IAT 3 Solution for ODD SEM 2022-23 (Subject CODE BCHEE102)

Roll No. | | | | |

Internal Assessment Test 3 – April 2023

Sub:	Chemistry				Sub Code:	BCHEE102	Branch:	ECE	
Date:	01-04-2023	Duration:	90 min's	Max Marks:	50	Sem / Sec:	I / M, N, O & P		OBE

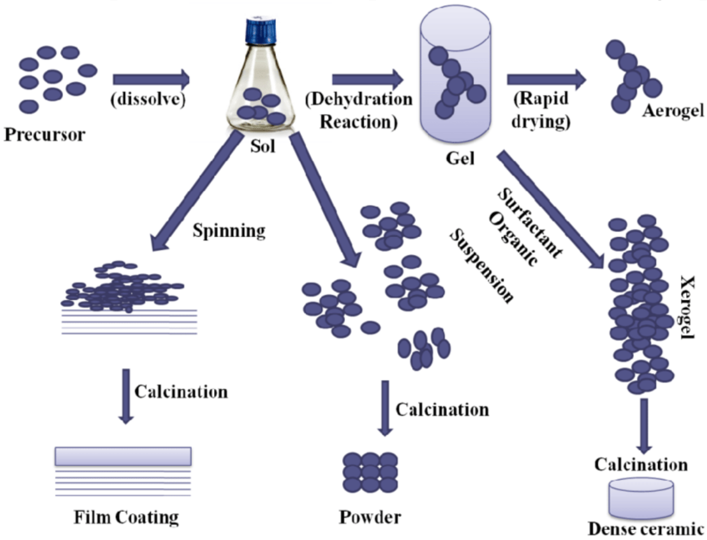
Question no. 1 is COMPULSORY and answer any THREE FULL Questions from the rest.

		Question	MARKS	CO	RBT
1	(a)	What are nanomaterials? Explain the preparation of nanomaterials by sol gel method giving suitable example.	[7]	CO1	L3
	(b)	Define liquid crystals? Describe the classification of liquid crystals with examples.	[7]	CO1	L2
2	(a)	Describe any 3 size dependent properties of nanomaterials.	[6]	CO1	L2
	(b)	Explain the synthesis of nanomaterials by co-precipitation method with suitable example.	[6]	CO1	L2
3	(a)	Write a note on properties and applications of nanofibers.	[6]	CO1	L2
	(b)	Describe the properties and explain the applications of Liquid crystals in LCD's with the help of diagram.	[6]	CO1	L3
4	(a)	Discuss the properties and applications of nanosensors.	[6]	CO1	L2
	(b)	What are QLED's. Explain the properties and applications of QLED.	[6]	CO1	L2
5	(a)	What are perovskite materials? Explain their properties and applications in optoelectronic devices.	[6]	CO1	L3
	(b)	What are OLED's. Discuss their properties along with applications.	[6]	CO1	L2

IAT 3 Solution for ODD SEM 2022-23 (Subject CODE BCHEE102)

Answer 1(a) Nanotechnology can be defined as the manipulation of atoms and molecules (one billionth) scale (1-100 nm) to produce devices, structures, or systems with at least one novel or superior property. Materials having at least one dimension in the nanoscale are called **nanomaterials**.

The sol-gel process, involves the evolution of inorganic networks through the formation of a colloidal suspension (sol) and gelation of the sol to form a network in a continuous liquid phase (gel). The precursors for synthesizing these colloids consist usually of a metal or metalloid element surrounded by various reactive ligands. The starting material is processed to form a dispersible oxide and forms a sol in contact with water or dilute acid. Removal of the liquid from the sol yields the gel, and the sol/gel transition controls the particle size and shape. Calcination of the gel produces the oxide.



Step1: Formation of different stable solutions of the alkoxide or solvated metal precursor (the sol).

M-OR + H2O -----------------► M-OH + HOR

Step 2: Gelation resulting from the formation of an oxide or alcohol bridged network (the gel) by polycondensation or poly esterification reaction. This results in a dramatic increase in the viscosity of the solution.

M-OH + M-OR ----------------- ► M-O-M + HOR

M-OH + M-OH -----------------► M-O-M + HOR

Step 3: Aging of the gel(synthesis), during which the polycondensation reactions continue until the gel transforms into a solid mass. This is accompanied by the contraction of the gel network and the expulsion of solvent from gel pores.

