New Engineering Materials

B.Tech First Year
Engineering Chemistry

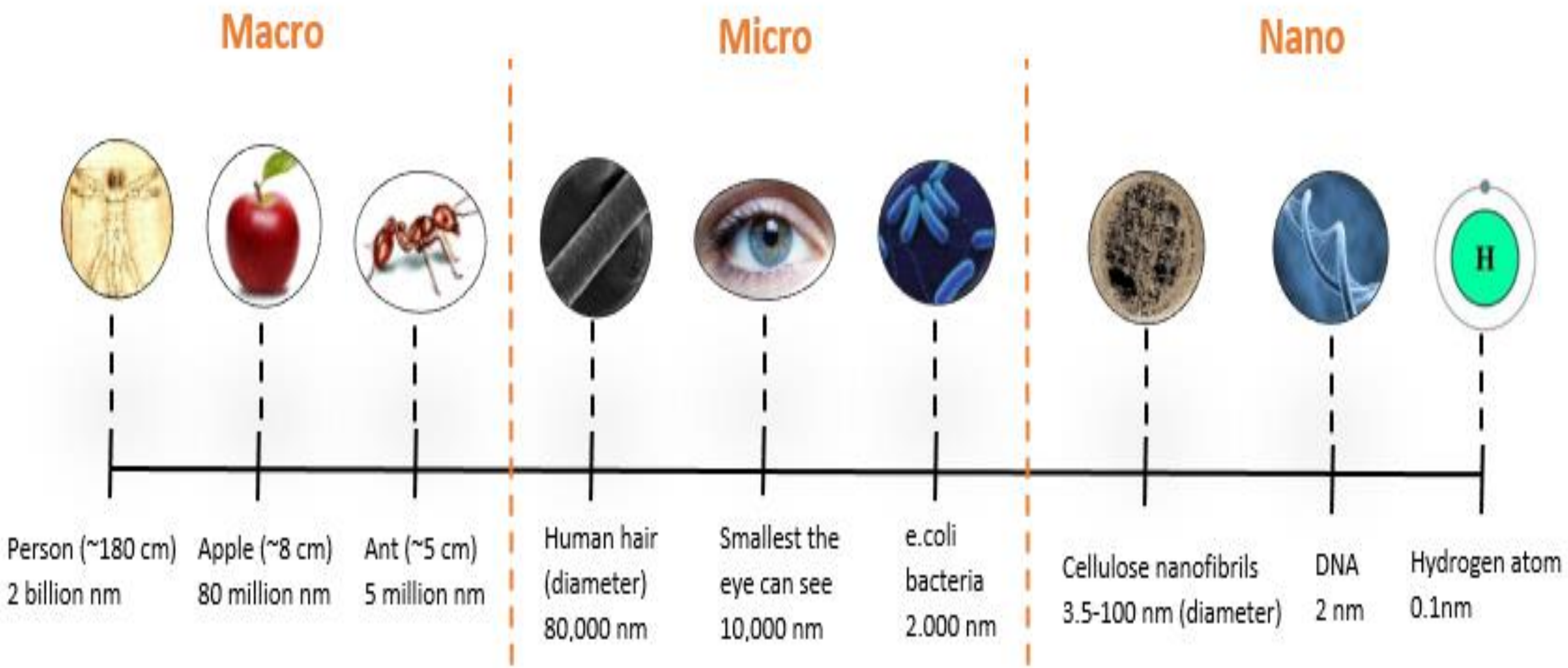
Content

- What is Nanotechnology?
- Why nanoscale?
- What is nanomaterial?
- Nanomaterials' characteristics
- Approaches of Nanotechnology
- Bottom-up or top-down?
- Applications of Nanotechnology

Nanomaterials

- "Nano" – derived from a Greek word "Nanos" meaning DWARF or small.
- Particles with one of its dimensions <100 nm shows new properties and behavior
- Nanoparticle is any material having at least one of its dimensions in the range of **1-100 nm.**
- Display new chemistry and behavior (**electronic structure, conductivity, reactivity, melting temperature and mechanical properties**). Size dependent behavior allow **engineering** of their properties.
- 1 nm = **1 billionth of a meter** (10^{-9} m)
- Potential **for technological advancement** to wide diverse range of applications **(stronger and lighter materials, shorting the delivery time of nanostructured pharmaceuticals in body, storage capacity of magnetic tapes and increasing the computing speed).**
- **Interdisciplinary** cover a wide variety of subjects **catalysis on nanoparticles to physics of quantum dots laser.**

Comparison of macro, micro and nanoscale



http://www.ntnutechzone.no/en/2016/02/did-you-know-that-the-north-sea-is-full-of-half-eaten-apples/

Nanotechnology

- **The design, characterization, and application of structures, devices, and systems** by **controlled manipulation of size and shape of materials** at the nanometer scale (atomic, molecular, and macromolecular scale)
- To produce materials with at least one **novel/superior characteristic or property**.
- The development of materials and devices by exploiting the characteristics of particles on the nano-scale
  - Nanoscience – is the study of nano-materials, their **properties** and related phenomena.
  - Nanotechnology – is the **application** of nanoscience to produce **devices and products**.

