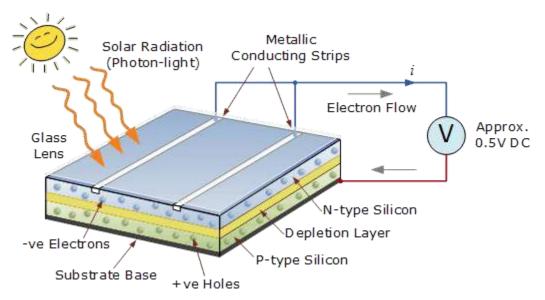


### **Solutions for IAT 3 (March-2022)**

Sub:	Engineering Chemistry			Sub Code:	21CHE12		Branch:		ECE, EEE, AIML and AI&DS
Date:	28/ 03 / 2022	Duration:	90 mins	Max Marks:	50	Sem	I	Section:	I to O

### Q1(a) Define Photovoltaic cell. Explain the construction, working and applications of PV cells. (CO4, Marks 7)

Answer: Photovoltaic cells or solar cells are semiconductor device that converts sunlight into direct current (DC) electricity. As long as light is shining on the solar cell, it generates electrical power. When light stops, electricity stops.



#### **Construction:**

Photovoltaic cells consist of a semiconductor diode (p-n junction) made of a silicon. Silicon wafer or very thin silicon slices are made by silicon blocks and they are doped by p-type and n-type dopants to make p-n junction. It has two electrical contacts, on one of its sides, a metallic grid is used and on the other side a layer of noble metal (such as Ag) is used. The metal grid permits the light to fall on the diode between the grid lines. The part between the metallic grid is coated with antireflective compound. eg  $TiO_2$ 

#### Working:

Electromagnetic radiation consists of particle called photon (hv). They carry certain amount of energy given by the Plank quantum equation.

 $E = hc/\lambda$ 



Where, h = Planck's constant, c = velocity of light,  $\lambda = wavelength$  of the radiation. The electromagnetic radiation (sunlight) falls normal to the plane of the solar cell, the photons which possess energy sufficient to overcome the barrier potential are absorbed, electrons are ejected and electron-hole pairs are formed. The electrons move towards the n-region (as it is positively charged). The electrons are driven into the external circuit and used for various applications or appliances.

#### Applications of PV cells: For producing electricity

- (i) In space stations and artificial satellites.
- (ii) In Street light in rural and remote areas.
- (iii). Solar Cell for Transportation: used in electric vehicles
- iv. For Operating water pumps for domestic and agricultural purpose.
- (v) For toys, watches, calculators solar water heaters etc.

#### Q1 (b). Describe any 6 basic principles of green chemistry. (CO4, Marks 7)

Answer: The term Green Chemistry is defined as -"The invention, design and application of chemical products and processes to reduce or to eliminate the use and generation of hazardous substances"

#### **Basic principles of green chemistry**

- 1) **Prevention of waste:** preventing the formation of waste products is always preferable to the clean-up of the waste once it is generated.
- 2) Atom economy: the synthetic processes and methods that are devices through green chemistry must always try to maximize the consumption and incorporation of all the raw materials into the final product. This must strictly be followed in order to minimize the waste generated by any process.
- 3) Avoiding the generation of hazardous chemicals: reactions and processes that involve the synthesis of certain toxic substances that pose hazards to human health must be optimized in order to prevent the generation of such substances.
- 4) **The design of safe chemicals:** during the design of chemical products that accomplish a specific function, care must be taken to make the chemical as non-toxic to humans and the environment as possible.
- 5) **Design of safe auxiliaries and solvents:** the use of auxiliaries in processes must be avoided to the largest possible extent. Even in the circumstances where they absolutely need to be employed, they must be optimized to be as non-hazardous as possible.
- 6) **Energy efficiency:** The amount of energy consumed by the process must be minimized to the maximum possible extent.
- 7) **Incorporation of renewable feedstock:** the use of renewable feedstock and renewable raw materials must be preferred over the use of non-renewable ones.
- 8) **Reduction in the generation of derivatives:** the unnecessary use of derivatives must be minimalized since they tend to require the use of additional reagents and chemicals, resulting in the generation of excess waste.