Step 4: Drying of the gel, when water and other volatile liquids are removed from the gel network. If isolated by thermal evaporation, the resulting is termed a xerosal. If the solvent (such as water) is extracted under supercritical or near supercritical conditions, the product is an aerogel.

Step 5: Dehydration, during which surface-bound M-OH groups are removed. This is normally achieved by calcination of the monolith at temperatures up to 800 0 C.

Step 6: Densification and decomposition of the gels at high temperature (T>800^0 C). The pores of the gel network collapse and the remaining organic species are volatilized.

The typical steps that are involved in sol gel processing are shown in fig. By different processes, one can get either nano film coating or nanopowder or dense ceramic with nanograins.

Example: Sol-Gel synthesis process ZnO NPs First of all, in a 100ml beaker 30 ml of water was added with 35 ml of triethanolamine(TEA) and drop wise ethanol was added with continuous stirring to get a homogeneous solution. After addition of 100 drops ethanol that was about 3 ml and continuous stirring results a homogeneous solution. Keeping the stoichiometry in mind a 2.0 gm batch of zinc oxide was prepared. Firstly, 30ml of water was mixed with 20 ml of TEA with constant stirring and drop wise addition of ethanol. The obtained homogeneous solution was kept at rest for 3.0 hours. For 2.0 gm batch of zinc oxide 5.49gm of zinc acetate dihydrate was mixed with 50ml water and 0.5M of solution was prepared which was subjected to continuous stirring to get a homogeneous solution. After that the two solutions were mixed together in 500ml beaker and drop wise ammonium hydroxide was added with continuous heating and stirring for 20minutesvia hot plate. Nearly 10ml of distil water was added during stirring. Then the solution was left for half an hour which results in the formation of white bulky solution. The obtained solution was then washed 10-12 times with distil water and filtered in a filter paper. The residue obtained waskept for drying in an oven at a temperature of about 95°C for 6 hours. The yellowish white powder obtained was then subjected to calcinations at a temperature of600°C for 5 hours

Answer 1(b) Liquid crystals (LCs) are a state of matter that has properties between those of a conventional liquid and a solid crystal.

2.1. Types of Liquid Crystals:

This classification is based on breaking order of the solid state and has two types:

1. Thermotropic liquid crystals 2. Lyotropic liquid crystals

2.1.1 Thermotropic liquid crystals

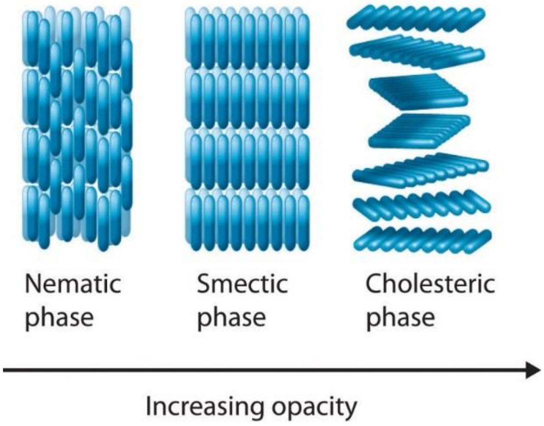
Thermotropic phases are those that occur in a certain temperature range. If the temperature is too high, the thermal motion may destroy the ordering in the LC phase and an isotropic liquid phase will occur. Ex: Cholesteryl benzoate, p-azoxy anisole etc. These have been classified into the following types.

a) Smectic liquid crystals
b) Nematic liquid crystals
c) Cholesteric liquid crystals

a) Nematic or thread-like liquid crystals: These are less ordered. These on heating lose their planar structure but retain a parallel alignment. Thus, they retain orientation but lose periodicity. The molecules tie parallel to each other but can move up or down or sideways or can rotate along their axes. N-paramethoxy benzylidene – p – butyl aniline changes to nematic liquid at 240C and this state persists up to 430C, after which it melts into an isotropic liquid. Nematic liquid crystals do not conduct electricity when they are in pure form. They flow like liquids, but their mechanical (like viscosity, elasticity) electrical (like dielectric constant) , optical properties and diamagnetism etc., depending upon the direction along which they are measured..