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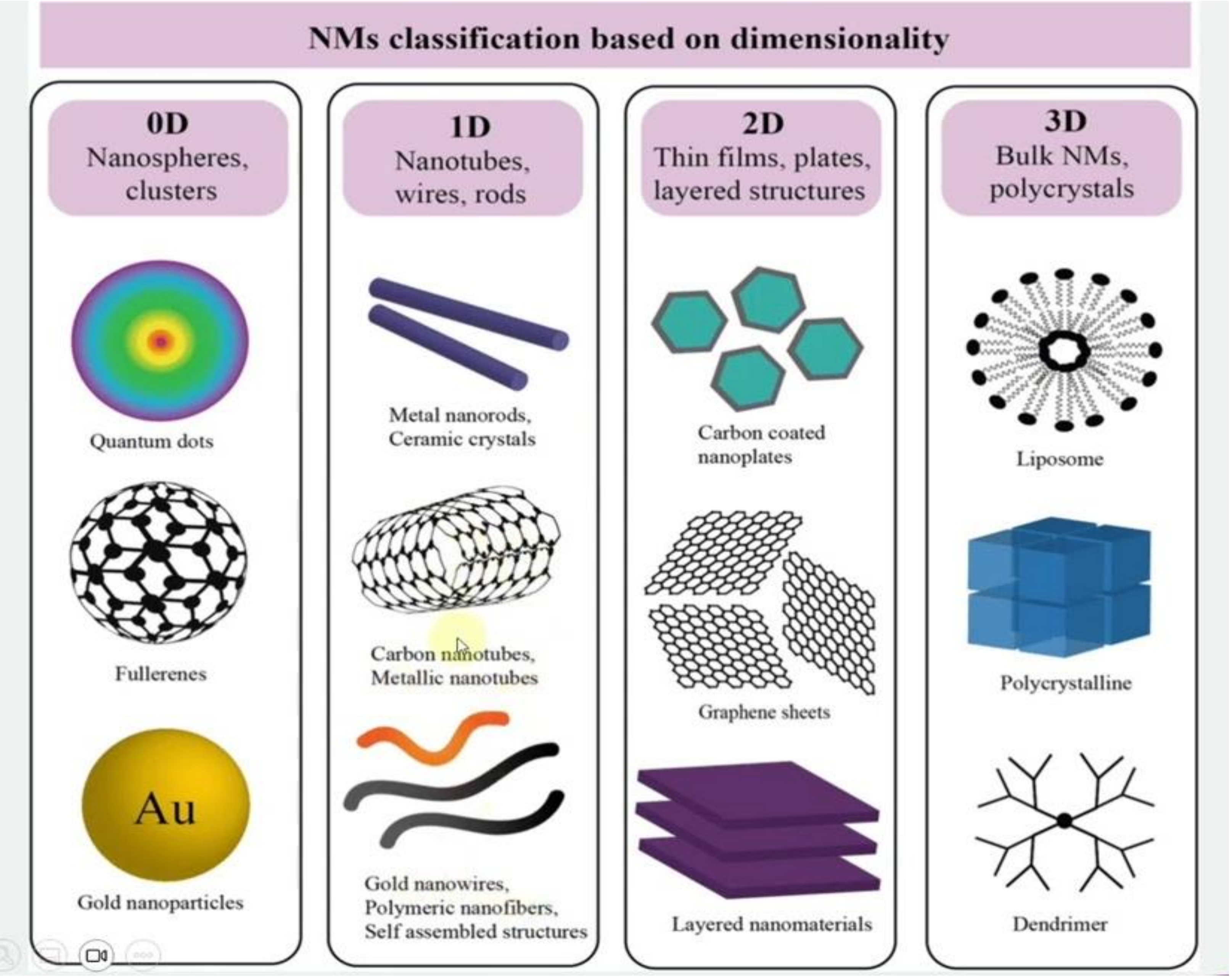
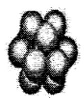
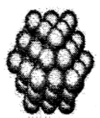
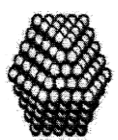
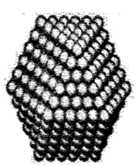
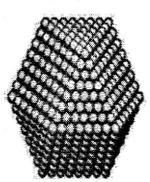


Why small is good?

