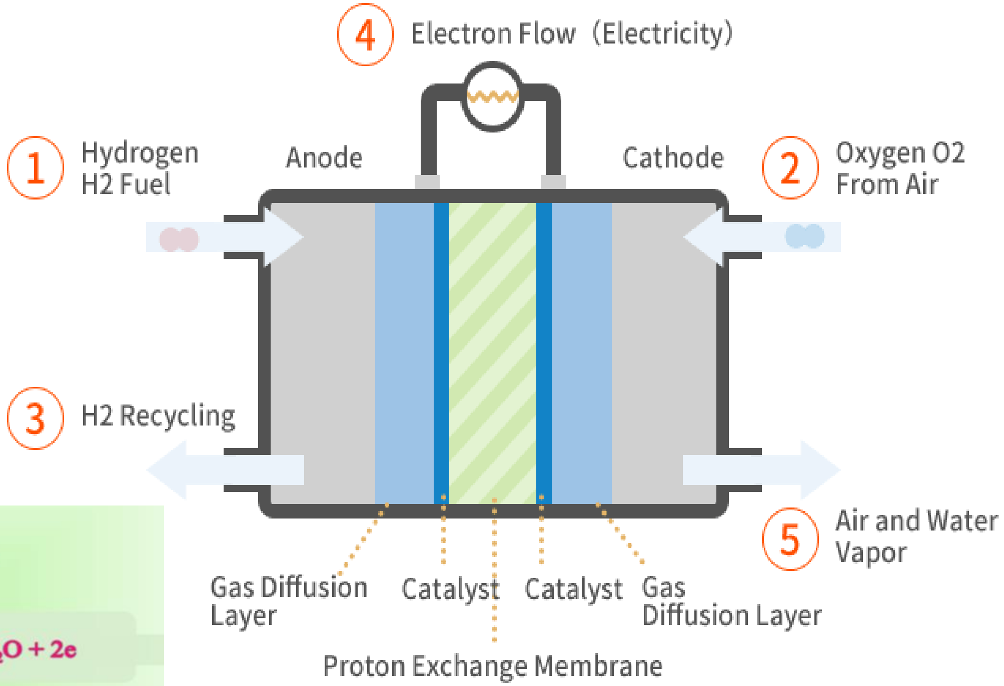


MODULE 3: Sustainable Energy Systems

Sustainable energy devices – Introduction to sustainable energy devices
Solid oxide Fuel Cell: Introduction, definition, construction and working with cell reaction and advantages.