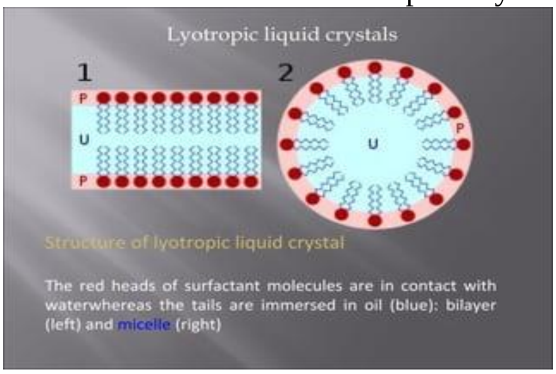
b) Smectic (or) soap-like liquid crystals: Smectic is the name given by G. Friedel for certain mesophases with mechanical properties similar to soaps. All smectic LCs have layered structures, with definite interlayer spacing. This can be measured by X-ray diffraction. Smectic liquid crystals on heating retain long-range order, yielding a smectic phase. They lose the periodicity within the planes but retain the orientation and arrangement in equispaced planes. Example: para-n-octyloxybenzoicacid

c) Cholesteric liquid crystals: These are optically active and possess the arrangement of molecules similar to those in the nematic type. Such liquid crystals are characterized by very high optical rotation, probably a thousand times greater than that of their crystalline variety. Moreover, on raising the temperature, the pitch decreases. This results in a corresponding change in the wavelength of reflection. They are named so because the skeleton of these substances pass through a state similar to that of cholesterol, a steroid present in blood. Example: Cholesteryl benzoate



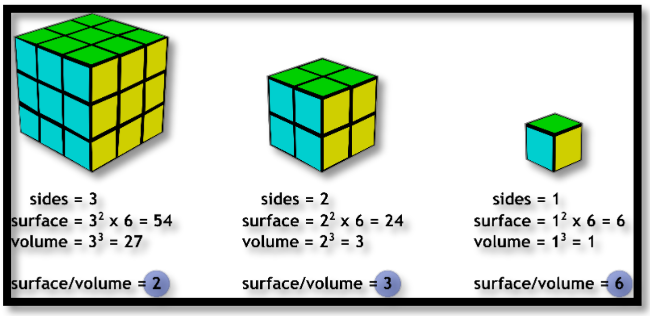
2. Lyotropic liquid crystals

Some compounds are transformed to an LC phase, when mixed with other substances (solvent) or when the concentration of one of the components is increased. Such compounds are called lyotropic LCs. A lyotropic liquid crystal exhibits liquid-crystalline properties in certain concentration ranges. Many amphiphilic molecules show a lyotropic liquid-crystalline phase. Examples are: Sodium laureate in water and Dhosphatidly choline in water.

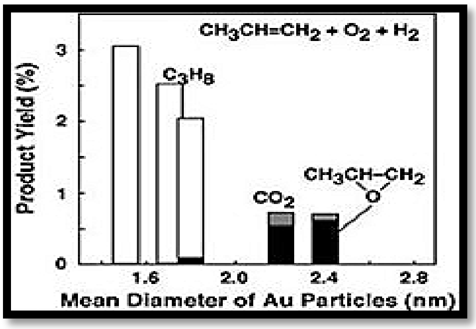


Answer 2a: Size-dependent properties

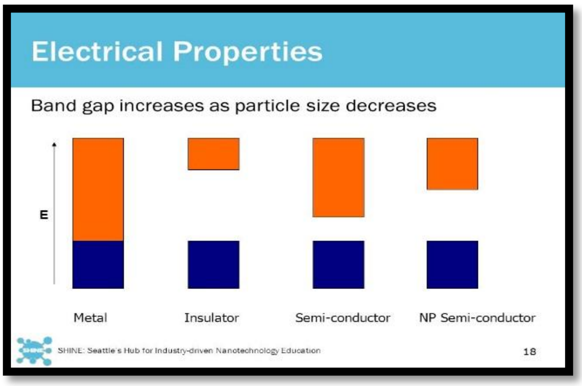
1). Surface area: In chemical reactions, this surface-to-volume ratio plays an important role. There is an enormous change in the properties of materials due to the increased surface area-to-volume ratio. The nanomaterials have a relatively larger surface area when compared to the same volume of the material produced in a larger form. So we know that material has high surface energy if it is small in size and vice versa. Therefore, nanoparticles have a large surface area to volume ratio and they possess large surface energy. Due to high surface energy materials are more reactive and also nanoparticles show enhanced stability and a broader scope of applications. In some cases, materials that are inert in their larger form are reactive when produced in their nanoscale form. This affects their strength or electrical properties. The ratio of surface area to volume of a material is given by $area/volume = 4\pi r2/\ 4/3\ \pi r3 = 3/r$