Full-shell Clusters		Total Number of Atoms	Surface Atoms (%)
1 Shell		13	92
2 Shells		55	76
3 Shells		147	63
4 Shells		309	52
5 Shells		561	45
7 Shells		1415	35

Surface area increases as size decreases

Nano-objects are:

- Faster

- Lighter

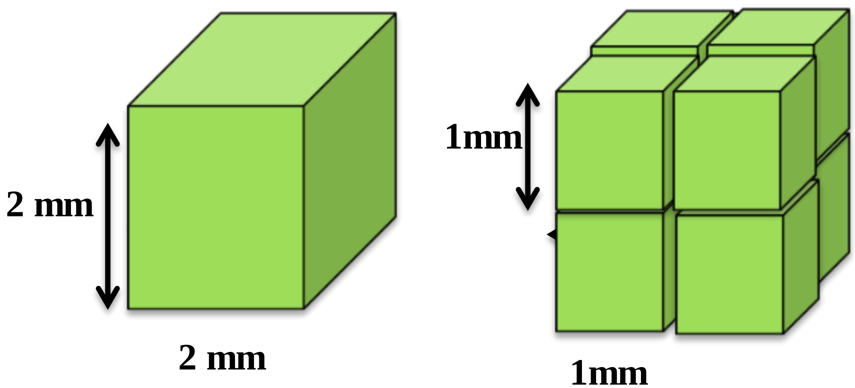
- Can get into small spaces

- Cheaper

- More energy efficient

- Different properties at very small scale

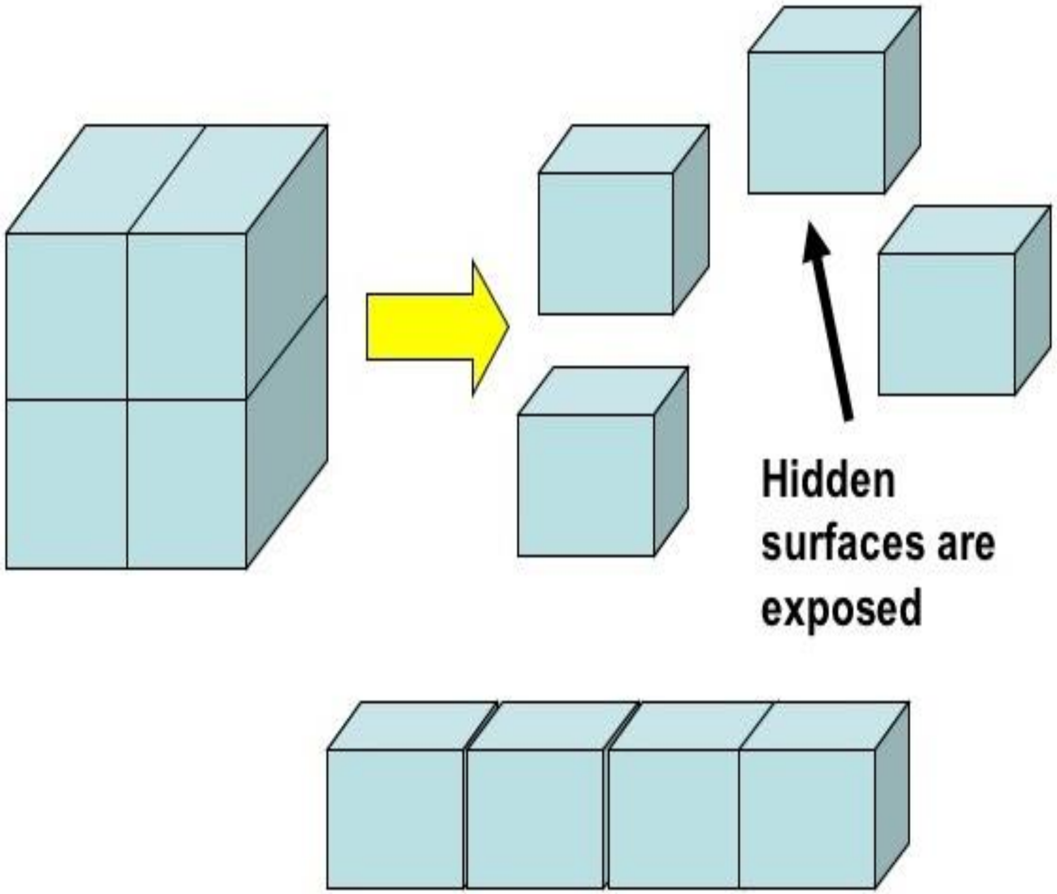
Surface area-to-volume ratio



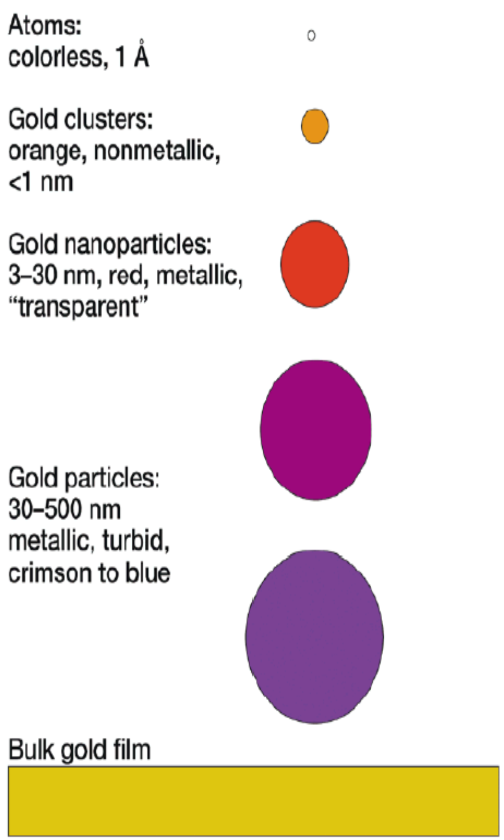
Surface Area (mm)	Surface area= Height x Width x No. of sides x No. of cubes	24 (2x2x6x1)	48 (1x1x6x8)
Volume (mm)	Volume=Height x Width x Length x No. of cubes	8 (2x2x2x1)	8 (1x1x1x8)
Surface Area/Volume ratio	Surface area/Volume	3 (24:8)	6 (48:8)

Surface area-to-volume ratio

- As surface to volume ratio increases
- A greater amount of a substance **comes in contact with surrounding material**
- This results in better **catalysts,** since a greater proportion of the material is exposed for potential reaction