9) **Incorporation of Catalysis:** in order to reduce the energy requirements of the chemical reactions in the process, the use of chemical catalysts and catalytic reagents must be advocated.

 $Q2\ (a)$  . With a neat diagram explain the hydrogen production by photo catalytic water splitting method. (CO4, Marks 6)

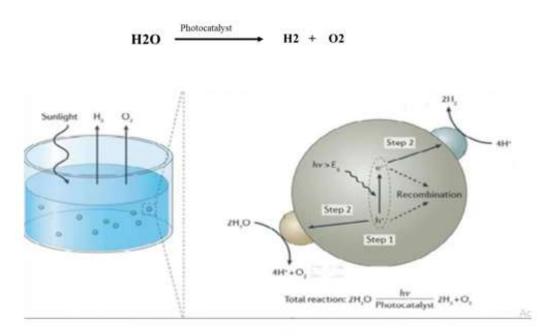
Answer: **Production of hydrogen:** Hydrogen is the future green fuel and does not cause environmental pollution.

Photocatalytic reaction

Input: Photocatalyst particles, sunlight and water

Output: Oxygen and hydrogen

Photocatalyst in the form of particles is immersed in water based electrolyte and it produces charge carriers holes and electrons after absorbing sunlight. Charges are moved to surface of the photocatalyst to start the chemical reaction. Holes are oxidizing the water and electrons reduces hydrogen ions to Hydrogen gas.



### Q2(b)Define fuel cell? Illustrate the construction, working mechanism and applications of methanol-oxygen fuel cell with a neat sketch. (CO4, Marks 6)

Answer: It is good example for liquid fuel cell. They use either acidic or alkaline medium. The preferred electrolyte is the acidic. Methanol is an efficient active organic fuel at low temperature.

Construction: Methanol – oxygen fuel cell consist of

Anode – It is a porous Nickel (Ni) electrode impregnated with Pt/Pd catalyst.

Cathode - It is a porous Nickel (Ni) electrode coated with Pt/Pd catalyst.

*Electrolyte* – Aqueous sulphuric acid (H<sub>2</sub>SO<sub>4</sub>), 3.7 M.



Fuel – Methanol mixed with sulphuric acid supplied at

Oxidant – Pure oxygen is supplied at cathode.

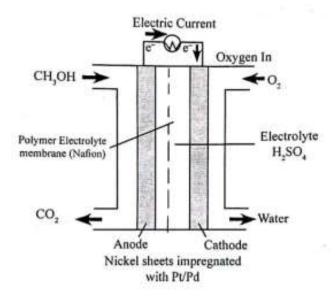


Figure. Methanol – oxygen fuel cell

Working: Cell reaction;

Anode reaction:  $CH_3OH + H_2O \rightarrow CO_2 + 6H^+ + 6e^-$ Cathode reaction:  $3/2 O_2 + 6 H^+ + 6e^- \rightarrow 3 H_2O$ Overall Cell reaction:  $CH_3OH + 3/2 O_2 \rightarrow CO_2 + 2 H_2O$ 

 $H_2O$  and  $CO_2$  are formed as by-products but they do not harm the cell functioning because they are removed as and when they are formed.

Cell Potential : 1.2 V

#### **Applications:**

- (1) used in automobiles, military applications.
- (2) Power backup and portable instruments.
- (3) in large scale power production.

### Q3 (a) Define nanomaterials. Discuss any 2 size dependent properties of nanomaterials. (CO3, Marks 6)

Answer: Nanomaterials or Nanoparticles are defined as substances which contain nano size particles with at least one dimension in the range of 1 nm to 100 nm.

Nanoparticles can exhibit size-dependent properties which is different from those of bulk materials.



Size dependent properties of Nanoparticles:

Optical Property: It is dependent on electronic structure. A change in the particle size, brings about change in electronic structure and band gap, which leads to the change in absorption and emission properties. Example: Bulk gold appears yellow in colour, where as nano gold appears red in colour.

Surface area and Catalytic Property: Surface area is enormously increased on moving from bulk to nanoscale. Nanomaterials have a significant proportion of atoms existing at the surface. Nanomaterials have high surface to volume ratio therefore they exhibit good catalytic activity. Example: Bulk gold is catalytically inactive while nano gold is catalytically very active for selective redox reactions.