2) Catalytic properties: The factors such as very small size, very high surface-to-volume ratio, and the increasing number of atoms on the surface are the most important reasons for the emergence of catalytic properties in nanomaterials. Basically, when particles become very small (nanoscale), due to the very high curvature they find, they have many atoms on their surface, which are very weakly bonded to the lattice atoms of the lattice. Therefore, these particles have very high surface energy and are highly active, and it is said that surface atoms are in a state of physical instability and are chemically active, and are prone to perform many chemical reactions. It can be said that the main and determining reason for the emergence of catalytic properties in nanomaterials is their very high surface-to-volume ratio. The higher this ratio, the higher the catalytic properties in nanomaterials due to the increase in surface energy. In principle, the reason for these changes is due to changes in the electronic structure of materials, which can be justified by quantum mechanics.The effect of gold nanoparticle size on catalytic activity in the propene epoxidation reaction has been investigated, which shows that by reducing the size of gold nanoparticles, the yield of the product increases.



3) Conducting properties: In bulk metals, the valence and conduction bands overlap, while in metal nanoparticles there is a gap between these bands. The gap observed in metal nanoparticles can be similar in size to that seen in semiconductors (< 2 eV) or even insulators (> 2 eV). This results in a metal becoming a semiconductor. For example, carbon nanotubes can be either conductors or semiconductors depending on their nanostructure. Another example is supercapacitors which have effectively no resistance and disobey ohm's law.



Answer 2b: Co-precipitation method:

The commonly used solution method for the synthesis of multi-component oxide ceramics is the co-precipitation method, which produces a "mixed" precipitate comprising two or more insoluble species that are simultaneously removed from the solution. The precursors used in this method are mostly inorganic salts (nitrate, chloride, sulfate, etc.) that are dissolved in water or any other suitable medium to form a homogeneous solution with clusters of ions. The solution is then subjected to pH adjustment or evaporation to force those salts to precipitate as hydroxides, hydrous oxides, or oxalates. The crystal growth and their aggregation are influenced by the concentration of salt, temperature, the actual pH, and the rate of pH change. After precipitation, the solid mass is collected, washed, and gradually dried by heating to the boiling point of the medium. The washing and drying procedures applied for co-precipitated hydroxides affect the degree of agglomeration in the final powder and must be considered when nanosized powders are the intended product. Generally, a calcination step is necessary to transform the hydroxide into crystalline oxides. In most of the binary, ternary and quaternary systems, a crystallization step is necessary, which is generally achieved by calcination or, more elegantly, by a hydrothermal procedure in high-pressure autoclaves.

Example: Precursor solution: 0.1 M Fe ion solution, prepared by dissolving ferrous and ferric chlorides in a 1:2 $FeCl_2 \cdot 4H_2O$: $FeCl_3 \cdot 6H_2O$ molar ratio in deionised (DI) water (pHprec = 1.8). Base solution:

IAT 3 Solution for ODD SEM 2022-23 (Subject CODE BCHEE102)

DI water mixed with 2 M NaOH in a 10:4 volumetric ratio (0.57 M NaOH). Neutralisation solution: 0.316 M citric acid solution, pHneutr = 1.8. All chemicals, the provider and lot numbers are listed in table S1. 5 IONPs were co-precipitated by mixing the precursor and base solution of the (standard) concentrations stated above (if not mentioned otherwise). Mixing was performed at a reaction temperature of 60 °C for all syntheses. The sequence of neutralisation solution addition and the added quantity varied with the experiment

Answer 3a: Nano-fibers are slender, elongated, threadlike material with a diameter between 50 and 300 nanometers.

Properties of Carbon Nanofibers:

- Nanofibers have diameter 1000 times smaller than that of human hair
- high surface area with tunable porosity,
- 3D topography
- flexible surface functionalities
- and better mechanical properties (i.e., stiffness and tensile strength).
- Carbon nanofiber has a low density.
- The thermal conductivity ranges between 1950 – 6000 W/m K and electrical resistivity from 1×10^{-3} to 1×10^{-4}.
- Activated CNFs have a specific surface area with high adsorption capacity.

