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Indian Society of Analytical Scientists Delhi Chapter

e-Bulletin



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From Editor's Desk......

It is with great enthusiasm; we publish the second issue of the ISAS-DC e-Bulletin. Following the encouraging response to our inaugural we reaffirm our resolve to bring to the forefront the constantly changing scenario of the analytical sciences and to highlight the evolving landscape of analytical sciences and their impact on research, industry, and society at large. New horizons are being explored as interface between conventional methods and t echnological advances. Artificial Intelligence (AI), machine learning, automation are no longer buzzwords. Now these are among the tools employed to resolve intricate analytical issues. The applications are for predictive analysis, simulations, data interpretation and process optimization which continue to redefine benchmarks in laboratories and industries across globe. the One area that is changing very quickly is monitoring the environment.

With the emphasis on sustainability and climate change, Analytical tools are being used to measure air and water quality, monitor the pollutants, and shape data driven environmental policy. All these are necessary for a cleaner, healthier future for all. Green energy storage and conversion is the need of the hour. Modern devices store the charge efficiently and deliver high charge density as well as power density that can transform the EVs and other transport.

We would like to thank all contributors and readers who have supported this platform. We invite you to explore the contents of this issue and encourage your continued contributions, feedback, and collaboration. Together, let us inspire innovation, share knowledge and shape the future of analytical sciences in India and beyond.

Warm regards,

The Editorial Team

About ISAS - Delhi Chapter



Greetings from Indian Soceity of Analytical Scientists - Delhi Chapter.

ISAS-Delhi Chapter (www.isasdelhi.org), was established in 1992 with headquarters at Indian Oil R&D Centre, Faridabad, Haryana to promote the growth of analytical sciences in the northern part of our country. Delhi Chapter of ISAS covers Delhi, Chandigarh, Punjab, Haryana, UP, Uttranchal, Jammu & Kashmir and other contiguous area. Among the 12 chapters of ISAS all over India, ISAS-Delhi Chapter is one of the most active Chapter. At present Delhi Chapter itself has more than 1600 life members from more than 100 research institutes, national laboratories, universities, industry etc.

The Chapter has organized more than 60 technical programs like one / two / three -days technical Seminars / Symposia / Conference / Workshops on various contemporary topics of science at diverse locations like Shimla, Agra, Dehradun, Palampur, Rohtak, Faridabad, Delhi, Ballabgarh, Noida, Dharamshala, Leh/Ladakh. The society also organizes summer and winter workshops on various analytical techniques for the benefit of students, researchers and faculty members. ISAS-Delhi Chapter has been adjudged as the Best Chapter by the parent body four times in the past based on our activities to promote analytical science in the country. Our Chapter also provides partial financial assistance of Rs. 25,000/- to students to present research work in international conferences abroad. We have also initiated Lifetime achievement award and young researcher award once in 2 years.

ISAS Delhi Chapter provides a common platform for analytical scientists to exchange ideas, keep themselves abreast of the latest developments, thus promoting growth of analytical sciences in the country. ISAS-DC is now an established scientific forum with sound financial and intellectual backing. We invite all scientists and researchers in the field of science to be part of this professional scientific society and achieve excellence in your sphere of activity.

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ISAS- Delhi Chapter Award Announcement (2024)

Since 2022, ISAS-DC has initiated Lifetime Achievement Awards and Young Researcher Awards, which are conferred upon to a Scientist/Researcher/Technocrat/Academician, who has been life members of ISAS-DC for their outstanding achievements, accomplishments & contributions to the field of science especially analytical sciences. The awards are given once in 2-years, 2 Number of Lifetime Achievement Awards (1 from academia and 1 from Industry) and 2 number of Young Researcher Awards (1 from academia and 1 from Industry).

For 2024 awards, applications were called recently and the status of applications received are as under:

Category	Lifetime Achievement Award	Young Researcher Award
Industry	6	3
Academia	2	7
Total	8	10

The composition of the Jury is as follows:

- 1. Prof K. K. Pant, Director- IIT, Roorkee
- 2. Dr Harinder Bist, Director- CSIR-IIP, Dehradun
- 3. Prof. S K Mehta, Panjab University, Chandigarh & former VC, University of Ladakh
- 4. Mr. S. K. Bose, CEO, Hydrocarbon Sector Skill Council

The Jury selected the following for the awards:

Category	Lifetime Achievement Award	Young Researcher Award
Industry	Dr. Anurag Ateet Gupta Advisory Board Member Indian Association of Nanoscience & Nanotechnology	Dr Sujit Mondal Indian Oil R&D Centre Faridabad
Academia	Prof. M Sarwar Alam Pro VC, Al-Karim University Katihar	Prof. Bhubaneswar Mandal Indian Institute of Technology Guwahati

