Sample Questions for reference (Engineering Chemistry)

Biomaterials

1. What are biomaterials?
   - Biomaterials are substances, either natural or synthetic, that are used in medicine to restore body function, promote healing, or replace damaged tissues and organs.
   - Their historical use dates back to ancient times, with examples like the Egyptians using animal sinew as sutures for medical purposes.
   - They are made from a wide range of materials, including metals, ceramics, plastics, glass, and even living cells and tissues, depending on the application.
   - Biomaterials can be engineered into various forms such as coatings, fibers, films, foams, or molded parts to suit specific medical needs.
   - Common biomedical applications include heart valves, hip joint replacements, dental implants, and contact lenses, which improve patients' quality of life.
   - Many biomaterials are biodegradable or bioabsorbable, meaning they naturally break down or are absorbed by the body after their intended function is complete, reducing long-term complications.
   - These materials are carefully designed to be biocompatible, ensuring they do not cause adverse reactions when interacting with human tissues.
   - Their versatility makes them essential in advanced medical devices and therapies, driving innovations in healthcare and improving patient outcomes

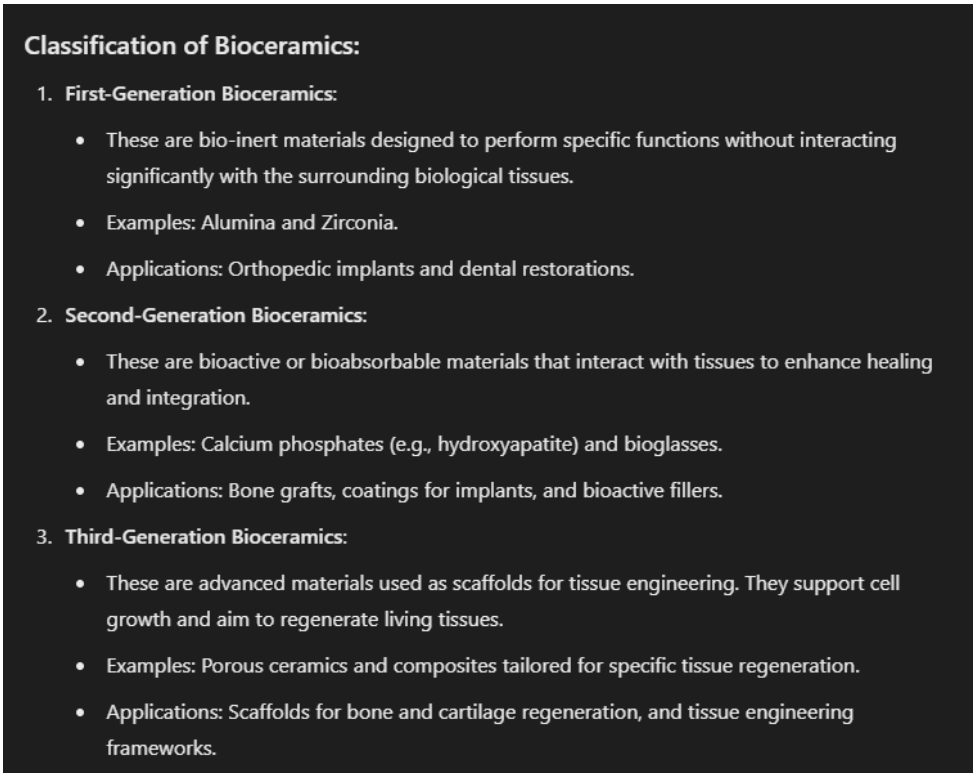
2. Applications of metals and alloys in biomedical field
   - METALS AND ALLOY are extensively used as biomaterial for their excellent strength and biocompatibility. Research is still being done to develop metallic biomaterials with the highest biocompatibility and least toxicity.
   - Various applications of metals and alloys in the biomedical field, categorized by body regions and their associated implants:

     1. Cranial Implants:

     Utilized for cranial reconstruction, typically made from 3D-printed titanium (Ti) and titanium alloy (Ti_6Al_4V).

2. **Stents:** Applied in cardiovascular procedures to maintain blood vessel patency, stents are fabricated from stainless steel, Co-Cr alloys, and nickel-titanium (Nitinol or NiTi).
3. **Joint Replacements:**
   Used for hip or knee replacement, these prosthetics are designed using stainless steel, Co-Cr alloys, and Nitinol.
4. **Bone Fracture Fixation:**
   Plates, screws, and rods for fracture repair are manufactured from stainless steel, Co-Cr alloys, and Ti_6Al_4V.
5. **Bone Scaffold:**
   Porous structures for bone regeneration are made from Co-Cr alloys, titanium (Ti), Ti_6Al_4V, and biodegradable metals such as magnesium (Mg).

3. What are bioceramics? Classify them
   - Bioceramics are ceramic materials specifically developed for use in medical and dental applications. These materials are known for their biocompatibility, high strength, resistance to wear, and ability to integrate with biological tissues.



Classification of Bioceramics:

1. **First-Generation Bioceramics:**
   - These are bio-inert materials designed to perform specific functions without interacting significantly with the surrounding biological tissues.
   - Examples: Alumina and Zirconia.
   - Applications: Orthopedic implants and dental restorations.
2. **Second-Generation Bioceramics:**
   - These are bioactive or bioabsorbable materials that interact with tissues to enhance healing and integration.
   - Examples: Calcium phosphates (e.g., hydroxyapatite) and bioglasses.
   - Applications: Bone grafts, coatings for implants, and bioactive fillers.
3. **Third-Generation Bioceramics:**
   - These are advanced materials used as scaffolds for tissue engineering. They support cell growth and aim to regenerate living tissues.
   - Examples: Porous ceramics and composites tailored for specific tissue regeneration.
   - Applications: Scaffolds for bone and cartilage regeneration, and tissue engineering frameworks.

4. Properties and Applications of bioceramics

Properties and Applications of Bioceramics

Bioceramics are a class of materials extensively used in various technological and biomedical applications due to their unique structural and functional properties. Here are the key properties and applications based on the provided text:

Properties of Bioceramics:

1. **High Performance in Extreme Conditions:**
   - Bioceramics exhibit exceptional performance under high loading rates, high temperatures, and chemically severe environments, which are typically unsuitable for metals.
2. **Brittleness and Fracture Toughness:**
   - A significant limitation is their inherent brittleness and low fracture toughness, which has historically restricted their use in specific applications.
3. **Material Innovations:**
   - To improve their mechanical performance, novel materials such as ceramic matrix composites and nanostructured ceramics are being developed.
4. **Nanostructure Features:**
   - Nanometric features in bioceramics can enhance functionality. For example, surfaces with nanostructures reduce the risk of prosthesis rejection and promote osteoblast proliferation (bone cell growth).

Applications of Bioceramics:

1. **Biomedical Use:**
   - Bioceramics are widely used in biomedical fields, particularly for applications such as prosthetics and implants, due to their biocompatibility and suitability for bone integration.
2. **Nanophased Ceramics:**
   - Research on nanophased or nanostructured ceramics shows promise for addressing structural and biological challenges in bioceramic applications. These materials can be produced using nanocrystalline methods or nanocomposites.
3. **Prosthesis Development:**
   - The incorporation of nanometric features in prosthetics not only improves biocompatibility but also reduces rejection risks, making them highly effective in medical applications.

Bioceramics, especially in their nanostructured form, are crucial for advancing both structural applications and biomedical solutions. Their development continues to address critical challenges such as brittleness and compatibility in demanding environments.

5. Applications of ceramic nano-biocomposites

Nano-Composites

Ceramic nanocomposites

➢Nanocomposites based on ceramic materials have been studied in order to improve mechanical properties and alter functional properties.

➢The ceramic nanocomposites reported until now are either a ceramic nanophase in a ceramic matrix, a carbonaceous nanophase in a ceramic matrix or a ceramic nanophase in a polymer matrix.

➢Enhancements in stability, hardness, strength, toughness and creep resistance compared to the unreinforced matrix material have been reported in nanocomposites (Narayan et al., 2004).

➢Moreover, the combination of properties can lead to a new generation of medical devices and implants combining mechanical properties with bioactive properties.

Some examples of ceramic based nanocomposite materials are as follows.

- Alumina-based nanocomposites: with the addition of several nano-reinforcements, alumina matrix materials with improved mechanical properties (higher resistance, hardness, wear resistance and fracture toughness) have been obtained.
- Alumina/silicon carbide nanocomposites: the incorporation of SiC nanoparticles to an alumina matrix increases wear resistance.
- Alumina/zirconia nanocomposites: also known as zirconia-toughened alumina (ZTA) nanocomposites, they consist of a fine-grained alumina matrix reinforced with zirconia particles. The addition of the zirconia nanoparticles is intended to increase the toughness of the alumina matrix.
- Alumina/titania nanocomposites: increased hardness, fracture toughness and fracture resistance have been achieved.