Applications of Carbon nanofibers:

- **Biosensors:** High sensitivity towards the target molecules, good electron transferability, a larger surface area for adsorption and being highly electrocatalytic towards the oxidation of small molecules like viruses, proteins and nucleic acids, glucose, hydrogen peroxide, dopamine, and cortisol they can be used efficiently in various clinical biosensing applications.
- **Wound dressing materials:** carbon-based nanofibers have been seeking more attention because of their excellent mechanical strength and biocompatibility. They are being used in the biomedical sector especially wound dressing, biomedicine and bioengineering.
- **Carbon nanofibers as supercapacitors:** PAN/polymethylmethacrylate (PMMA)/carbon composite nanofiber mats used as electrode material in a supercapacitor, characterized by a low loss after 10,000 charge-discharge cycles.
- **Carbon nanofibers for electrocatalytic applications**
- **Carbon nanofibers for CO_2 adsorption:**
- **Carbon nanofibers as cathode and anode material in advanced batteries:**

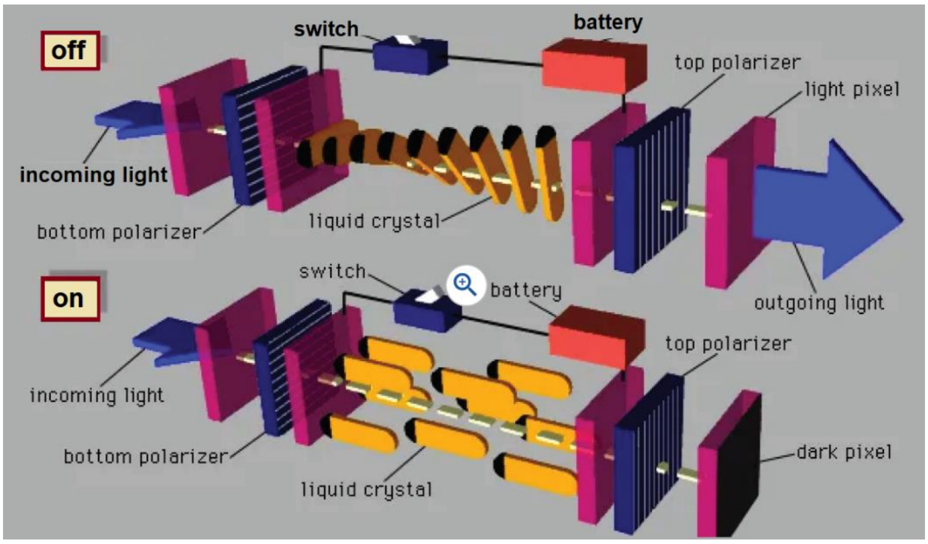
Answer 3b Properties of liquid crystals:

- These compounds display properties of both solid and liquid.
- Anisotropic: possess some orientational or positional order but with a lower degree of organisation compared with a crystalline solid.
- liquid crystal possesses liquid-like flowing behaviour,
- compounds are often more viscous.
- Liquid crystals are attributed to their sensitivity to various stimuli, such as temperature, electric and magnetic fields.
- Exhibit birefringence. That is, light that enters the crystal is broken up into two oppositely-polarized rays that travel at different velocities. Observation of a birefringent material between crossed polarizing filters reveals striking patterns and color effects.

Applications of LCs

IAT 3 Solution for ODD SEM 2022-23 (Subject CODE BCHEE102)

(1) Working principles of LCD: The properties of liquid crystals which make them suitable for use in displays are; their ability to affect the path of plane polarized light and their reaction to changes of temperature. Thermotropic liquid crystals are a type of liquid crystal which reacts to changes in temperature. This class of liquid crystals is subdivided into isotropic, where molecules have a random order and nematic liquid crystals where all the axes through the centre of the molecules are aligned. The nematic phase of liquid crystals is the one most often used in LCD displays. The molecules are rod-shaped and can move with respect to each other but with their molecular long axes, n, remaining aligned . Changes in this alignment of the nematic phase are seen when an external electric field is applied. Twisted versions of these nematic phases are used in the formation of pixels. A twisted nematic liquid crystal is trapped between two parallel glass sheets with polarizers at 90° to each other placed on either side of this sandwich. The nature of the liquid crystal is such that the orientation of a beam of polarized light will be turned through 90° allowing it to pass, unchanged, through the pixel as it will now be at the correct angle to pass through the second polariser. This causes the device to be in an on state and glowing. On application of an external electric field the liquid crystal molecule will realign so that polarized light is not transmitted by the molecule and as such does not pass through the second polarizer turning that pixel off. A series of transistors is used to turn on and off pixels in order to make up an image.