ISAS- Head Quarter Award Announcement (2024)

Best Performance Award

Dr Ravindra Kumar Indian Oil R&D Centre Faridabad

Best Scientist Award

Dr J Christopher
Hindustan Petroleum Green R&D Centre
Bangalore

Hearty congratulations to all award winners

Editorial Series

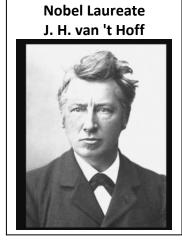
Nobel Laureate

First Nobel Prize in Chemistry (1901) Jacobus Henricus van 't Hoff: A Pioneer of Physical Chemistry

First Nobel Prize in Chemistry was awarded in 1901, and the awardee was Jacobus Henricus van 't Hoff of the Netherlands. He received the prize for his discovery of "the laws of chemical dynamics and osmotic pressure in solutions."

About Jacobus Henricus van 't Hoff: A Journey

Jacobus Henricus van 't Hoff (1852-1911) was a brilliant Dutch physical chemist who laid much of the foundational groundwork for modern physical chemistry. His work bridged the gap between physics and chemistry, bringing rigorous mathematical and thermodynamic principles to the understanding of chemical phenomena. Jacobus Henricus van 't Hoff



was born in Rotterdam, TheNetherlands, on August 30, 1852. He was the third child in a family of seven children of Jacobus Henricus van 't Hoff, a physician, and Alida Jacoba Kolff. After his attaining large part of the curriculum, he returned to Holland in 1874 and obtained his doctor's degree that same year under E. Mulder in Utrecht.

In 1876 he became lecturer at the Veterinary College at Utrecht, but left this post for a similar position at the University of Amsterdam the following year. In 1878 came his appointment as Professor of Chemistry, Mineralogy, and Geology at the same university. After having occupied this chair for 18 years he accepted an invitation to go to Berlin as Honorary Professor, connected with a membership of the Royal Prussian Academy of Sciences. At his new post he remained till his last breath i.e. on March 1, 1911, at Steglitz near Berlin, Germany.

Achievements: Peeping into the past

Of the numerous distinctions he himself mentioned the award of the first Nobel Prize in Chemistry (1901) to him as the culmination-point of his career. In 1885 he was appointed member of the Royal Netherlands Academy of Sciences, after his nomination had been withheld in 1880 because of an insufficient number of votes – a proof that his ideas initially found little acceptance in his own country. Among his other distinctions were the honorary doctorates of Harvard and Yale (1901), Victoria University, Manchester (1903), Heidelberg (1908); the Davy Medal of the Royal Society (1893), Helmholtz Medal of the Prussian Academy of Sciences (1911); he was also appointed Chevalier de la Legion d'Honneur (1894), Senator der Kaiser-Wilhelm-Gesellschaft (1911). He was also memberor honorary member of the Chemical Society, London (1898), Royal Academy of Sciences, Gottingen (1892), American Chemical

Society (1898), Académie des Sciences, Paris (1905). In 1887, he, alongwith Ostwald, founded the influential journal Zeitschrift für Physikalische Chemie (Journal of Physical Chemistry), which became a crucial platform for the dissemination of research in this emerging field.

Key Achievements and Contributions:

Stereochemistry (1874):

- ➤ One of his earliest and most groundbreaking contributions was the development of the theory of the tetrahedral carbon atom. Independently, and almost simultaneously, with Noble LaureateJ. H. van 't Hoff French chemist Joseph Le Bel, van 't Hoff proposed that the four valencies of a carbon atom are directed towards the corners of a tetrahedron.
- ➤ This revolutionary concept explained the phenomenon of optical isomerism (chirality) in organic compounds, where molecules have the same chemical formula but different spatial arrangements that cause them to rotate plane-polarized light in opposite directions. It provided a three-dimensional understanding of molecular structure, which was crucial for the development of organic chemistry.

Chemical Dynamics and Equilibrium (1884):

Van 't Hoff's seminal work, "Études de Dynamique chimique" (Studies in Chemical Dynamics), published in 1884, was a landmark in the field of chemical kinetics. He applied the principles of thermodynamics to chemical reactions, demonstrating how the rates of reactions are influenced by factors like temperature and concentration. He introduced concepts such as chemical affinity and showed how the equilibrium constant for areversible reaction changes with temperature, leading to the famous van 't Hoff equation (relating the equilibrium constant to temperature and enthalpy change:

$$\frac{d(\ln K)}{dT} = \frac{\Delta H^{\circ}}{RT^2}$$

This equation is fundamental to understanding how chemical equilibria respond to temperature changes. He also developed a graphical method for determining the order of a chemical reaction.