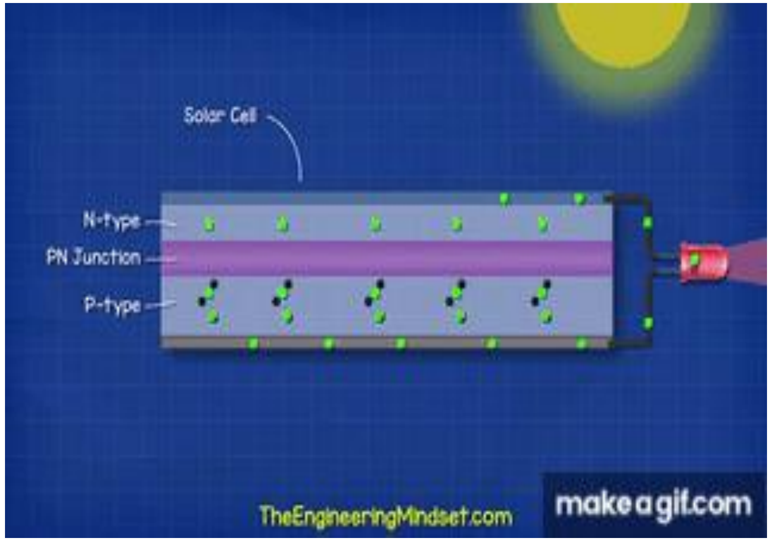


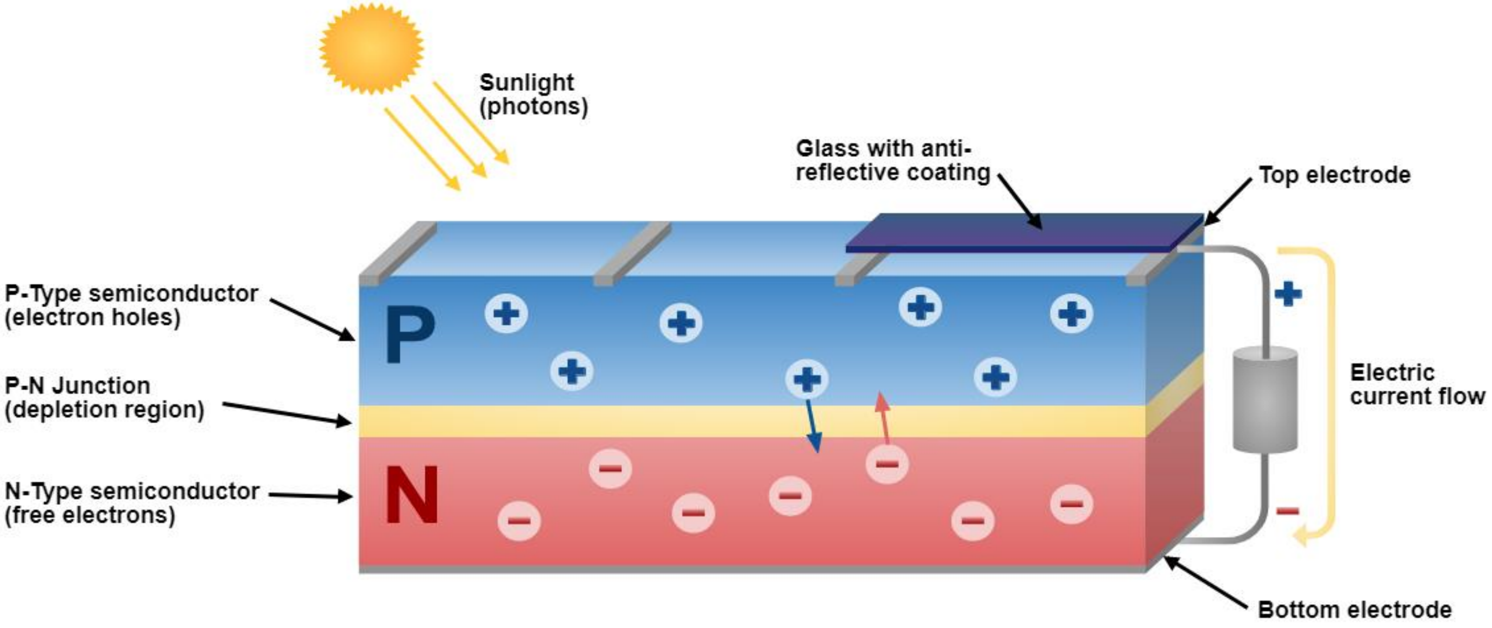
At Cathode	$\frac{1}{2} O_2 + 2e \longrightarrow O^{2-}$
At anode	$H_2 + O^{2-} \longrightarrow H_2O + 2e$
Overall Reaction	$H_2 + 1/2O_2 \rightarrow H_2O$



Sustainable energy devices – Introduction to sustainable energy devices

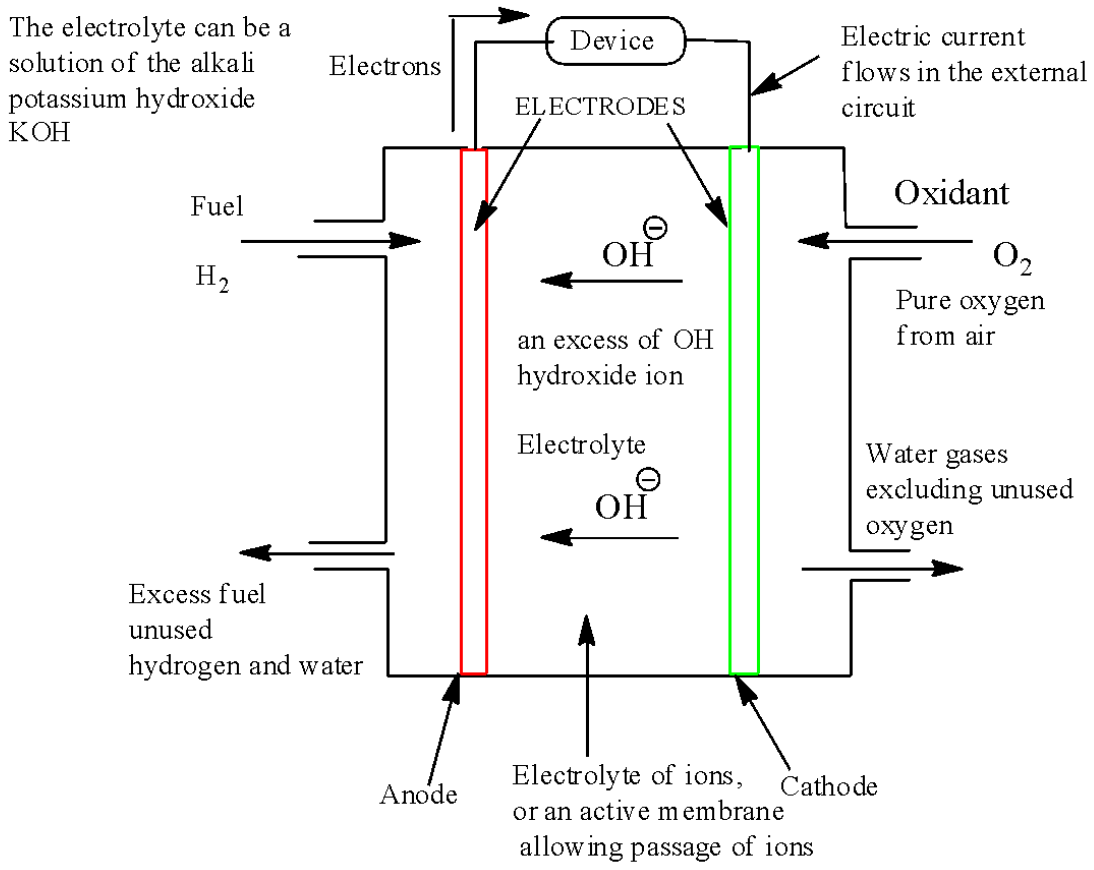
Solar/PV cell: Introduction, definition, construction and working with advantages.