- Zirconia/alumina nanocomposites: also known as alumina-toughened zirconia (ATZ), they consist of a zirconia matrix reinforced with alumina nanoparticles. They show exceptional resistance and extraordinary toughness.
- Silicon nitride/silicon carbide nanocomposites: the obtained results are controversial.
- Ceramic/carbon nanofibre composites: widely used, there is an improvement in properties (Pace et al., 2002).
- Ceramic/carbon nanotube (CNT) composites: mechanical and electrical properties are enhanced, but biocompatibility issues are still contro- versial (Streicher et al., 2007; Garmendia et al., 2008, 2009, 2010, 2011).
- Ceramic in polymer composites: especially relevant for tissue engineering applications.

For nanocrystalline:

Properties and Application of nanocrysatlline ceramics

- In the case of nanocrystalline ceramics, as the grain size is reduced, the grain volume at grain boundaries is increased (Meyers et al., 2006).
- Thus, due to the high density of interfaces, an important fraction of atoms will be at the interface.
- This fact allows nanocrystalline materials to offer unusual and improved properties when compared to microscale materials.
- There are studies (Webster et al., 1999) that provide evidence that nanophase ceramics could promote osseointegration, which is critical for the clinical success of orthopaedic/dental implants.
- Webster et al. (2000) synthesized dense nanophase alumina (Al2O3) materials and showed a significant increase in protein absorption and osteoblast adhesion on the nano-sized ceramic materials compared to traditional micron-sized ceramic materials.
- Other studies (Du et al., 1999) have suggested that better osteoconductivity would be achieved if synthetic Hydroxyapatite(Hap) could more resemble bone minerals in composition, size and morphology.

Advantages

The use of nanocrystalline materials can thus offer advantages for use in biomedical applications, such as:

a. increased resistance/hardness
b. improved toughness
c. lower elastic modulus and lower ductility
d. reduced risk of rejection
e. enhanced proliferation of osteoblasts
f. promotion of ossointegration

With ceramic nanocomposites, even greater improvements can be achieved and the use of new ceramic matrix nanocomposites has been suggested (Gleiter, 1995; Narayan et al., 2004;

6. Write two advantages and two limitations of using stainless steel as biomedical implant.

STAINLESS STEEL

- ALLOY of Fe,, Cr, Ni and C.
- It has good corrosion resistance due to formation of passive layer on these material (due to Cr).
- Used as permanent surgical implant for decades. Eg. 316 L (316 LOW CARBON STEEL)
- The biocompatibility in this implants due to protective layer of Chromium oxide.
- The advantages of SS are that it is cheap, easily available and has excellent fabrication properties, is biocompatible and has great strength.

- Limitation:

1. Within the body, the SS implants are exposed to rather complex body fluids, which contain chloride ions, reduced sulfur, etc. and when SS reacts with these ions, toxic elements like nickel and chromium are released. (to over counter these alloy can coated with transition metal nitrides eg. TiN, VN, TiAlN)

- Another major concern in using SS as a biomedical implant is the presence of nickel, which is toxic, and many patients are nickel sensitive. Research is also going on in developing nickel-free SS. Nitrogen, which is also an austenite stabilizer like nickel, is being used instead of nickel.

MEMS

1. What is MEMS?
    - Micro-electromechanical systems (MEMS) is a process technology used to create tiny integrated devices or systems that combine mechanical and electrical components. It can range in size from a few micrometers to millimeters.
    - These devices (or systems) have the ability to sense, control and actuate on the micro scale, and generate effects on the macro scale.
    - MEMS consist of mechanical microstructures, micro sensors, micro actuators and microelectronics, all integrated onto the same silicon chip.
    - Micro sensors detect changes in the system's environment by measuring mechanical, thermal, magnetic, chemical or electromagnetic information or phenomena.
    - Microelectronics process this information and signal the micro actuators to react and create some form of changes to the environment.
    - The device's electronic components are crafted using computer chip technology, whereas the small mechanical parts are created using a technique called micromachining. This involves carefully manipulating materials like silicon to either carve away sections or add new layers.

2. Discuss the applications of silicon as a substrate in MEMS

Silicon as a Substrates

The most common substrate material for micromachining is silicon. It has been successful in the microelectronics industry due to following reason:

- **i) silicon is abundant, inexpensive, and can be processed to unparalleled purity**
- **ii) silicon's ability to be deposited in thin films is very amenable to MEMS**
- **iii) high definition and reproduction of silicon device shapes using photolithography are perfect for high levels of MEMS precision**
- **iv) it can be readily oxidized to form a chemically inert and electrically insulating surface layer of SiO2 on exposure to steam.**

3. Discuss the applications of MEMS as chemical and biological sensors
   - Chemical and biological sensors encompass a large and wide variety of devices that interact with solids, gases and liquids of all types and are therefore extremely diverse and interdisciplinary.

   Some applications of chemical and biosensor technology include:

   - General healthcare monitoring
   - Screening for disease
   - Clinical analysis and diagnosis of disease
   - Veterinary and agricultural applications
   - Industrial processing and monitoring
   - Environmental pollution control
   - Glucometers are a type Biosensors, which measure the concentration of glucose in blood.
   - Agriculture Industry: Biosensors used for detection of pesticides and concentration of important nutrients.

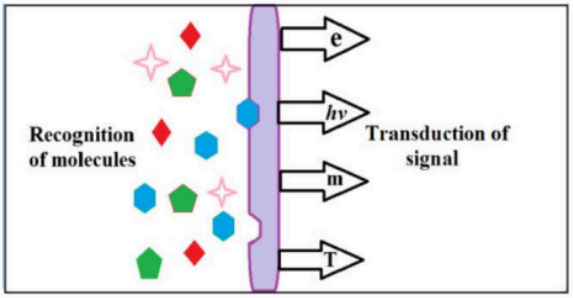
4. Describe the working principle of chemical and biosensors

   Working principle of Chemical sensors

Chemical sensors are sensor devices that convert chemical information (i.e., the amount of some individual compound) into a signal that can be analyzed. The sensing material and the transducer are generally the two main components. The target molecule interacts with the sensing material. This binding contact causes changes in a material attribute, such as mass and electrical conductivity, which will be converted into a quantifiable signal, generally an electronic signal, by the transducer

The ideal chemical sensor should be an inexpensive, portable, reusable, and reliable device that quickly responds with a perfect choice for a certain target analyte present in any medium, at any concentration level.

The magnitude of the measurable signal is proportional to the concentration of analyte. There are two major detection mechanisms in chemical sensors. They are photochemical and photometric, and are used to find the concentration or changes in the chemical reactions with most accuracy



Working principle of Bio sensors:

Biological Sensors

The short form of the biological sensor is known as a biosensor. In this sensor, a biological element is maybe an enzyme, a nucleic acid otherwise an antibody. The bio-element communicates through the analyte being checked & the biological reply can be changed into an electrical signal using the transducer. Based on the application, biosensors are classified into different types like bio-computers, glucometers & biochips.

The working principle of biosensors involves a few key components:

Recognition: The biological element selectively interacts with the target analyte present in the sample.

Transduction: This interaction leads to a change in the biological element, such as a change in electrical conductivity, pH, or light emission.

Signal Amplification: Sometimes, additional components in the biosensor amplify the signal generated by the interaction between the biological element and the analyte.

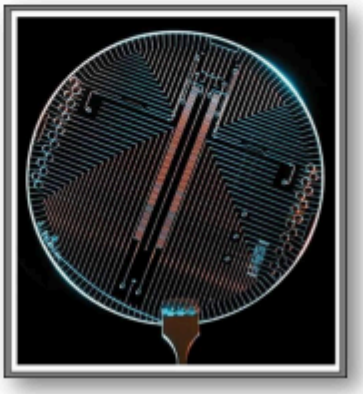
Detection and Output: The transducer detects the change and converts it into a measurable signal, which is then displayed or processed for interpretation by the user or an electronic device.

5. Applications of MEMS as chemical and biological sensors

Clinical Laboratory Testing

A lab-on-a-chip (LOC) takes the laboratory testing of biomolecular samples (e.g. blood, urine, sweat, sputum) out of the clinical lab and places it in the field or point-of-care (POC).

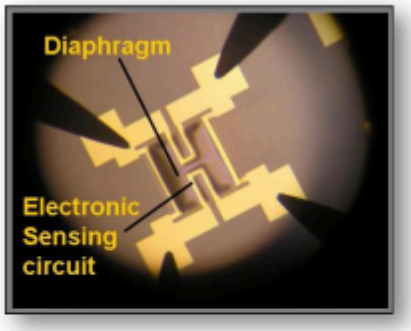
LOCs use microfluidics and chemical sensors to simultaneously identify multiples analytes (substances being analyzed).