Material properties vary with size of material



- **(Bulk) Gold is a shiny yellow metal**
- **Gold (Au) nanoparticles appears red**
- **Bulk gold does not exhibit catalytic properties**
- **Au nanoparticle is an excellent low temperature catalyst**

Nanoscale size effect

- Manifestation of novel phenomena and properties, including changes in:

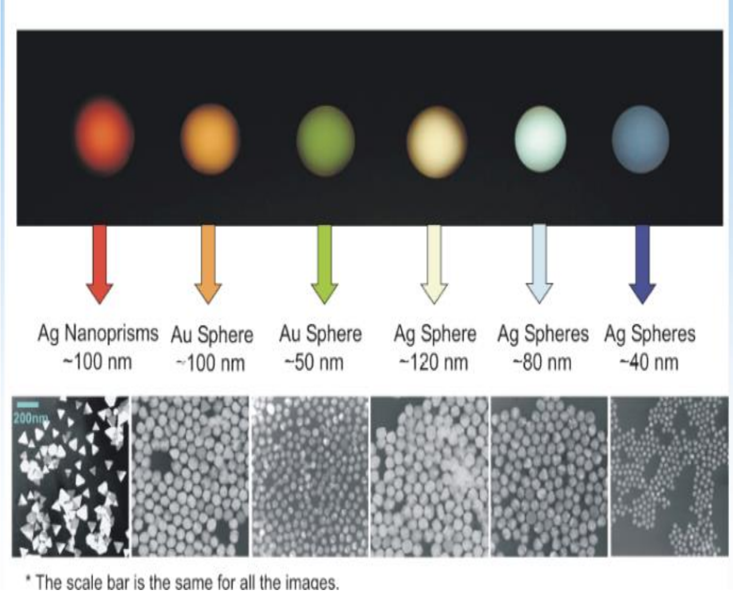
Physical Properties (e.g. melting point)

Chemical Properties (e.g. reactivity)

Electrical Properties (e.g. conductivity)

Mechanical Properties (e.g. strength)

Optical Properties (e.g. light emission)



Thermal properties

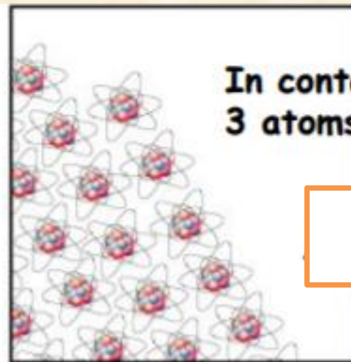
Nanocrystal size decreases

↓

surface energy increases

↓

melting point decreases



$$E_{total} = E_{bulk} + E_{surface}$$

Surface atoms require less energy to move because they are in contact with fewer atoms of the substance

Example:

3 nm CdSe nanocrystal melts at **700 K** compared to bulk CdSe at **1678 K**

How to make nanostructures?