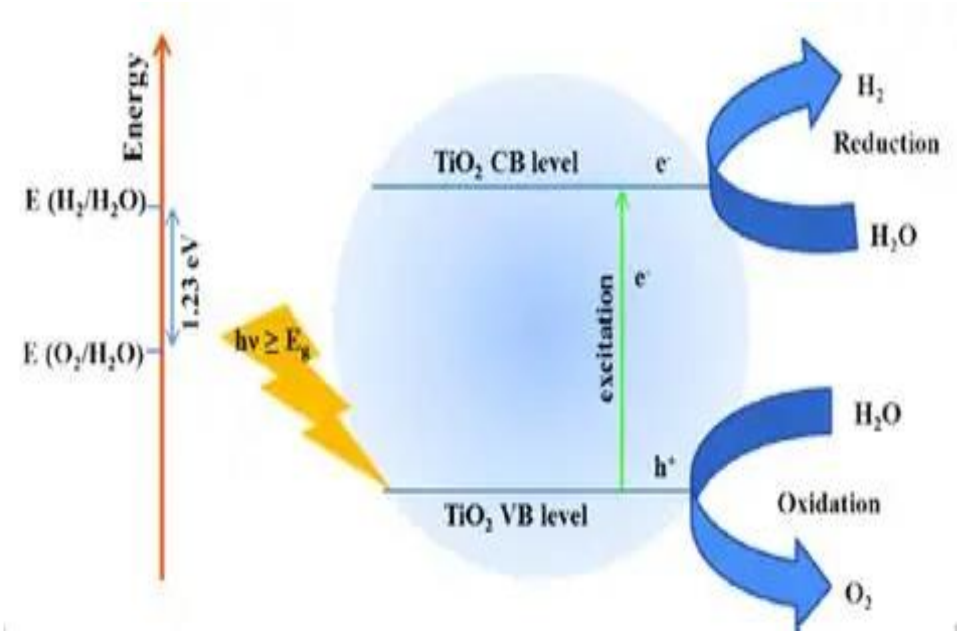
Sustainable energy devices – Introduction to sustainable energy devices

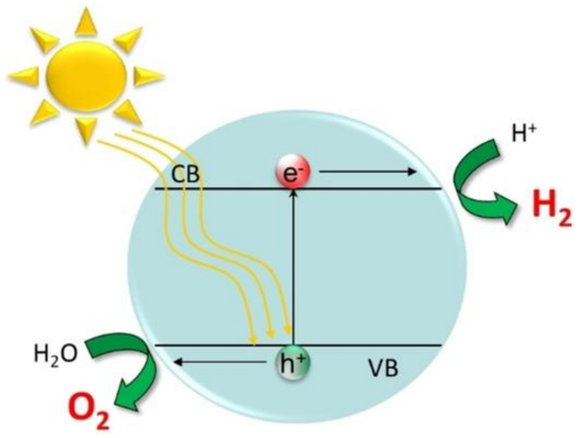
Fuel Cell: Introduction, definition, construction and working with cell reaction.



An alkaline hydrogen-oxygen FUEL CELL

Sustainable energy devices – Introduction to sustainable energy devices
Production of green hydrogen by photocatalytic water splitting by TiO_2 method and its advantages.





Production of green hydrogen by photocatalytic water splitting by TiO2 catalyst and its advantages

Photocatalytic water splitting uses sunlight and a semiconductor catalyst to split water into hydrogen (H_2) and oxygen (O_2). TiO_2 is one of the most widely used photocatalysts due to its stability and strong oxidation ability.

Process Using TiO_2

Step-by-Step Mechanism

1.Light Absorption: TiO_2 absorbs UV light (band gap ~3.2 eV).→ Generates electron (e^-)–hole (h^+) pairs.

2.Charge Separation: Electrons move to the conduction band (CB). Holes remain in the valence band (VB).

3.Reduction Reaction (Hydrogen Generation):

$2H^+ + 2e^- \rightarrow H_2$

4.Oxidation Reaction (Oxygen Formation): $2H_2O + 4h^+ \rightarrow O_2 + 4H^+$

5.Overall Water-Splitting Reaction: $2H_2O \rightarrow 2H_2 + O_2$


THANK YOU!