Lab-on-a-chip (LOC)

MEMS Pressure Sensor

- MEMS pressure sensors use a flexible diaphragm as the sensing device.
- One side of the diaphragm is exposed to a sealed, reference pressure and the other side is open to external pressure.
- The diaphragm moves with a change in the external pressure.



MEMS Pressure Sensor

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Pressure Sensors in BioMedical Applications

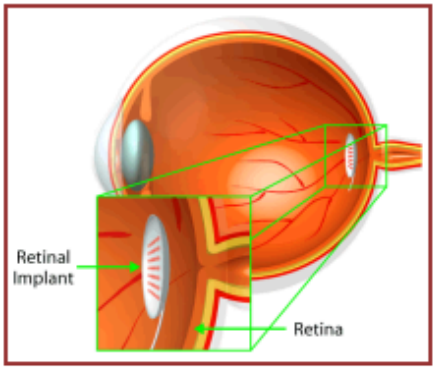
- Blood PS
- Intracranial PS
- PS in endoscopes
- Sensors for infusion pumps

RF (radio frequency) elements incorporated into the MEMS device allow the sensor to transmit its measurements to an external receiver.

Retinal Prosthesis

- Medical MEMS – aka BioMEMS - can consist of in vivo (internal) components and in vitro (external) components such as this retinal prosthesis
- A microarray or retinal implant is implanted in vivo on the retina.
- An external camera and processor are mounted in a pair of glasses.
- Watch this video to see how it works.

https://youtu.be/Bi_HpbFKnSw



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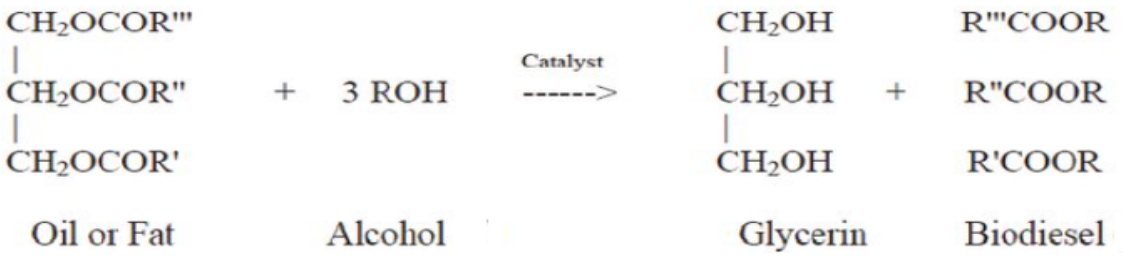
[Module-3] Sustainable Energy

1. State five advantages and five limitations of Renewable energy resources.

Advantages	Disadvantages
Reduces consumption of fossil fuels.*	Currently, electricity from PV systems is more expensive than electricity produced from fossil fuel or nuclear power plants.
Reduces production of greenhouse gases.*	Expensive to buy.
Reduces production of various pollutants.*	Requires engineering expertise to design and install systems.
Good for remote applications: satellites, rural hospital equipment in developing countries, telecommunication equipment, etc.	Production of PV systems from single silicon crystals is technically challenging, and energy- and time-consuming.
Reduces the loss of electricity due to power line resistance (distribution losses) because it can be sited where the electricity is used.	Sunlight is not constant, so must get electricity from other sources at night or on cloudy days or store it (such as batteries, etc.)
Reduces water consumed in electrical generation processes by displacing electrical demand.	Sunlight is diffuse; PV would take much space to produce enough electricity to meet our current needs (an area ~one sixth the size of Arizona)
Does not contribute to thermal pollution of waterways.	* Once manufactured, PV systems produce no waste products. Manufacturing of almost any device uses some nonrenewable resources, consumes energy and produces waste products. PV systems consume some nonrenewable resources if a system component needs repair or maintenance (such as batteries, inverter, etc.).
No hidden costs.	
Can provide energy independence.	
PV cells last ~ 30 years.	
Uses a renewable energy source.	

Renewable resources	Non- renewable resources
Resources which can be renewed or can be reused are renewable resources.	Resources which cannot be renewed or reused once utilized are called non-renewable resources.
These include components like air, water, wind, sunlight etc.	These include components like fossil fuels, LPG gases.
They are sustainable resources.	They are exhaustible resources.
Their rate of renewal is greater than the rate of getting exhausted.	Their rate of renewal is slower than the rate of getting exhausted.
They are mostly environmental friendly and does not cause pollution.	They are the main cause of pollution.

2. Give eight characteristics of ideal fuel.
3. Explain the synthesis method of Biodiesel. State the advantages and limitations of biodiesel.
   - Biodiesel is a liquid biofuel obtained by chemical processes from vegetable oils or animal fats and an alcohol that can be used in diesel engines, alone or blended with diesel oil
   - The production of biodiesel chemical reaction is known as transesterification.
   - Transesterification is the chemical process, which converts natural fats and oils into Biodiesel. Most of the biodiesel is produced from waste animal fats and vegetable oils obtained from restaurants, and industrial food producers.



- **Advantages**

  - Some of the advantages of using biodiesel as a replacement for diesel fuel are Renewable fuel, obtained from vegetable oils or animal fats.
  - Low toxicity, in comparison with diesel fuel. □ Degrades more rapidly than diesel fuel, minimizing the environmental consequences of biofuel spills.
  - Lower emissions of contaminants: carbon monoxide, particulate matter, polycyclic aromatic hydrocarbons, aldehydes.
  - Lower health risk, due to reduced emissions of carcinogenic substances. □ No sulfur dioxide (SO2) emissions.
  - Higher flash point (100C minimum).
  - May be blended with diesel fuel at any proportion; both fuels may be mixed during the fuel supply to vehicles.
  - Excellent properties as a lubricant.
  - It is the only alternative fuel that can be used in a conventional diesel engine, without modifications.

2. Cost Issues

- **High Production Costs:** Producing biodiesel is often more expensive than petroleum-based diesel due to raw material costs and processing requirements.
- **Economies of Scale:** Small-scale biodiesel production facilities may struggle to compete with large-scale fossil fuel operations.

3. Energy Content

- **Lower Energy Density:** Biodiesel typically has a slightly lower energy content (about 8-12% less) compared to petroleum diesel, which can reduce engine performance and fuel efficiency.

4. Cold Weather Performance

- **Gelling in Cold Temperatures:** Biodiesel has a higher cloud point and pour point than conventional diesel, making it prone to gelling in cold climates unless treated.

5. Engine Compatibility

- **Potential Engine Modifications:** Older engines may require modifications to run on biodiesel blends due to material incompatibilities with rubber and seals.
- **Fuel Quality Issues:** Poorly processed biodiesel can lead to deposits, clogging, and wear in engines.

6. Environmental Concerns

- **Land Use Change:** Converting land for biodiesel crops (e.g., deforestation) can result in significant carbon emissions, offsetting the fuel's environmental benefits.
- **Biodiversity Loss:** Monoculture plantations for biodiesel crops can harm biodiversity.

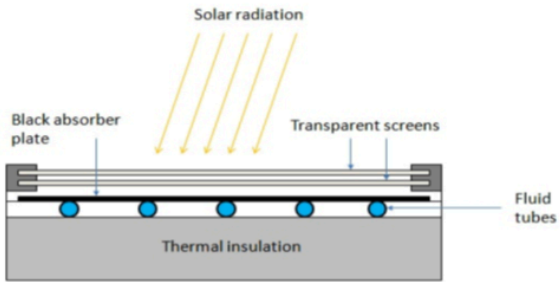
4. Calculate GCV and NCV for sample of coal containing: Carbon: 82%, Hydrogen= 5%, Nitrogen= 2.5%, Sulphur=1.5% and ash =3%.
5. Explain the construction and working of solar water heater with the help of suitable diagram.

   Construction and application:

Flat Plate Collector (Solar Heater):

The device works on the principle of black body in which heat absorbing capacity and tendency of a black surface is utilized to achieve benefits for human.

Diagram:



Construction:

These are the main components of a typical flat-plate solar collector:

Black surface - absorbent of the incident solar energy

Glazing cover - a transparent layer that transmits radiation to the absorber, but prevents radiative and convective heat loss from the surface

Tubes containing heating fluid to transfer the heat from the collector

Support structure to protect the components and hold them in place

Insulation covering sides and bottom of the collector to reduce heat losses

Application

- Some advantages of the flat-plate collectors are that they are:
- Easy to manufacture
- Low cost, Collect both beam and diffuse radiation
- Permanently fixed (no sophisticated positioning or tracking equipment is required)
- Little maintenance

Working:

Working of a Flat Plate Collector (Solar Heater)

1. Sunlight strikes the blackened absorber plate, converting solar energy into heat.
2. Heat is transferred to a fluid (usually water or antifreeze solution) flowing through tubes attached to or embedded in the absorber plate.
3. A glass or plastic cover traps heat by allowing sunlight in but reducing heat loss through convection and radiation.
4. The back and sides are insulated to minimize heat loss and improve efficiency.
5. The heated fluid is circulated through the system by natural convection (thermosiphon) or a pump.
6. The heated fluid is stored in a tank or used directly for applications like water heating, space heating, or industrial processes.