Osmotic Pressure in Solutions (1886):

Van 't Hoff conducted extensive research on the behaviour of dilute solutions, particularly focusing on osmotic pressure. He remarkably demonstrated a profound similarity between the behaviour of dilute solutions and ideal gases. He derived the van 't Hoff equation for osmotic pressure (Pi (π) = iMRT), which is analogous to the ideal gas law (PV = nRT). Here, π is osmotic pressure, M is molarity, R is the gas constant, T is absolute temperature, and i is the van 't Hoff factor (accounting for the dissociation of

solutes into ions). This work was crucial in establishing the thermodynamic validity for solutions and provided a powerful tool for determining the molecular weights of solutes.

Founding of Physical Chemistry:

Van 't Hoff, along with Wilhelm Ostwald and Svante Arrhenius, is considered one of the founders of physical chemistry as a distinct scientific discipline.

Later Work on Oceanic Salt Deposits:

After moving to Berlin in 1896, van 't Hoff applied his understanding of chemical equilibria to practical problems, and his work on the study of the Stassfurt salt deposits in Germany had significant implications for the chemical industry.

Nobel Prize Recognition:

Conferring Nobel Prize in 1901 was a testament to the profound impact of his work in establishing quantitative laws for chemical processes, particularly his insights into chemical dynamics and the properties of solutions, paving the way for countless advancements in various fields.

Future Energy Storage and Conversion Device, Supercapacitor

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Abstract:

Energy storage and conversion is required for performing day to day activities as well as for enhanced applications like satellite launch and in hybrid vehicles. We generally use battery as main source of energy. But battery suffers with many problems that majorly include its fast discharging and less shelf life. In spite of storage of lot of energy in the batteries, we cannot use it where high power density is required. Supercapacitors have high power density, high efficiency, and extended shelf and cycle life than normal batteries and that's why they are used as efficient device for energy conversion and storage. There are various materials that can be used as active electrode material for supercapacitor device. Some of them are Metal Oxides, Carbon Materials and its other forms, Conducting Polymers and Composite materials. This article describes how an Electrochemical Supercapacitor store charge, its applicability, various materials used for developing supercapacitor and its future scope.

Introduction:

Many applications, such as standby power systems, electric/hybrid automobiles, and telecommunication devices, require electrical energy storage [1–3]. There are two ways to store this electrical energy: indirectly in batteries and directly using a mechanism known as non-faradaic electrical energy storage, which involves negative and positive charges on a capacitor's plate [4]. Due to specific constraints, simple energy and simple capacitors cannot be employed in applications where a considerable amount of energy is required. As a result of these constraints, high power energy storage systems such as high power batteries and high power electrochemical capacitors were developed. The electrochemical capacitor is the more practical of these two high power energy storage devices.

A battery's compact size and weight allow it to store a lot of energy. However, the cycle life of batteries is quite short and varies depending on the kind of battery. Therefore, electrochemical capacitors are being developed to get around this restriction. Compared to batteries, these capacitors are far more powerful and have a longer cycle life. However, the low energy density of these capacitors dictates their employment in a specific high power application. Due to self-discharge and corrosion, the majority of secondary batteries will deteriorate significantly and become nearly unusable after many months of being stored unused. Over time, electrochemical capacitors will self-discharge to low voltage, but they will still be able to recharge to their initial state since they will still have capacitance. With only a minor change in characteristics, an electrochemical capacitor can undergo deep cycling at high speeds for 500,000–1,000,000 cycles. On the other hand, batteries cannot accomplish this [5].

For a given application, electrochemical capacitors have high power density, high efficiency, and extended shelf and cycle life than normal batteries. Their low energy density, which restricts their usage to specific applications where a tiny amount of energy is needed before the electrochemical capacitor can be charged, is their main drawback. Table 1 under illustrates significant advantages and disadvantages of both, the supercapacitor and battery.