2) When a beam of light strikes a film of a smectic liquid crystal, the properties of the reflected light depending on this characteristic distance. Since this distance is temperature sensitive, the reflected light changes with changing temperature. This phenomenon is the basis of liquid crystal temperature sensing devices, which can detect temperature changes as small as $0.01^{O}C$ with ordinary light.

3) Liquid crystals are used in gas-liquid chromatography because their mechanical and electrical properties lie in between crystalline solids and isotropic liquids.

4) Liquid crystals are employed as solvents during the spectroscopic study of the structure of anisotropic molecules.

5) Cholesteric liquid crystals are used in thermography a method employed for detecting tumors in the body.

Answer 4a Nanosensors are sensors that make use of the unique properties of nanomaterials and nanoparticles to detect and measure materials and components on the nanoscale. The signals can be biomedical, optical, electronic, electrical, physical or mechanical.

IAT 3 Solution for ODD SEM 2022-23 (Subject CODE BCHEE102)

Properties of Nanosensors:

- Available in small sizes
- Requires less power to operate
- Less weight
- Works as data storage systems
- Great sensitivity, accuracy, scalability, efficiency, precision, and specificity
- Easy to execute.
- Provides a high-volume ratio.
- Response time is low.

Nanosensor Applications

They are used:

- To detect various chemicals in gases for pollution monitoring.
- Nanosensors have potential applications in the food sector, in food processing monitoring, food quality assessment, food packaging, food storage, shelf-life monitoring, and viability, as indicators of food safety and microbial contamination.
- For medical diagnostic purposes either as bloodborne sensors or in lab-on-a-chip type devices. The nanosensors provide an understanding of a person's health status through noninvasive detection of clinically relevant biomarkers in several biofluids such as tears, saliva, and sweat without sampling, complex manipulation, and treatment steps.
- To monitor physical parameters such as temperature, displacement and flow
- To monitor plant signaling and metabolism to understand plant biology
- To study neurotransmitters in the brain for understanding neurophysiology

Answer 4b: Quantum dot light-emitting diode (QLED) use quantum dots for emission and attracted much attention for the next generation of display

Properties:

- high color saturation
- tunable color emission
- high stability.
- QLED display has advantages in flexible and robust application, which makes wearable and stretchable display possible in the future.
- energy efficient, thin-film display and solid-state lighting applications.
- facile scale-up capability
- Wide-viewing angle

Applications of QLED

- quantum dot light-emitting diodes (QLED) are cost-effective electroluminescence devices ideal for large-area display and lighting applications.
- For photomedical applications: facilitate widespread clinical applications of photodynamic therapy (PDT) or photobiomodulation (PBM).
- Consumer electronics: Used in smart phones, tablets, laptops, and televisions.
- Lighting: Used in lighting applications
- Wearable devices:Used in smart watches and fitness trackers.
- Automotive displays:Used in automotive displays
- Medical devices: OLEDs are used in medical devices

IAT 3 Solution for ODD SEM 2022-23 (Subject CODE BCHEE102)

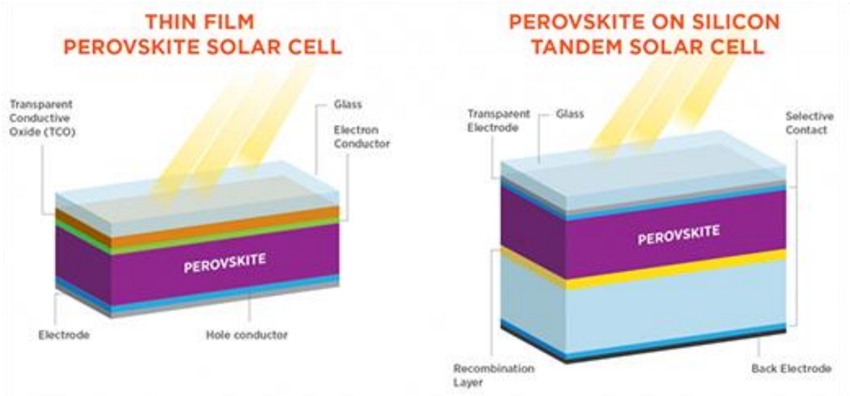
Answer 5a: Perovskite Materials is a material that has the same crystal structure as the mineral calcium titanium oxide (Perovskite).