6. What is power alcohol? State four advantages and four limitations of power alcohol.

- Power alcohol, also known as ethanol or ethyl alcohol, is a type of renewable biofuel derived from plant materials such as sugarcane, corn, barley, wheat, or cellulose-rich materials like wood chips and agricultural residues.

Advantages

- **Reduced Greenhouse Gas Emissions:** When compared to fossil fuels, ethanol generally produces lower net carbon dioxide emissions, contributing to mitigating climate change.
- **Domestic Production:** Many countries aim to promote ethanol production from locally grown crops, reducing dependence on imported oil and enhancing energy security.
- **Fuel Properties:** Ethanol has high octane ratings and can be used as a blending component in gasoline to enhance its octane level and reduce emissions.
- **Renewable and Environmentally Friendly:** Power alcohol is considered a renewable fuel as it is derived from plant matter that can be grown and harvested repeatedly. It is also relatively cleaner burning compared to fossil fuels, emitting fewer greenhouse gases and pollutants like carbon monoxide and particulate matter.

Limitations

- **Lower Energy Density:** Ethanol has a lower energy density (calorific value 7000 Kcal/Kg as compared to gasoline (12000 Kcal /Kg), resulting in decreased fuel efficiency when used as a standalone fuel. Vehicles running on ethanol may experience reduced mileage compared to gasoline-powered vehicles.
- **Cold Weather Performance:** Ethanol has a higher water content, making it prone to issues in cold weather conditions, such as difficulties in starting engines and potential corrosion of fuel system components.
- **Infrastructure and Compatibility Issues:** While some vehicles are designed to run on ethanol (flex-fuel vehicles), the widespread use of ethanol as a fuel requires significant changes in infrastructure, including fuel distribution systems and vehicle engines, which might not be readily available or cost-effective.
- It must be noted that these disadvantages are significantly reduced when biodiesel is used in blends with petrol.

7. Calculate GCV and % Hydrogen for coal sample having NCV= 7890 Kcal /Kg and following composition: Carbon = 80 %, Nitrogen = 4%, oxygen = 5 %, Sulphur = 3%.
8. Li-ion battery
9. Ni-Cd battery
10. Lead Acid battery

11. Solar Photovoltaic cell for the generation of electricity

[Module-4] Spectrophotometery

1. What is spectroscopy and spectrophotometery? What are electroanalytical techniques?

Definitions

- **Spectroscopy** is the branch of science that deal with the study of interaction of matter with electromagnetic radiation of particular wavelength and vice-versa
- **Spectrophotometry** is a method to measure intensity of light absorbed by a chemical substance when a beam of light passes through a sample solution.

  It is the combination of spectrometry (interaction of electromagnetic radiation of particular wavelength) and photometry (measurement of intensity of transmitted radiation in terms of absorbance). The basic principle is that each compound absorbs or transmits light over a certain range of wavelength.
- **Electro-analytical** methods are a class of techniques in analytical chemistry, which deals with study of an analyte (test solution) by using suitable instrumental techniques. Eg. pH-Metry, Conductometry etc.

2. State and derive Beer's law.

Beer's Law

Equal changes in concentration of absorbing species in paths of constant length absorb equal fractions of the incident radiation.

OR

Equal fractions of the incident radiation are absorbed by successive layers of the medium containing equal concentration of absorbing species provided the layers have same thickness.

The decrease in the intensity of incident radiation due to absorption is directly proportional to the concentration of absorbing species.

Mathematically,

$$\frac{-dI}{I} = k_2\, dc$$

After integration,

$$-\int \frac{dI}{I} = \int k_2\, dc$$

3.

$$-\ln I = k_2\, c + C_2$$

$$\text{at } c = 0 \quad I = I_0$$

$$\ln I_0 = 0 + C_2$$

$$-\ln I = k_2\, c - \ln I_0$$

$$\ln \frac{I_0}{I} = k_2\, c$$

$$\log \frac{I_0}{I} = \frac{k_2}{2.303}\, c$$

Beer's Law Expression

4. State and derive Lambert's law

Lambert's Law

Successive layers of equal thickness of a light absorbing species (solution) absorb equal fractions of the incident radiation

OR

When a monochromatic radiation is passed through a light absorbing species (solution), the decrease in the intensity of radiation with thickness of the light absorbing species (solution) is directly proportional to the intensity of incident light

OR

~~Equal fractions of the incident radiation are absorbed by successive layers of equal thickness containing the same number of absorbing species~~

Derivation of Lambert's law

The radiation absorbed is directly proportional to the distance covered by the beam.

Mathematically, the law can be expressed as,

$$\frac{-dI}{I} = k_1\, dl$$

Here, **dI** is the decrease in the intensity of the beam of initial intensity $\mathbf{I_0}$ after passing through the solution of thickness *dl*.

Negative sign indicates the decrease in the intensity with increase in path length.

After Integration,

$$-\int \frac{dI}{I} = \int k_1\, dl$$

$$-\ln I = k l + C_1$$

where, C_1, is the constant of integration.

When $l = 0$ $I = I_0$ the intensity of the incident beam

$$-\ln I_0 = 0 + c$$

$$-\ln I = k_1 l - \ln I_0$$

$$\ln \frac{I_0}{I} = k_1 l$$

$$2.303 \log \frac{I_0}{I} = k_1 l$$

$$\log \frac{I_0}{I} = \frac{k_1}{2.303} l$$ ____ Lambert's Law Expression

5. State and derive Beer -Lambert's law

Beer-Lambert Law Statement

The Beer-Lambert law states that:

> for a given material sample path length and concentration of the sample are directly proportional to the absorbance of the light.

Combining Both Laws we will obtain expression for Beer-Lambert's Law

$$\log \frac{I_0}{I} = \frac{k_1}{2.303} l$$ ___ Lambert's Law Expression

$$\log \frac{I_0}{I} = \frac{k_2}{2.303} c$$ Beer's Law Expression

$$2.303 \log \frac{I_0}{I} = K.C.l$$

$$\log \frac{I_0}{I} = \frac{K}{2.303} C.l$$

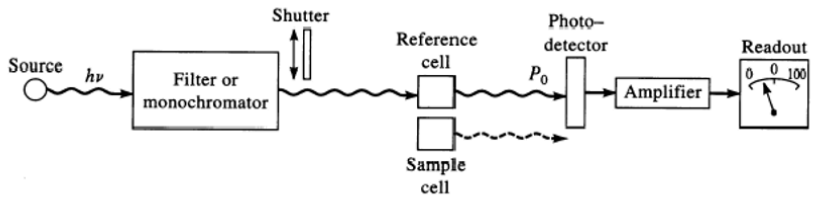
Where, $\log \frac{I_0}{I} = A$ ___ Absorbance

$\frac{K}{2.303} = \varepsilon$ ___ Molar extinction coefficient

$$A = \varepsilon.C.l$$

6. Explain the construction and working of a single-beam spectrophotometer with neat labelled diagram.

Single beam spectrophotometer



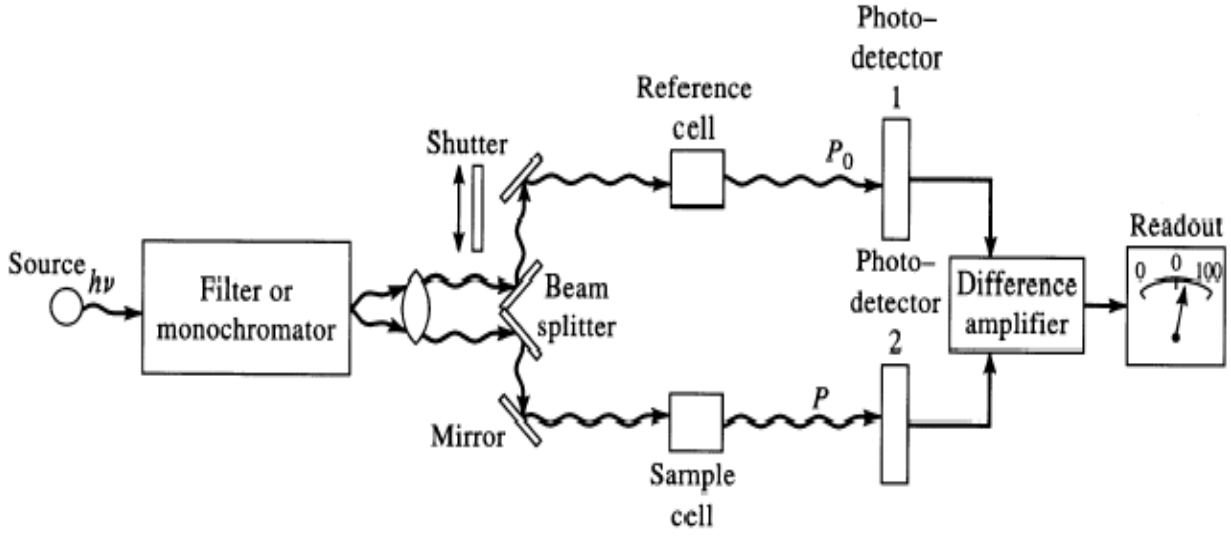
Construction:

- **Light source**
  - Deuterium and hydrogen lamps (190-400 nm)
  - Tungsten filament lamp (300-750 nm)
- **Sample containers**
  - Cuvettes (Quartz)
- **Mono-chromators**
  - Prisms can be used as mono-chromator
  - Diffraction gratings
- **Detectors**
  - Photomultiplier tube
  - Photodiode
  - Photodiode array

Working of Single beam spectrophotometer

- The instrument is useful for both Ultraviolet and Visible regions.
  - For UV light Deuterium lamps (190-400 nm)
  - For Visible light Tungsten filament lamp (380-750 nm) are used depending on the requirement.
- Light beam is focused on the mono-chromator, where after reflection and dispersion nearly monochromatic beam emerges out.
- This emergent monochromatic beam passed through a quartz cuvette containing a sample solution
- Transmitted radiation from the cuvette is allowed to fall on a photoelectric cell, which converts radiant energy into electrical signal as absorbance.
- Water is generally used as blank solution.

7. Explain the construction and working of a double-beam spectrophotometer with neat labelled diagram.



Construction:

- **Light source**
  - Deuterium and hydrogen lamps (190-400 nm)
  - Tungsten filament lamp (300-750 nm)
- **Sample containers**
  - Cuvettes (Quartz)
- **Beam splitters**
  - Mirrors
- **Mono-chromators**
  - Prisms can be used as mono-chromator
  - Diffraction gratings
- **Detectors**
  - Photomultiplier tube
  - Photodiode
  - Photodiode array

Working of Double beam spectrophotometer

- The instrument is useful for both Ultraviolet and Visible regions.
  - For UV light Deuterium lamps (190-400 nm)
  - For Visible light Tungsten filament lamp (380-750 nm) are used depending on the requirement.
- The variation in the intensity of the source light is compensated by splitting the incident beam into **two light beams** by passing through beam splitter.
- One of the beam passes through the blank solution while other through the sample solution.
- Transmitted radiations from the cuvette is allowed to fall on a photoelectric cell, which converts radiant energy into electrical signal as absorbance.
- Simultaneously, absorbance of blank and sample solution can be measured.
- Water is generally used as blank solution.

8. State the Applications of Beer -Lambert's law?

Application of UV-Visible Spectroscopy

- Quantitative determination of analyte concentration
- Identification of inorganic and organic species
- Magnitude of molar absorptivity
- Used as a detector in HPLC
- Used in semiconductor industry to measure thickness and optical properties of thin films.
- To study absorbance of organic compounds

9. State the advantages and limitations of UV-Vis spectrophotometery.

Advantages of UV-Vis Spectrophotometry

1. **Wide Range of Applications**: It is used in various fields such as chemistry, biology, environmental science, and pharmaceuticals for qualitative and quantitative analysis.
2. **High Sensitivity**: Can detect even low concentrations of analytes, making it ideal for trace analysis.
3. **Non-Destructive**: The sample is typically not altered or destroyed during analysis.
4. **Fast and Convenient**: Provides rapid results with relatively simple sample preparation.
5. **Versatile**: Applicable for both liquid and solid samples (with proper accessories like integrating spheres).
6. **Cost-Effective**: Instruments are generally affordable compared to other spectroscopic methods like NMR or mass spectrometry.
7. **Accurate and Reproducible**: With proper calibration and maintenance, it provides reliable and consistent results.

Limitations of UV-Vis Spectrophotometry

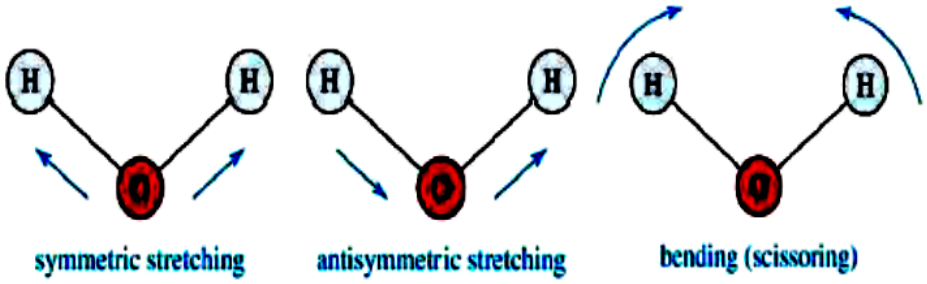
1. **Limited to UV-Vis Region:** Cannot analyze compounds outside the UV (200-400 nm) and visible (400-700 nm) spectrum.
2. **Interference from Other Species:** Overlapping absorption spectra from multiple components in a mixture can complicate analysis.
3. **Requires Transparent Samples:** Turbid or highly scattering samples can lead to inaccuracies unless special techniques are used.
4. **Solvent Effects:** The choice of solvent can influence absorption characteristics, requiring careful selection.
5. **Lower Specificity:** May not provide detailed structural information about a molecule compared to IR or NMR spectroscopy.
6. **Sample Limitations:** UV-absorbing impurities can interfere, and samples must be UV-active to be detected.
7. **Maintenance Needs:** Requires periodic calibration, lamp replacement, and careful handling to ensure accuracy.

10. What is fundamental modes of vibrations in IR spectroscopy?

Fundamental Modes of Vibration

- A **molecular vibration** is a periodic motion of the atoms of a molecule relative to each other, such that the center of mass of the molecule remains unchanged.
- The typical **vibrational frequencies**, range from less than 10^{13} Hz to approximately 10^{14} Hz, corresponding to wavenumbers of approximately 300 to 3000 cm^{-1}.
- In general, a non-linear molecule with N atoms has **$(3N - 6)$** normal modes of vibration, but a *linear* molecule has **$(3N - 5)$** modes, because rotation about the molecular axis cannot be observed.
- A diatomic molecule has one normal mode of vibration, since it can only stretch or compress the single bond.
- Vibrations of polyatomic molecules are described in terms of normal modes, which are independent of each other, but each normal mode involves simultaneous vibrations of different parts of the molecule.

VIBRATIONAL MODES



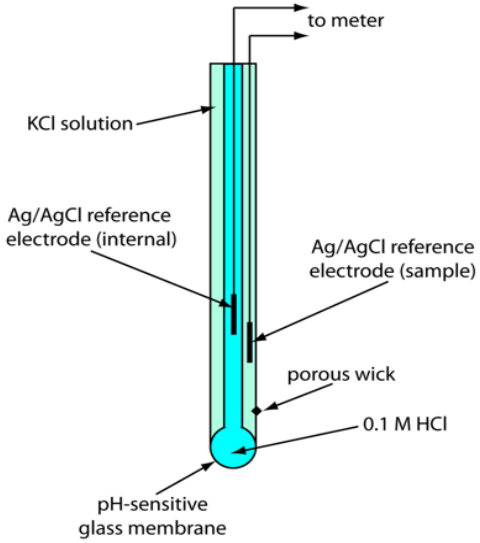
Stretching : in which the distance between the two atoms increases or decreases but the atoms remain in the same bond axis.
Bending: in which the position of the atom changes relative to the bond axis. Covalent bonds can vibrate in several modes, including stretching, rocking, and scissoring.

11. Discuss finger print region in IR spectroscopy with suitable examples.
    - IR is most useful in providing information about the presence or absence of specific functional groups.
    - IR can provide a molecular fingerprint that can be used when comparing samples. If two pure samples display the same IR spectrum it can be argued that they are the same compound.
    - Although the entire IR spectrum can be used as a fingerprint for the purposes of comparing molecules, the 600 - 1400 cm^{-1} range is called the fingerprint region.
    - This is normally a complex area showing many bands, frequently overlapping each other.
    - Examples: idk

12. Explain with the help of neat diagram construction and working of combined glass electrode in pH meter.

Ion Selective electrode

A **glass electrode** is a type of ion-selective electrode made of a doped glass membrane that is sensitive to a specific ion.