Top-down Approach

Building something by starting with a larger component and carving away material (like a sculpture)

In nanotechnology: patterning (using photolithography) and etching away material, as in building integrated circuits

Rock

Statue

How to make nanostructures?

Bottom-up

Building something by assembling smaller components (like building a car engine), atom by atom assembly.

In nanotechnology: **self-assembly of atoms and molecules**, as in chemical and biological systems

Brick

Building

Self-assembly refers to the spontaneous bonding of **molecules to metal surfaces**, forming an organized array of molecules on the surface. Self-assembly of thiol and **disulfide compounds on gold has been most widely studied**.

2- Applications of Nanotechnology:
2.1 General Applications

Application	Examples
Medicine	Diagnostics, Drug delivery, Tissue engineering
Information and communication	Memory storage, Novel semiconductor devices, Novel optoelectronic devices, Displays, Quantum computers
Heavy Industry	Aerospace, Catalysis, Construction Vehicle manufacturers
Consumer goods	Foods, Household, Optics, Textiles, Cosmetics, Sports
Environment	

2.2- Environmental Applications

Check http://www.nanowerk.com/products/product.php?id=160 for more details

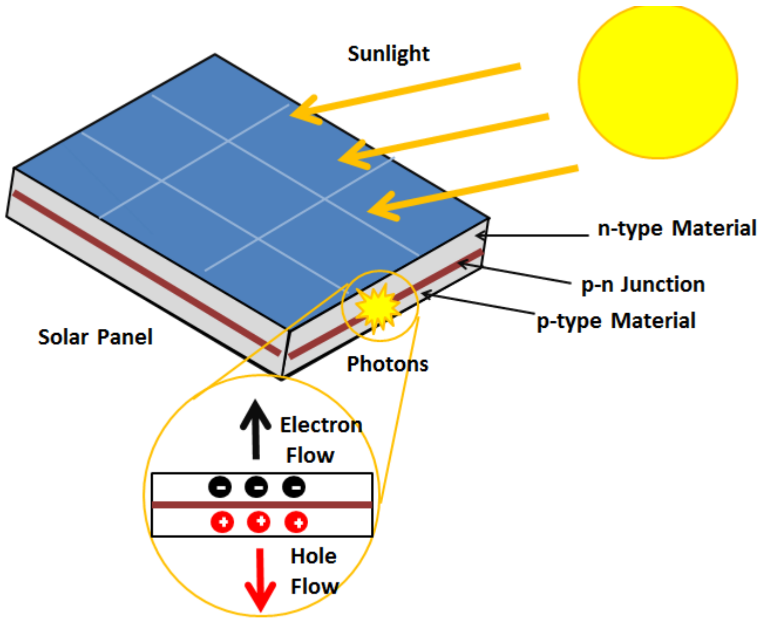
Application	Examples
Carbon capture	Photocatalyst consisting of silica Nanosprings coated with a combination of titanium dioxide
Sensors	Pollutants sensors that able to detect lower limits with low cost
Remediation (decontamination, oil spill management)	Heavy metal decontaminant removes heavy metals such as lead, cadmium, nickel, zinc, copper, manganese and cobalt in a neutral pH environment without using any form of sulphur .
Wastewater treatment	Inorganic microfiltration and ultrafiltration membranes.
Energy	Heat distribution e.g. ceramic-like materials that provide sufficient reliability and durability of the entire structure
Drinking water purification	

Organic/ Hybrid Photovoltaic

- Through the ages mankind need more and more energy
- **Oli, gas and coal** will not last forever, and it takes number of years until new fossil fuel are formed.
- The earth receives 1,74,000 TW (terawatts) of incoming solar radiations at the upper atmosphere, so as a solution sun become an important source of renewable energy.

Photovoltaics is the conversion of light into electricity using semiconducting materials that exhibit the photovoltaic effect

The photovoltaic effect is a process of converting light, i.e., photons, into electricity.