Properties of Perovskite Materials:

- Generally, perovskite compounds have a chemical formula of ABO_3, where B is a transition metal ion with a small radius, a larger A ion is alkali earth metals or lanthanides with a larger radius, and O is the oxygen ion with a ratio of 1:1:3. In the cubic unit cell of ABO_3 perovskite, atom A is located at the body center, atom B is located at the cube corner position, and oxygen atoms are located at face-centered positions.
- Optical Properties: As one of the unique properties of metal-organic halide perovskites, the optical properties of photo-generated charge carriers have been researched. The specific excitonic absorption peaks of the metal-organic halide perovskite could be transited to various absorption spectra, and it changed significantly in visible light through the adjustment of metal atoms and halogens
- Electroneutrality; the perovskite formula must have a neutral balanced charge therefore the product of the addition of the charges of A and B ions should be equivalent to the whole charge of the oxygen ions.
- Dielectric properties: There are some properties inherent to dielectric materials like ferroelectricity, piezoelectricity, electrostriction, and pyroelectricity. One of the important characteristics of perovskites is ferroelectric behavior.
- Electrical conductivity: Some perovskites exhibited great electronic conductivity
- Superconductivity: One of the obvious properties of perovskites is superconductivity.
- Catalytic Activity: Perovskites exhibited high catalytic activity.
- Piezoelectric property: Piezoelectric Effect is the ability of certain materials to generate an electric charge in response to applied mechanical stress. Various applications such as capacitors, piezoelectric devices, and ferroelectric devices have been designed by using traditional inorganic perovskite materials.

Applications in Optoelectronic devices

1. Solar cells: A perovskite solar cell is a type of solar cell, which includes a perovskite structured compound, most commonly a hybrid organic-inorganic lead or tin halide-based material, as the light-harvesting active layer.



Perovskite materials are usually cheap to produce and relatively simple to manufacture. They possess intrinsic properties like broad absorption spectrum, fast charge separation, long transport distance of electrons and holes, long carrier separation lifetime, which make them very promising materials for solid-state solar cells.

2. Photodetectors: Lead halide perovskites have also been used to fabricate high-performance photodetectors.

3. Apart from these perovskite materials can be used in Light-emitting devices, Lasers, Water splitting applications such as Oxygen reduction and oxygen evolution reactions, Hydrogen evolution reactions and solid oxide fuel cells.

4. Nanoperovskites are recently utilized in electrochemical sensing of alcohols, gases, amino acids, acetone, glucose, H_2O_2, and neurotransmitters exhibiting good selectivity, sensitivity, unique long-term stability, excellent reproducibility, and anti-interference ability.

Answer 5b: Organic Light Emitting Diodes (OLED's) operates on the principle of converting electrical energy into light, a phenomenon known as electroluminescence. OLED is a semiconductor device, in which the emissive electroluminescent layer is a film of organic compound which emit light in response to an electric current.

Properties of OLED's

•Very thin solid-state device.
•Lightweight: the substrates are shatter resistant unlike glass displays of LCD devices.
•High luminous power efficiency: an inactive OLED element does not generate light or consumes power, hence allowing true blacks.
•Fast response time making entertaining animations- LCDs reach as low as 1ms response time for their fastest colour transition.
•Wide-viewing angle: OLEDs enable wider viewing angle in comparison to LCDs because pixels in OLEDs emit light directly. The colours appear correct.
•Self-emitting hence, removing requirement of a backlight source.
•Colour tuning for full colour displays
•Flexibility- OLED displays are fabricated on flexible plastic substrates producing flexible organic LEDs.
•Cost advantages over inorganic devices- OLEDs are cheaper in comparison to LCD or plasma displays.
•Low power consumption

Applications of OLEDs

1. To build digital displays in TV screens, cell phones, PDAs, monitors, car radios, digital cameras.
2. OLEDs have wide applications in lightning
3. It is used in watches.
4. OLEDs have replaced CRTs (Cathode Ray Tubes) or LCDs (Liquid Crystal Display).