Construction:

It consists of glass membrane, it separates an internal solution and silver / silver chloride electrode from the studied solution

Ag|AgCl|HCl|glass||probed solution|reference electrode

$$E = E^0 - \frac{2.303RT}{F}\text{pH}$$

Applications:

Glass electrodes are commonly used for pH measurements. There are also specialized ion sensitive glass electrodes used for determination of concentration of lithium, sodium, ammonium, and other ions. Glass electrodes have been utilized in a wide range of applications — from pure research, control of industrial processes, to analyze foods, cosmetics and comparison of indicators of the environment and environmental regulations: a microelectrode measurements of membrane electrical potential of a biological cell, analysis of soil acidity, etc.

13. Calculate absorbance and molar absorptivity of KMnO4 solution having 3.5 x 10-4 g/litre concentration which absorbs 60 % of incident radiation at 545 nm of 1 cm path length cuvette. [Mol. Wt. = 158 g/mol]
14. Explain the principle of conductometric titration with suitable example.
    - Conductometric titration is a type of titration in which the electrolytic conductivity of the reaction mixture is continuously monitored as one reactant is added to the other.

Principle

- When solution of one electrolyte is added to another electrolyte, the conductance of the solution will alter, if an ionic reaction occurs.
- If no ionic reaction takes place then the conductance of the solution will simply increase.
- If an ionic reaction occurs, the ion added may replace another ion and hence bring about change in the conductance.
- Let A^+B^- be the ions of titrand and C^+D^- be ions of the titrant, the ionic reaction in the titration is combination of A^+ and D^-, AD formed may be insoluble or weakly ionized.

$$\mathbf{A^+B^- + C^+D^- \rightarrow AD + C^+B^-}$$

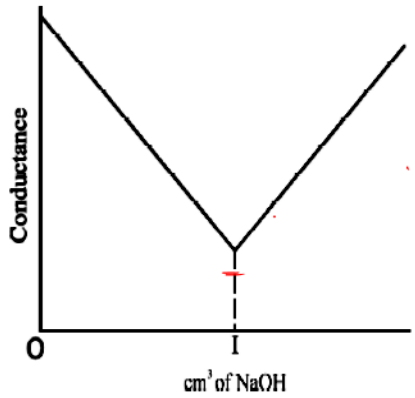
Principle

- Thus as the titration proceeds, A^+ are replaced by C^+. The conductance of the solution increases or decreases depending on whether conductance of C^+ is greater than or less than that of A^+. After equivalence point the ionic reaction does not occur and hence, the conductance of the solution will raise due the excess addition of titrant C^+D^-.
- The principle of conductometric titration is changes in the conductance of the solution due to difference in the ionic conductance or due to production of more number of ions in the solution.

Example:

Strong Acid with a Strong Base
[HCl with NaOH]

Before NaOH is added, the conductance is high due to the presence of highly mobile hydrogen ions. When the base is added, the conductance falls due to the replacement of hydrogen ions by the added cation as H^+ ions react with OH^- ions to form undissociated water. This decrease in the conductance continues till the equivalence point. At the equivalence point, the solution contains only NaCl. After the equivalence point, the conductance increases due to the large conductivity of OH^- ions



Conductometric titration of a strong acid (HCl) vs. a strong base (NaOH)

15. If the molar absorptivity of a given substance is 4700 dm3mol-1cm-1. The transmittance of this solution is 0.7 in the cell of path length 1 cm. calculate the concentration of the

solution. What will be the concentration of the solution if the transmittance will be 0.8 and the cell path length will be increased to 2 cm.

16. What is the condition for a molecule to be IR active? Explain with suitable examples. Give the IR frequency range for mid, far and finger print regions.\

Condition for a Molecule to Be IR Active

For a molecule to be **IR active**, it must exhibit a change in its **dipole moment** during the vibration of its bonds. When infrared radiation interacts with a molecule, only those vibrations that cause a fluctuating dipole moment can absorb IR radiation and contribute to the IR spectrum.

IR Active Molecule: Carbon Dioxide (CO_2)

- **Asymmetric Stretching:** The dipole moment changes during asymmetric stretching, so this vibration is IR active.
- **Symmetric Stretching:** No change in the dipole moment occurs during symmetric stretching, making it IR inactive.

IR Inactive Molecule: Diatomic Gases (e.g., O_2, N_2)

- **Reason:** Homonuclear diatomic molecules like oxygen and nitrogen are nonpolar and do not have a dipole moment. Their vibrations do not create any dipole change, making them IR inactive.

- Near IR 15000 cm^{-1} to 3000 cm^{-1}
- **Mid IR 4000 cm^{-1} to 400 cm^{-1}**
- Far IR 200 cm^{-1} to 10 cm^{-1}
- Most used 4000 cm^{-1} to 670 cm^{-1}

[Module-5] Computers and Chemistry

1. What is computational chemistry? State its advantages

- Computational chemistry is a branch of chemistry that uses computer simulations to assist in solving chemical problems. It incorporates methods of theoretical chemistry into computer programs to calculate the structures and properties of molecules, groups of molecules, and solids.

Advantage of Computational Chemistry

1) It allows the medicinal chemist for use the computational power of computer for measurement of

- Mol. geometry
- electron density
- electrostatic potentional
- conformational analysis
- different types of energies.

2) Determination of structure of ligand and target through X-ray crystallography and NMR spectroscopy.

3) Docking of ligand in rececpter active sites and exact measerment of geometric and energetic favor ability of such interaction.

4) Comparssion of various ligands throgth various parameters.

2. Describe various computational methods
    - **Refer pdf**
3. Discuss the various quantum mechanics methods

Quantum Mechanics Method

1. *Ab inito* method
2. Semiemperical method
3. Density functional theory

Ab Initio method

- *Ab initio* translated from Latin means from "first principles".
- This refers to the fact that no experimental data is used and computations are based on quantum mechanics.
- It derived directly from theoretical principle.

Semiempirical Method

This method simplifies quantum mechanics calculations by using empirical data. It blends theoretical principles with experimental results to approximate how electrons behave in molecules. Because it relies on parameters derived from experimental data, semiempirical methods require less computational effort than fully theoretical (ab initio) methods.

Density Functional Theory (DFT)

DFT is a quantum mechanical modeling method used to study the electronic structure of atoms, molecules, and condensed phases. It addresses the many-electron problem by using functionals, which are functions of the electron density. DFT strikes a good balance between accuracy and computational cost, making it a popular choice for examining large systems.

4. Elaborate on the scope of Cheminformatics and Bioinformatics

Scpoe in Cheminformatics

- CI is the latest area is now becoming a reality in India too
- Till data advance countries like US, UK, Japan and few European countries were working on this .
- In India CI is making inroad in Indian software, Department of Bio-Tech Govt of India , R& D organizations pharmaceuticals and other industries too.
- With thousands of jobs and crores of grants by Govt of India, CI professionals are growing day by day not only in India but also in abroad .
- CI companies are in great need of people with knowledge of chemistry and computer skills to handle the data generated by chemical researchers.

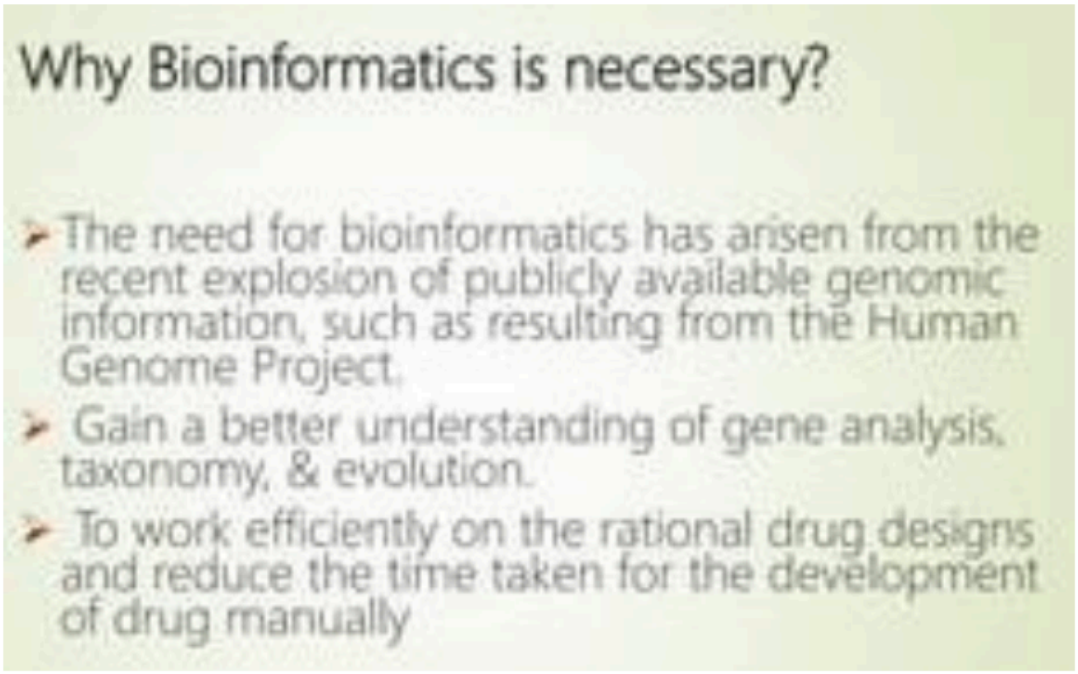
Chemical Information System(CIS)