Why Organic Photovoltaic (OPV) solar cell

- Organic Photovoltaic cell (OPVC) or organic solar cell is a class of solar cell that uses **conductive organic polymers** or small organic molecules for light absorption and charge transport to produce electricity from sunlight by the photovoltaic effect.
- **Organic PV solar cell** aims to provide an earth abundant and low energy production PV solution.
- This new technology has the theoretical potential to provide electricity at a **lower cost** than the classical solar cells (Inorganic PV cells).

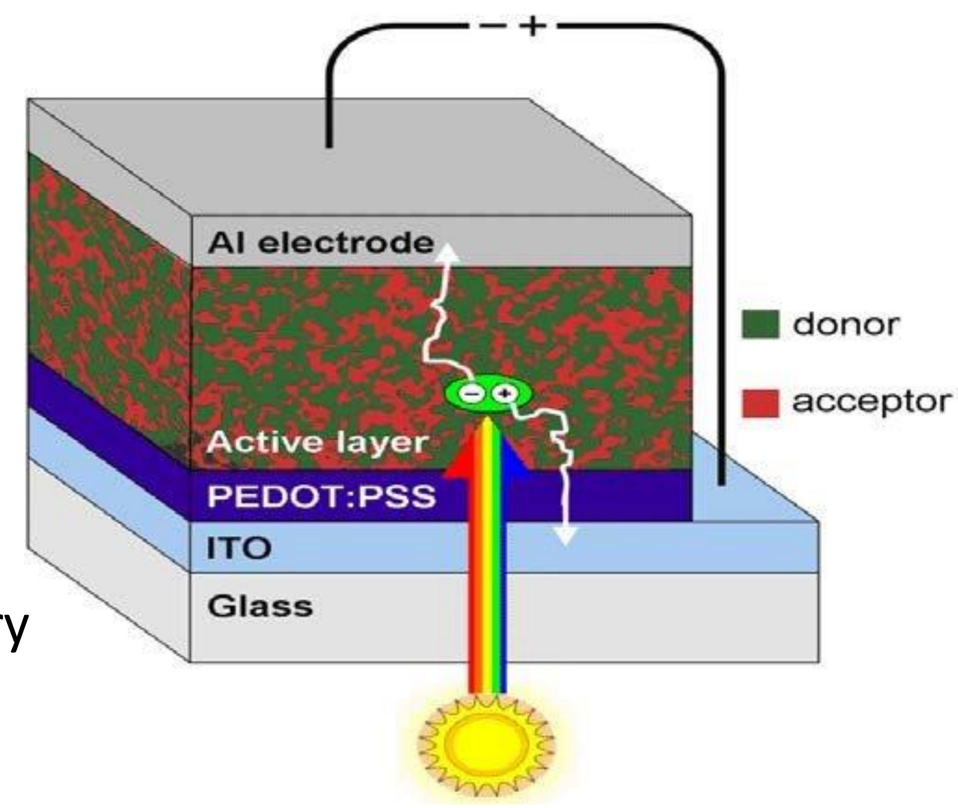
Structure of Organic Photovoltaic Solar cell

- The external behavior of organic photovoltaic is same as inorganic PVs, But the **voltage and current** are generated is quite different.
- The organic PV material is not crystalline, so there are not nice bands for the electrons and there isn't electric field to drive them.
- Because of that, when an excited electron is created by incident light it will quickly recombine with its hole unless something causes them to separate before recombination can happen.
- For that reason OPVs consist of two materials, one that electrons prefer and another that holes prefer.
- Once the electron and hole are separated into distinct materials, they can just diffuse apart due to their respective concentration gradients.

- There are three roles that will need to be filled by the materials:
  I. Absorption of light in the **visible spectrum,**
  II. A semiconducting material that will take the electrons (the acceptor)
  III. A semiconducting material that will take the holes (the donor).

If the charge carriers are generated far from the electrodes, the materials will also need to be efficient charge conductors (long carrier lifetimes) so that the charges are not lost before collection.

Many material combinations have been tried that fit these requirements.



They can be classified into three primary categories: molecular, polymer and hybrid

- In the construction of a working solar cell the **organic layer** is just one of the necessary components.
- The device must also be designed to efficiently **get light in and charge out.**
- On the side where light will come from there is a transparent conducting electrode. Indium tin oxide (ITO) is very commonly used for this purpose.
- There is also often a glass substrate that provides mechanical support.
- **Anti-reflection coatings** can help minimize losses due to non-absorption.
- On the other, dark side the electrode usually consists of a thin film of metal (such as Au or Al) that has been evaporated in to the device.