Table 1: Advantages and Disadvantages of Battery and Supercapacitor

Battery		Supercapacitor		
Advantage	Disadvantage	Advantage	Disadvantage	
Fixed Output Voltage	Thermal Sensitivity	Good Thermal Stability	Less Energy Density	
Low Energy Density	Short Service Life	High Life Span	Rapid Self Discharge	
Low Self Discharge	Slow Charge and	High Current and Fast	Consistent Voltage	
	Discharge Rate	Charging	Discharge	

Principle and Mechanism:

A basic capacitor uses a dielectric substance sandwiched between two metal electrodes to store energy. Q = C is the fundamental equation and the another equation is C = KA/D where A is surface area, D is thickness, K is the dielectric constant, Q is charge and the C is capacitance. The energy stored in a capacitor is given by the equation 1/2CV² where V is the voltage between two plates. Similar to how a battery stores energy, so does an electrochemical capacitor. Two solid electrodes submerged in a liquid electrolyte make up an electrochemical capacitor. Materials with a large surface area and high porosity, such as carbon nanotubes, are used to produce these solid electrodes. An ionic conductor separates these electrodes, which have a somewhat larger surface area. The interface between the liquid electrolyte and solid electrode is where the charge is kept. The charge storage equation is identical to that of a basic capacitor. The following is an explanation of the charge and discharge mechanism. Electrons begin to move when a battery is coupled to a capacitor. Because of its negative charge, the electron moves toward the battery's positive end and the power source. Consequently, an electron excess forms at the negative site, which becomes negatively charged, and an electron deficit forms at the positive side, which becomes positively charged. Until the potential difference between the two electrodes equals the battery voltage, this electron flow will continue. Capacitor charging is the term for this process. When the battery is disconnected, electrons travel from the side with excess electrons to the side with insufficient electrons. Capacitor discharging is the term for this procedure [6-7]. It is appropriate to talk about double layers and pseudocapacitance separately when discussing the energy storage process in supercapacitors.

Double Layer Capacitor:

Charge separation in the double layer that forms at the interface between the liquid electrolyte in electrode micropores and the solid electrode material surface is how energy is stored in double layer capacitors [5]. The electrode material, surface area, and pore size all affect a double layer capacitor's capacitance. As was previously said, C = KA/D, in other words, capacitance is also influenced by the thickness and dielectric constant. Therefore, the double layer's thickness must be minimal for high capacitance values. A significant portion of the pore volume of porous carbon used in ultracapacitors should be found in

pores with a diameter of 1–5 nm. A lower capacitance is displayed by materials with smaller pores. According to the charge storage method, there are primarily two types of double layer capacitors which are explained in details as under [5,7,8].

Electrical Double Layer Capacitor:

One type of battery is an electric double layer capacitor, EDLC [9]. Two polarizable electrodes, a current collector, a separator, and a liquid electrolyte are all components of an EDLC. In EDLC, carbon is often utilized as the electrode material. In EDLC, several kinds of carbon, including as carbon aerogel, activated carbon, and carbon nanotubes, can be utilized as electrode materials [10]. The kind of electrolyte also affects the carbon electrode's electrochemical capacitance in EDLC. The list of several carbon types that have been tested as electrodes in EDLCs is as follows: Hallocyte templated porous carbon, multibranched porous nanofiber, nanostructured graphite, bamboo-based activated carbon, woven cloth, carbon nanotubes, nanostructured mesoporous carbon, activated carbon nanotube, polymer/carbon composites, multiwalled and single-walled carbon nanotube, carbon nanotube/activated carbon, CNT array, and double-walled CNT/activated carbon [11-12]. Figure 1 given below is the schematic representation of an electrochemical double layer capacitor (A) and a pseudocapacitor (B) [13].

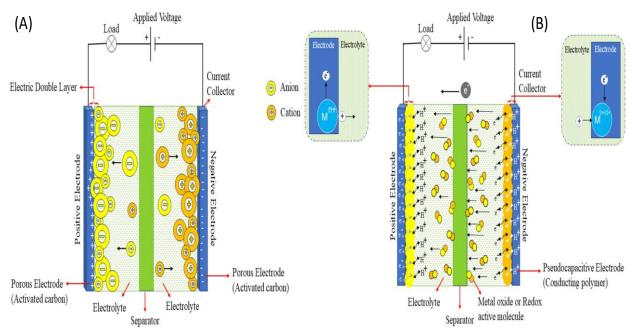


Figure 1. Schematic Representation of Electrochemical Double Layer Capacitor and Pseudocapacitor [13]

Pseudocapacitors:

Other names for this include pseudocapacitor, supercapacitor, and ultracapacitor. Carbon-based EDLCs have a lower specific storage energy, which is their primary drawback. Hence, pseudocapacitors are created to get over this drawback. Metal oxide capacitors and conducting polymer capacitors are the two primary groups into which we may separate capacitors using pseudocapacitance.

Surface-treated carbons have been used in some work on ultracapacitors that use pseudocapacitance, although mixed metal oxide material has been used in the majority of these studies [14-15]. RuO₂ is the most promising metal oxide for such supercapacitor. However, the high price of ruthenium has led to a quest for other metal nitrides and oxides [16-17]. The scarcity of ruthenium metal is another factor driving the hunt for alternative metal oxides.