#### Q3(b)Write a note on carbon nanotube. Discuss their properties and applications. (CO3, Marks 6)

Answer: Carbon Nanotubes (CNTs): Carbon Nanotubes (CNTs) are cylindrical tubes with a central hollow core formed by rolling up of graphene sheets. The CNT is a one dimensional material like nanowire, but with the length to width ratio greater than 1000. CNTs are categorized as Single-Walled CNTs (SWCNTS) and multi-walled nanotubes (MWCNTs).

1. Single-Walled CNT (SWCNTs): They are formed by rolling up of single graphene layer. The diameter of

SWCNT is 1-4 nm and length can go up to few micrometers.

2. Multi-Walled CNT (MWCNTs): They consist of two or more concentric graphene cylinders. The diameter of MWCNTs is in the range of 30-50 nm and length can go up to few micrometers. **Properties:** 

1. CNTs exhibit high electrical and thermal conductivity.

2. They have low density and very high mechanical strength due to these properties they are used as electrode material.

3. CNTs can emit electrons when subjected to high electrical field. Due to this property they are used in X-ray tubes.

3. The CNTs are about 20 times stronger than steel and hence find applications in making automobiles and aircraft body parts.

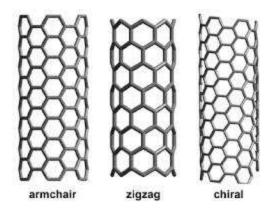
4. SWCNTs absorb radiation in the near IR range (700-1100 nm) and convert it to heat. This property is used in caner thermotherapy to selectively kill cancer cells.

- 5. SWCNTs are used in solar panels.
- 6. CNTs are used for hydrogen storage to be used as fuel source.

#### Applications: In the field of

- 1. Biosensors, chemical sensor and gas sensors,
- 2. Water purification
- 3. Cancer treatment
- 4. Drug delivery
- 5. Battery
- 6. Construction with steel





## Q4(a) What are Fullerenes? Describe their properties and applications of fullerenes. (CO3, Marks 6)

#### **Answer: Fullerenes:**

1). Fullerenes are class of molecules made only carbon atoms having closed cage like structure. Fullerenes can be of a different type  $C_{60}$ ,  $C_{70}$ ,  $C_{76}$ ,  $C_{78}$ ,  $C_{80}$  etc. depending on the number of carbon atoms. The most important fullerene is  $C_{60}$  containing 60 carbon atoms.

Fullerenes having spherical shape resemble soccer ball and are also called buckyballs. Fullerenes structure is built of fused pentagons and hexagons.

2). Fullerenes contain carbon atoms arranged as a combination of 12 pentagonal rings and n hexagonal rings. All the C-atoms are sp2 hybridized. The  $C_{60}$  molecule has two bond lengths. The hexagonal ring bonds can be considered double bonds and are shorter than the pentagonal bonds. Fullerene  $C_{60}$  is molecule is composed of 60 carbon atoms arranged as 12 pentagons and 20 hexagons and is commonly known as Buckminster fullerene

3) Fullerenes are stable, but not totally unreactive. The characteristic reaction of fullerenes is electrophilic addition. Fullerenes are heat-resistant and

4) Solubility: Fullerenes are soluble in many organic solvents, such as toluene, chlorobenzene etc. Solutions of pure buckminsterfullerene have a deep purple color. Solutions of C70 are a reddish brown. The higher fullerenes  $C_{76}$  to  $C_{84}$  have a variety of colors.

5) Superconductivity: Fullerenes are normally electrical insulators, but when crystallized with alkali metals, the resultant compound can be conducting or even superconducting

Applications: In the field of 1.Biosensors, chemical sensor and gas sensors, 2.Water purification 3. Cancer treatment 4. Super conductor 5. Fuel cells 6.Textiles, Food packaging etc..



Figure: Fullerene C<sub>60</sub>



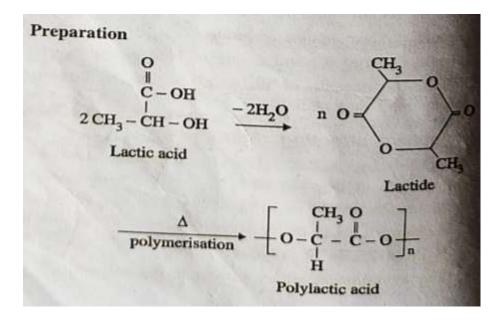
### Q4(b) What are biodegradable polymers? Explain synthesis, properties and applications of polylactic acid. (CO3, Marks 6)

**Answer:** Biodegradable polymers are defined as materials who's chemical and physical characteristics undergo deterioration and completely degrade when exposed to microorganisms, aerobic, and anaerobic processes.