Working of Organic Photovoltaic Solar Cell

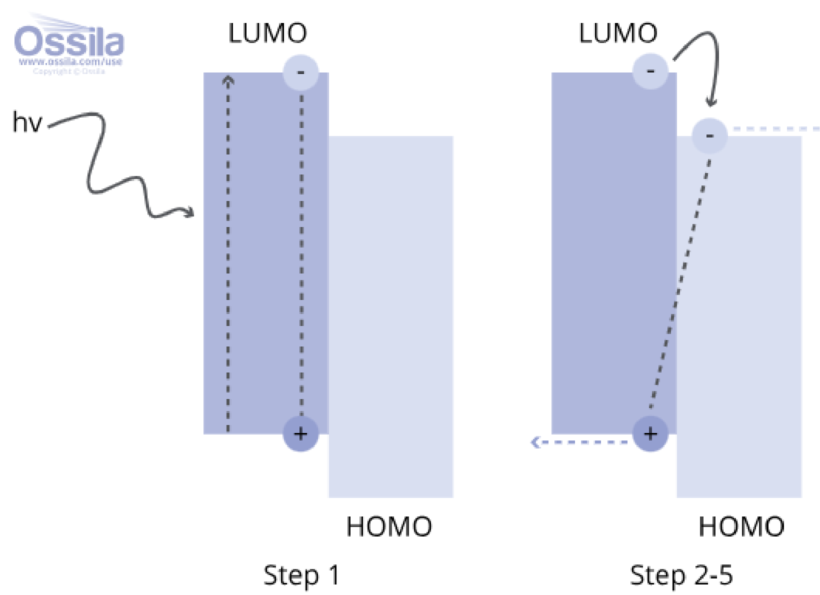
- The purpose of an OPV is to **generate electricity from sunlight**.
- This is achieved when the energy of light is equal to or greater than the band gap, leading to the absorption and excitation of an electron- from **HOMO to the LUMO**.
- The excited electron will leave behind a positively charged space known as a "hole".
- Due to the opposite charge of the hole and electron, they become attracted and form an electron-hole pair, also known as "exciton".
- To remove the charged particles from the solar cell, the electron-hole pair must be separated, and this process is known as "exciton dissociation".

1. Absorption of incident, light leading to exciton generation

- Light with enough energy will be **absorbed** by the OSC and excite electrons from the HOMO to the LUMO to form an exciton.
- If the energy of light being absorbed is greater than the band gap, the electron will move to a higher energy level than the LUMO and decay down.
- This process is known as 'thermalization' (or thermalisation) during which the energy is lost as heat.
- Thermalization is a key energy-loss mechanism in photovoltaics.

2. Diffusion of the exciton to a donor-acceptor interface

- Once formed, the exciton diffuses through the OSC component to the donor-acceptor interface, where the offset between LUMO levels will drive exciton dissociation.
- This must occur within a certain amount of time.
- If not, the excited electron will return to the empty energy state (known as the hole), a process known as ‘**recombination.**’
- The time taken is known as the ‘**exciton lifetime**,’ which is often represented as the distance that the exciton can diffuse in this time (which is around 10 nm).