- The main purpose of this is to identify a chemical substance, find compounds similar to the target compounds and demine the location of the compound, and it is an inventory system.
- **Chemical similarity** searching databases by chemical similarities is among the oldest and most useful techniques in molecular modeling as practiced by the pharmaceutical industry. It works because it is generally true that molecules with similar structure have similar biological activities

SCOPE:

- Bioinformatics consists of two subfields:
- The development of computational tools and databases.
- The application of these tools and databases in generating biological knowledge to beter understand living systems.

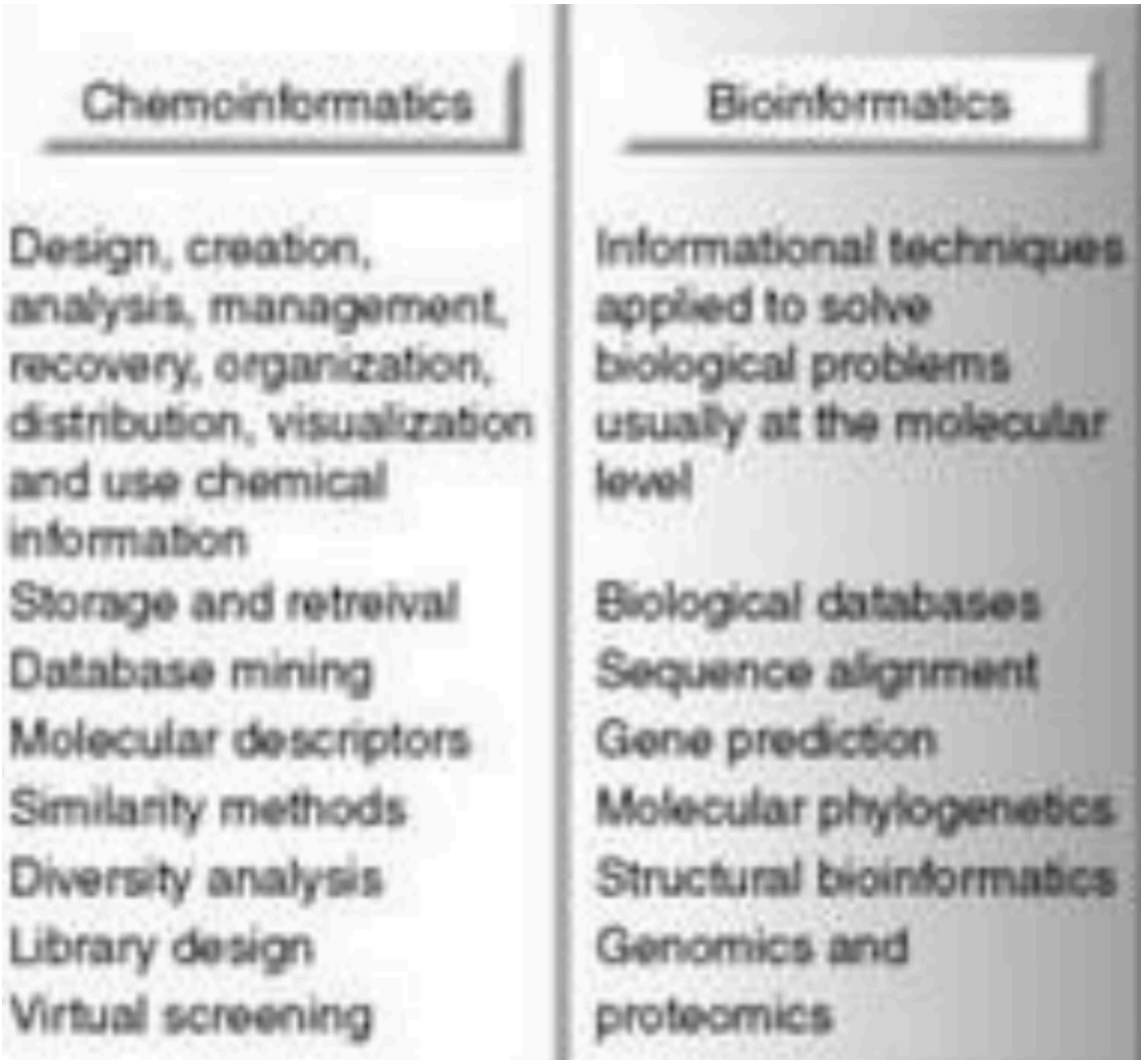
5. State the limitations and applications of Bioinformatics



LIMITATIONS

- Bioinformatics has a number of inherent limitations.
- Bioinformatics is by no means a mature field.
- Most algorithms lack the capability and sophistication to truley reflect the reality.
- Errors in sequence alignment, an affect the outcome of structural or phyligenetic analysis.
- Many accurate but exhausitive algorithms cannot be used because of the slow rate computation. Instead, less accurate but faster algorithms have to be used.
- IT IS A GOOD PRACTICE TO USE MULTIPLE PROGRAMS, IF THEY ARE AVAILABLE, AND PERFORM MULTIPLE EVALUATIONS.
- A MORE ACCURATE PREDICTION CAN OFTEN BE OBTAINED IF ONE DRAWS A CONSENSUS BY COMPARING RESULTS FROM DIFFERENT ALGORITHMS.

6. Distinguish between Cheminformatics and Bioinformatics



Cheminformatics	Bioinformatics
Design, creation, analysis, management, recovery, organization, distribution, visualization and use chemical information	Informational techniques applied to solve biological problems usually at the molecular level
Storage and retreival	Biological databases
Database mining	Sequence alignment
Molecular descriptors	Gene prediction
Similarity methods	Molecular phylogenetics
Diversity analysis	Structural bioinformatics
Library design	Genomics and proteomics
Virtual screening	

7. What is e-waste? elaborate on the various sources of e-waste

- **'E-Waste' is a term generally used for electrical and electronic appliances, gadgets, devices which are near or at the end of their useful life.**
- E-waste comprises of both hazardous and non-hazardous elements as their components.

Sources of E-waste

- Actually all humans are the source of E-waste. Technology has become a need now due to constant modernizing of technology with a very fast speed and for all of us to keep up with this quick change we have to keep throwing out the old electronic products and purchasing new products.
- In today's society it is necessary to have a laptop and phone, this leads to rapid growth of E-waste. Laptops and phones allow people to connect with the other parts of the world as well as to extend the knowledge. Printers, photocopiers and home equipment are there to make our life easier at the work place as well as home.
- Some of the products like refrigerators; televisions were once a lifetime purchase. Purchase a new one rather than repairing or upgrading old one which leads to 'replace-rather-than-repair' attitude.
- The accessibility of the latest technology plays a big part in increasing the amount of electronic waste. People are always keen to buy what is latest and the best in the market.
- Hence as the demand grows the production also grow which leads to produce a lot of electronic goods and hence the E-waste.