Polylactic Acid (PLA)

Polylactic acid is a biodegradable aliphatic thermoplastic polymer. It is derived from renewable sources such as starch, sugarcane etc.,

#### Preparation



It is prepared by the catalytic dimerization of lactic acid resulting in the formation of lactide monomer.

Polymerisation of lactide monomer in presence pf stannous octate to give polylactic acid as a final product.

#### Properties

- 1. PLA possess good biocompatibility, process ability and high strength.
- 2. D-isomer of PLA is crystalline and L-isomer is amorphous
- 3. Biodegradation of D-isomer is slower than L-isomer.

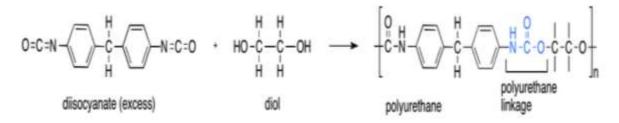
#### **Applications:**

- 1. PLA is used for making medical implants like screws, pins and anchors etc.,
- 2. It is used in a number of biomedical applications like drug delivery devices and dialysis media
- 3. It is used in the preparation of bioplastic for packaging food and disposable tableware.
- 4. It is also used for making compostable packaging materials and food packaging items etc.,



#### Q5(a) Explain the synthesis, properties and applications of Polyurethanes. (CO3, Marks 6)

**Answer:** Polyurethanes, along with phenolics, epoxies, and unsaturated polyesters, can be classified as reaction polymers. They can be prepared via the chemical reactions between isocyanates (that contain at least two isocyanate groups per molecule) and polyols (that contain at least two hydroxide groups per molecule). These reactions usually require the presence of a catalyst or some ultraviolet light in order to overcome the activation energy barrier.



#### **Properties of polyurethane**

1. If polyol chain is long and flexible, the polyurethane will be soft and elastic.

2. If cross-linking is very high, the polyurethane will be tough and rigid.

3. The cross-linked three-dimensional networks of polyurethane attribute very high molecular weights and has in thermosetting nature.

4. Polyurethanes have the ability to make foams.

5. resistance to organic solvents but attacked by strong acids & alkalies.

#### **Applications of polyurethanes**

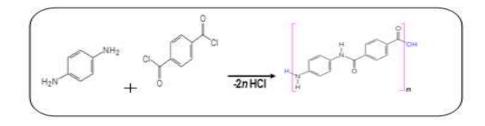
- The primary application of polyurethane is in the production of foams. These foams are used in a variety of materials such as upholstery fabrics, domestic furniture, and refrigerator sheets.
- Polyurethane is also used in some garments.
- Polyurethane mouldings are also used in columns and door frames. In fact, it is not uncommon for such mouldings to be employed in window headers and balusters.
- The low-density foams of polyurethane which exhibit flexibility are widely used in mattresses and other forms of bedding. They are also used in automobile seats and upholstery.
- Flexible polyurethane is also used in the manufacture of partially elastic straps and bands.
- The low-density elastomers of polyurethane are widely used in the footwear industry.
- Another notable application of polyurethane is in the manufacture of bathroom and kitchen sponges. It is also used in seat cushions and couches.



### Q5 (b) Define polymer composite. Explain synthesis, properties and applications of Kevlar. (CO3, Marks 6)

**Answer:** Polymer composites are a combination of polymers (i.e., thermosets or thermoplastics) with various continuous and noncontinuous reinforcements/fillers, principally added to polymers to improve the material performance.

**Synthesis of Kevlar:** Kevlar is made by a condensation reaction of an amine (1, 4-phenylenediamine) and acid chloride (terephthaloyl chloride). The Kevlar chains are relatively rigid and tend to form mostly planar sheets, similar to those of silk. This is due to the Para-orientation of the benzene rings. When Kevlar is spun the chains lock together via H-bonds to form a sheet that has a very high tensile strength. The sheets also stack radically, like the spokes on a wheel, allowing additional interactions between the face-to-face aromatic groups on neighbouring sheets to help to increase the strength of the overall fibre.