3. Dissociation of the exciton across this interface

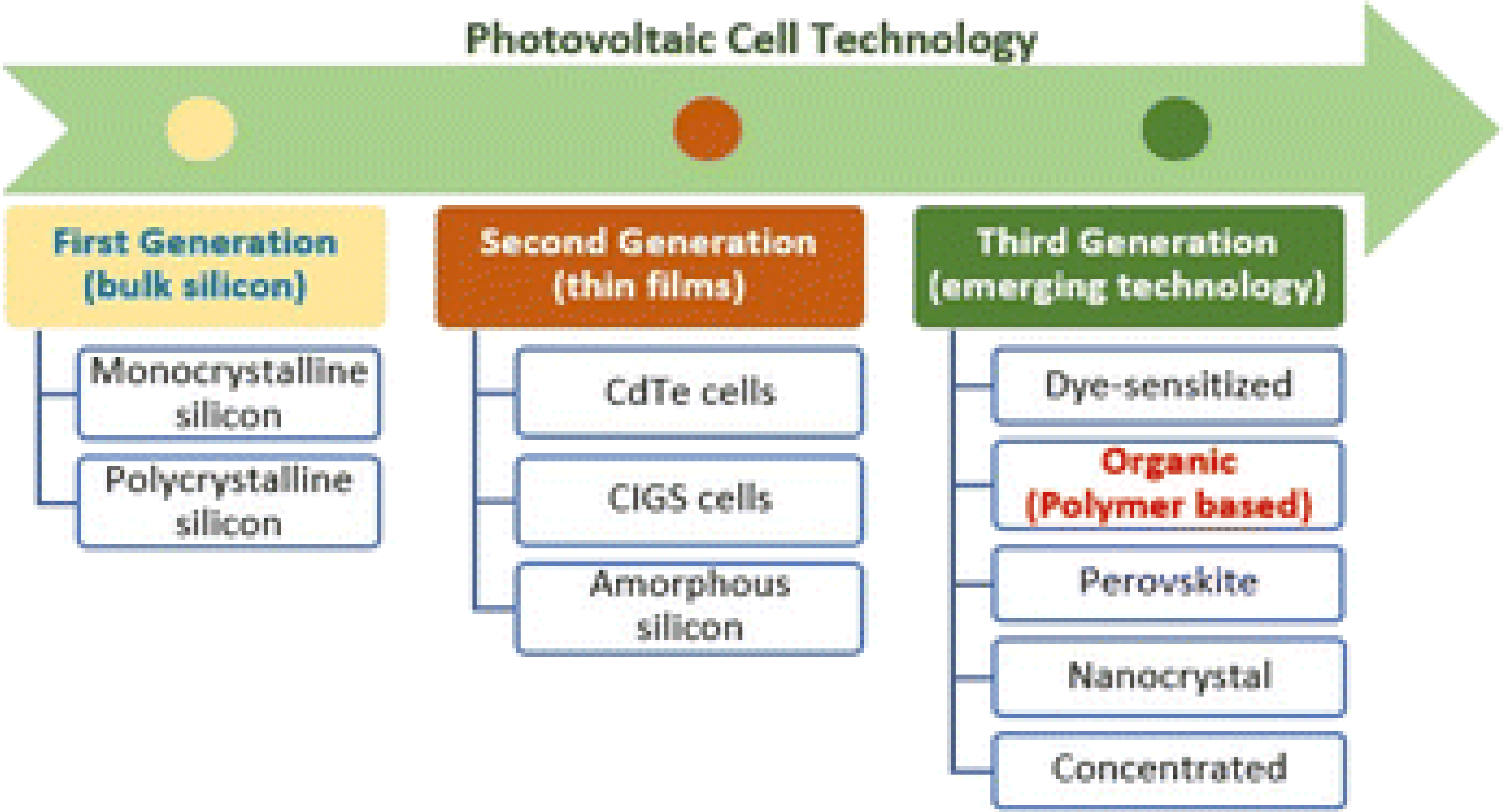
- At the interface, the electron will move to the **acceptor material** and the hole will remain on the donor.
- These charge carriers will still be attracted, and so form a **charge-transfer** state.
- When the **distance between the pair increases**, the attraction decreases. Eventually, the binding energy between them is overcome by thermal energy, and a **charge-separated state is formed**. While the electron-hole pair are still attracted in the charge-transfer state, recombination can occur across the interface between the two materials.

4. Charge-carrier transport

The charge-carriers will then **diffuse to the appropriate electrodes** (i.e. the holes to the anode and electrons to the cathode) through the relevant interfacial layers.

5. Charge-carrier collection

At the electrodes, the charge carriers are collected and used to do work in the external circuit of the cell – producing a current.


Photovoltaic Cell Technology
First Generation (bulk silicon)
Monocrystalline silicon
Polycrystalline silicon
Second Generation (thin films)
CdTe cells
CIGS cells
Amorphous silicon
Third Generation (emerging technology)
Dye-sensitized
Organic (Polymer based)
Perovskite
Nanocrystal
Concentrated

Advantages of Organic Photovoltaic Solar Cell

1. **Environmental sustainability:** Clean and green energy source as no harmful gases such as CO_2, NO_2, etc. are emitted. No noise pollution, which make them ideal for applications in residential area.

2. **Economically viable:** Operation and maintenance cost of cells are very low.

3. **Accessible:** Solar panels are easy to set up and can be made accessible.

4. **Renewal:** energy is free and abundant in nature.

5. **Cost:** Solar panel have no mechanically moving parts, the solar panel price for maintenance and repair is negligible.

Disadvantages of Organic Photovoltaic Solar Cell

1. Low efficiency
2. Power generation reduced during cloudy weather
3. Long range emission of solar radiations is inefficient and difficult to carry.
4. Photovoltaic panels are fragile and can be damaged relatively easily.
5. Current [produced is DC in Nature. So additional inverter is required for the conversion of DC to AC