8. Discuss about the composition of e-waste

Composition of E-waste

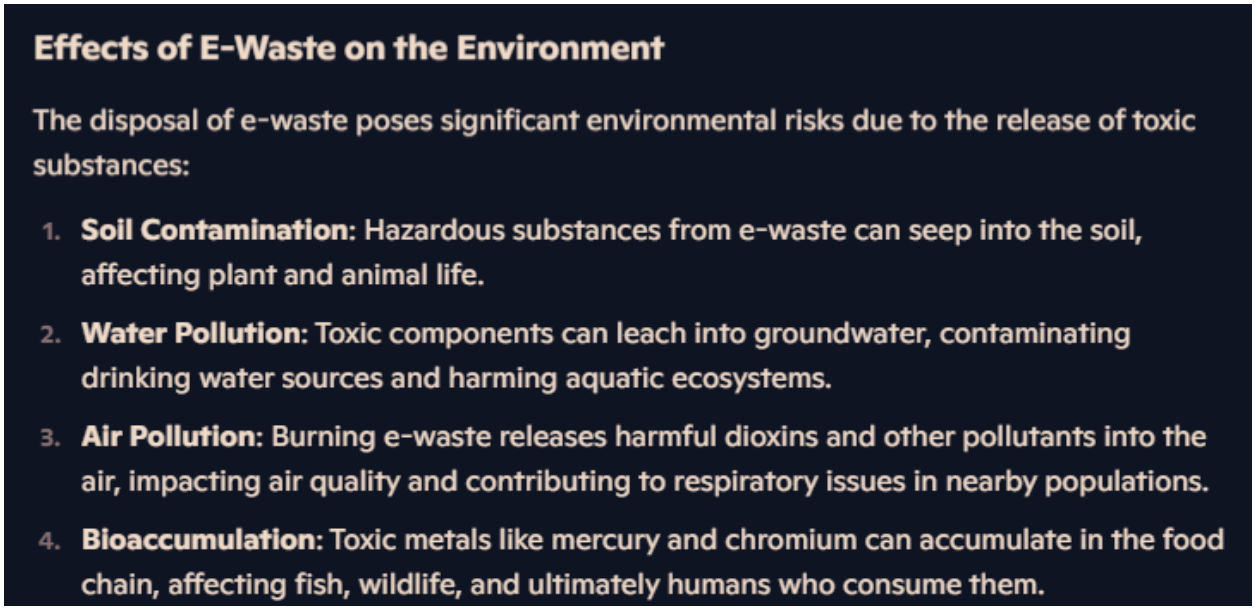
- E-waste contains all waste from electronic and electrical machines which have gotten end of their life period and are no longer suitable for their original future use and are intended for salvage, reprocessing or discarding.
- It comprises computer and its parts (like monitors, printers, keyboards, central processing units), typewriters, mobile phones and chargers, remotes, compact discs, floppies, headphones, batteries, LCD/Plasma TVs, air conditioners, refrigerators and many other household machines.
- It is very clear from the studies that most of the E-waste comes from computers, cell phones, TVs, Refrigerators and washing machines.
- If we know the composition of E-waste then it is easy to find the hazardous component of E-waste and metal retrieval from E-waste.
- So it is required to know about the composition of E-waste.

9. Describe the effects of e-waste on Human health and environment

Effects of E-Waste on Human Health

E-waste contains a multitude of hazardous materials that can seriously harm human health:

1. **Lead**: Found in printed circuit boards, monitors, and gaskets, it can affect the nervous system, cause kidney damage, and impair children's brain development.
2. **Cadmium**: Present in chip resistors and semiconductors, cadmium can accumulate in the kidneys and liver, causing irreversible damage and neural issues.
3. **Mercury**: Common in relays, switches, and circuit boards, mercury exposure can damage the brain and cause chronic neural issues.
4. **Chromium**: Used in galvanized steel and steel housing, it can lead to respiratory disorders and bioaccumulates in aquatic life.
5. **Plastics and PVC**: Present in cabling and computer housings, burning these materials releases dioxins, which affect reproductive and developmental health.
6. **Brominated Flame Retardants**: These disrupt endocrine system functions and are used in electronic equipment and circuit boards.
7. **Other Heavy Metals (Barium, Phosphorus, etc.)**: Found in CRTs, these materials can harm muscles, heart, liver, and spleen.
8. **Copper**: Used in wires and circuit boards, it can cause stomach cramps, nausea, liver damage, or Wilson's disease.
9. **Nickel**: Found in rechargeable batteries, nickel can trigger skin allergies and lung conditions like asthma.
10. **Lithium**: Present in lithium-ion batteries, it can harm nursing babies and cause lung problems when inhaled.
11. **Beryllium**: Used in motherboards, beryllium is carcinogenic and can cause lung cancer and chronic beryllium disease.



10. Need of E-waste Management

What is E- Waste Management?

E-Waste management is the art and science of efficacious and safe handling of the thousands of tonnes of extremely harmful electronic waste.

E-Waste is a gigantic problem already gaining momentum at a speed that is scary. Yet most of us aren't cognizant about its gravity. These reasons have given rise to the necessity of E-waste management.

E-waste management helps to recover and reprocess as much usable material as possible. It confirms that all the energy and water used to create these products is not totally futile.

It also scavenges for the rare metals, which are not replenish-able resources. Thus, E-waste management is not only advantageous but important.

Why E-Waste Management is Essential?

- Proper discarding of E-waste has become a priority. Many of us are not cognizant of the fact that electronic appliances like cell phones and computers actually comprise of many toxic substances that can leach out into the soil and cause harm to the environment.
- The problem has been increased so much because of the fact that the elements that are used in the fabrication of these electronics are usually quite expensive. Because of this reason, many leading companies often try to pull out these elements from the rejected electronics by using the ways that are unsafe.
- Heavy metals such as cadmium, lead, and mercury that are part of E-waste pose a great threat to the environment and human health.
- In addition to the toxins E-waste also contains the elements which take many years to biodegrade, which could mean that landfills with electronic waste could stay like that for centuries.
- According to the law, electronic waste matters can only be discarded in a landfill that is well-found to handle toxic substances. Many companies have started taking proper actions to significantly reduce the amount of E-waste that they produce.
- Producers of electronic items have started taking products back when they have outlived their usefulness. Producers safely remove elements like copper and other unsafe metals from the electronics and then dispose of the rest of the materials in a safe manner. Such actions need to be taken efficiently in other parts of the world.

11. Roles and Responsibilities of consumers / citizens in e-waste management

C. What Should Be The Responsibilities of the Consumers?

- Consumers can donate used electronic items; donating electronics for reuse extends the lives of valuable goods and also keeps them out of the waste management system for a longer time. Care should be taken while donating such products i.e. the products should be in working condition.
- Reuse of these products also benefits society. By donating the used electronics, many lower-income families can afford to use these devices that they otherwise could not pay for.
- E-wastes should never be dumped with the other household wastes. This should be separated and sold or donated to various organizations.
- While buying electronic products consumers can opt for those products which are made with fewer lethal substances, products which uses reprocessed content. Products which are energy efficient. Products which are easy to disassemble. Products which utilizes nominal packaging. Products which offer take back options. Products that have been certified by regulatory authorities.
- Consumers should opt for upgrading their computers or other electronic items to the modern version rather than purchasing new equipment.

12. Roles and Responsibilities of industries in e-waste management

B. What Should Be Responsibility and Role of Industries?

- It is a reverse fabrication system that designs infrastructure to recover and recycle every material confined within E-wastes metals such as lead, copper, aluminum and gold, and various plastics, glass and wire.
- Researchers have explained that such a closed loop production and recovery system offers a win-win state for everyone, a reduced amount of the earth will be mined for raw ingredients and groundwater will be protected.
- Producers, distributors and retailers should take the responsibility of recycling and disposal of their own products.
- Producers of computer monitors, TV sets and other electronic appliances containing harmful materials must be responsible for educating users and the general public regarding the potential danger to public health and the environment because of their products. For this all computer monitors, TV sets and other electronic devices containing harmful materials must be clearly labeled to mention the environmental hazards and proper materials management.
- Producers should provide contact details such as address, helpline numbers and e-mail Id of distributors and authorized collection centers so that consumers can return used electrical and electronic equipment.

13. Roles and Responsibilities of government in e-waste management

RESPONSIBILITIES & ROLES OF GOVERNMENT, INDUSTRIES & CITIZENS

It is imperative to adopt certain management options to handle the bulk E-wastes. Following are some of the suggested management options for the government, manufacturing industries and the public.

A. What Should Be the Responsibilities of Government to Reduce the E-Waste?

- Governments should set up regulatory organizations in each district, which are vested with the responsibilities of coordinating and consolidating the regulatory roles of the various government authorities regarding dangerous E-waste.
- Governments should be accountable for providing a satisfactory system of laws, controls and administrative processes for harmful waste management.
- Existing laws concerning disposal of E-waste should be reviewed and refurbished. A comprehensive law is required which provides E-waste regulation, management and proper disposal of unsafe wastes.
- Such a law should empower the agency to control, manage and regulate the related activities of government sectors.

- Under this law, the agency concerned should be to collect basic statistics of the materials from producers, processors and importers and to maintain a record of these materials, to identify harmful substances and industry should test them for adverse health and environmental effects, to control dangers from production, processing, distribution, use and dumping of electronic wastes, to encourage advantageous reuse of E-waste and encouraging commercial activities that use waste and to educate E-waste producers on reuse and recycling options.
- Governments should apply strict guidelines against dumping of E-waste in the country by outsiders. Where the laws are broken, stringent punishments must be imposed.
- Governments should enforce strict guidelines and heavy penalties charges on industries, which do not practice waste prevention and recovery in the manufacture facilities.
- Governments should encourage and support NGOs and other organizations to participate actively in solving the problem of E-waste.