#### **Properties of Kevlar**

1. It is strong but light in weight; 2. It is crystalline and non-flammable; 3. It has good impact and abrasion resistance

4. It is thermally stable and withstand high temperatures; Not affected by very low temperatures.

3. Long exposure to ultraviolet light causes discoloration & degradation of the fibres.

- 4. It can resist chemical attacks, however long exposure to strong acids/bases causes degradation.
- 5. Kevlar remains unaffected by hot water & moisture.
- 6. Kevlar fibre is five times stronger than steel and have high tensile strength

#### Applications

**1. Military Body Armor & Jackets:** Kevlar fibre is five times stronger than steel on an equal weight basis, offering superior protection in military body armour and flak jackets.

**2. Protection Vests:** From higher-level bullets to knives, needles and explosions, protection vests made with Kevlar



**3. Military Helmets:** Kevlar meet demanding requirements for protection against a wide range of threats, including bullets, shrapnel and fragmentation.

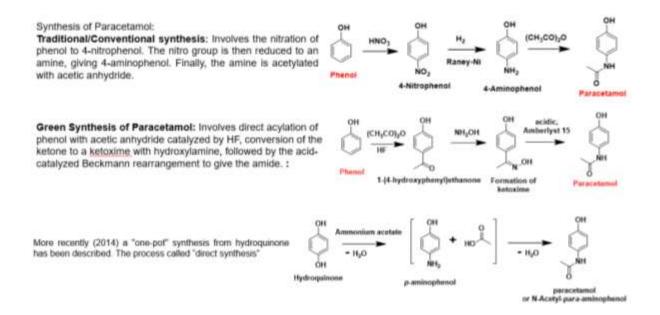
**4. Automotive Uses:** It is not uncommon for a new vehicle to have several crucial parts that employ products Belts, Brake pads, Clutches, Gaskets, Hoses made of Kevlar brand fibre.

**5. Kevlar as a Composite:** Formula 1 cars and HANS Device uses Kevlar straps to supports the driver's head and neck— Kevlar absorbs impact forces that are strong enough to pulverize neck vertebrae.

**6. Kevlar in Fiber Optics:** Kevlar is used to safeguard against mechanical stresses in optical fibre cables.

**7. Ropes and Cables:** Its resistance to chemicals and temperature extremes make it an ideal component for ropes and cables under severe loads in harsh environments,

### Q6(a) Explain the synthesis of paracetamol by conventional and green route from phenol. (CO4, Marks 6)



### Q6 (b)With suitable example explain microwave synthesis and bio catalyzed reactions. (CO4, Marks 6)

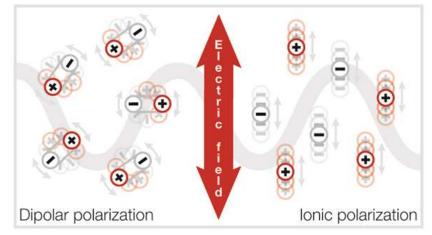
#### Answer: Microwave synthesis:

Microwave chemistry is based on the efficient heating of materials (in most cases solvents) by dielectric heating effects. Dielectric heating works by two major mechanisms:

i) Dipolar polarization



For a substance to be able to generate heat when irradiated with microwaves it must be a dipole, since, the microwave field is oscillating, the dipoles in the field align to the oscillating field. This alignment causes rotation, which results in friction and ultimately in heat energy.



#### ii) Ionic Conduction:

During ionic conduction, dissolved (completely) charged particles (usually ions) oscillate back and forth under the influence of microwave irradiation. This oscillation causes collisions of the charged particles with neighboring molecules or atoms, which are ultimately responsible for creating heat energy

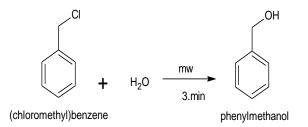
Microwave dielectric heating uses the ability of some liquids and solids to transform electromagnetic radiation into heat to drive chemical reactions.

#### General applications of Microwave Chemistry are,

- 1. Microwave assisted synthesis using Water.
- 2. Microwave assisted synthesis using Organic Solvents.
- **3.** Solvent free Reactions.

#### Hydrolysis of Benzyl Chloride:

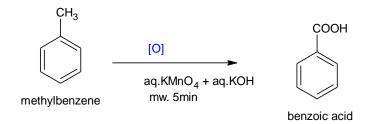
Hydrolysis of Benzyl Chloride with water in Microwave oven gives 97% yield of Benzyl alcohol in 3 min. Whereas conventional method takes about 35 min.



#### Oxidation



Oxidation of toluene by conventional method takes 10 - 12 hr. but by Microwave irradiation the reaction completed in 7 min. with 40% yield.



Bio-Catalyzed reaction: Bio-Catalyst is an enzyme which alters the rate of chemical or bio-chemical reaction. Enzymes are biocatalyst. These biocatalysts (enzymes) are used in the industrial preparation of ethanol. Ethanol is prepared by the fermentation of molasses -a dark brown coloured syrup left after crystallization of sugar which still contains about 40% of sugar. The process of fermentation actually involves breaking down of large molecules into simple ones in the presence of enzymes. The source of these enzymes is yeast.

The various reaction taking place during fermentation of carbohydrates are

$$\begin{array}{ccc} & & INVERTASE \\ C_{12}H_{22}O_{11} & \longrightarrow & C_{6}H_{12}O_{6} + C_{6}H_{12}O_{6} \\ Sucrose & glucose & fructose \end{array}$$

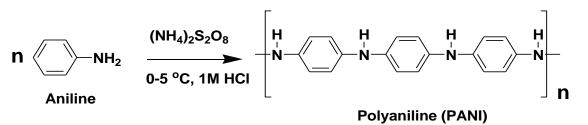
 $\begin{array}{ccc} ZYMASE \\ C_6H_{12}O_6 & \longrightarrow & 2 C_2H_5OH + 2 CO_2 \end{array}$ 

# Q7(a)What are conducting polymers? Explain the synthesis and mechanism of conduction in polyaniline. Mention any 2 factors influencing conduction in organic polymers. (CO3, Marks 6)

Ans: Conducting polymers are organic polymers that conduct electricity. Example: polyaniline (PANI)

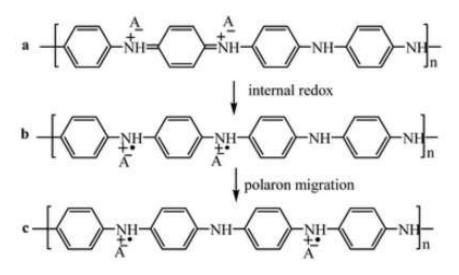
Preparation of Polyaniline: Polyaniline (PANI) is synthesized by polymerization of distilled aniline dissolved in precooled 1M HCl at 0-5  $^{\circ}C(HCl)$  in the presence of ammonium persulfate (APS) as initiator. The reaction is exothermic and the polymer formed is a mixture of different polyanilines





Mechanism of Conduction: These conjugated organic polymers in there pure state are insulators or semi-conductors. The  $\pi$ -electrons are normally localized and do not take part in conductivity. But, these electrons delocalize on doping and conduct electricity.

Polyaniline exists in a variety of forms (Oxidation states) that differ in their conductivity. The emeraldine form of polyaniline can also be electrochemically oxidized or reduced in aqueous acid resulting in pernigraniline (PS) and leuco-emeraldine (LS) salts, respectively. This process is known as protonic acid doping. The addition of protons and electrons to nitrogen is observed during the reduction. This leads to change of ring from phenyl to quinoid structure upon oxidation and vice versa during reduction. The generation of these charged carriers is responsible for conductivity of the polymer.



Mechanism of Conduction : (a) bipolaron (dication); (b and c) polaron (cation radical)

Factors influencing the conductivity of organic polymers:

(i) Conjugation and chain length : In general conductivity of a polymer increases with increase in polymer chain length and conjugation.

(ii) Doping level: The conductivity of a polymer increases with the increase in doping level till the saturation point is reached.

Q7(b)Explain the synthesis of adipic acid by conventional route from benzene and green route from glucose. (CO4, Marks 6)



Synthesis of adipic acid

(A) Traditional pathway : Using Benzene (Carcinogenic solvent)