Other metal oxides such as NiO, Ni(OH)₂, MnO₂, Co₂O₃, IrO₂, FeO, TiO₂, SnO₂, V₂O₅, and MoO can be utilized as materials for supercapacitor applications. Mixed metal oxide, metal oxide with a large surface area conducting substance, and numerous organic electrolytes are the subjects of ongoing study in this area. In organic electrolytes like V₂O₅, some researchers have done a fantastic job combining Carbon Nanotube (CNT) with a variety of metal oxides. Pseudocapacitor applications benefit from thin layers on conductive materials, such as carbonaceous materials. Numerous metal oxides, including tin oxides, nickel oxides, and many more, have literature accessible. Manganese oxide has a sp. capacitance of up to 600F/g for thin films and 150–300F/g for powder-based electrodes in aqueous electrolytes, making it another material that shows promise for supercapacitor applications. For MnO₂ as a higher sp. capacitance and material for supercapacitor, there is a wealth of further information accessible. Many transition metal oxides are being researched for use as electrode materials for supercapacitors because they are rare, inexpensive, and have high sp. Capacitance [16-23].

For the supercapacitor, electronically conducting polymers (ECP) like polyaniline, polypyrrole, polythiophene, and their derivatives are suitable materials [24]. These conductive polymers are less costly than metal oxides and activated carbon. ECP has the benefit of forming a thin layer across a large portion of the substrate. Furthermore, the ECP can hold the charge across their full volume because to their electrochemical feature of quickly reversible doping and dedoping ability [9]. Figure 2 below is the schematic representation of a Supercapacitor [13].

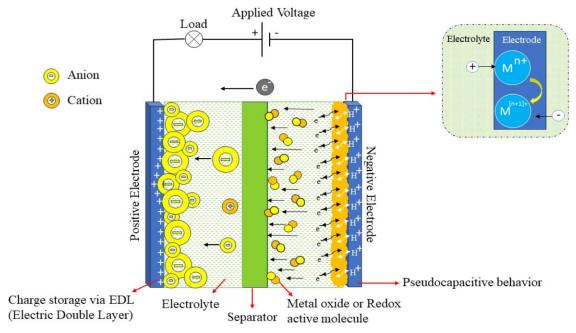


Figure 2: Schematic representation of a Supercapacitor [13]

Because the redox site in the polymer backbone is not robust enough for several repeated redox processes, ECP has drawbacks such as a shorter cycle life and sluggish ion transport. Nevertheless, this ECP displays an extremely high sp. capacitance value of up to 588F/g at a scan rate of 30mvs, as reported by J.H. Kim et al. for Polypyrrole (PPY) coated on VGCF [24] and 1600F/g for polyaniline by S.K. Mondel et al [25]. Therefore, we may conclude that ECP serves as a useful resource for supercapacitors.

Hybrid capacitors are those that have a double-layer material on one electrode and pseudo-capacitance material on the other. Nickel oxide was employed as a pseudo capacitance material in the majority of hybrid capacitors. These hybrid capacitors have a much higher energy density than double layer capacitors, but they have very nonlinear charge/discharge characteristics. Additionally, two dissimilar mixed metal oxides or doped conducting polymer materials can be used to build these capacitors [5].

Applications of Supercapacitor:

Applications needing short power bursts are well suited for supercapacitors, often referred to as ultracapacitors, which are energy storage devices with a high rate of energy storage and release. They are perfect for a variety of applications in many industries due to their special qualities, which include high power density, long cycle life, and quick charge/discharge times. The following as given in figure 3 are some important applications for supercapacitors:

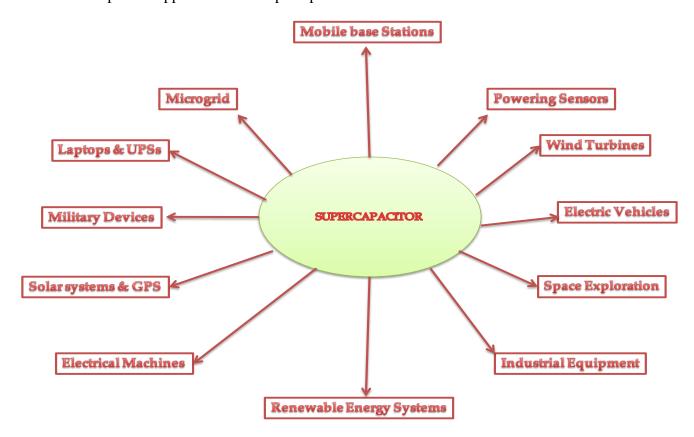


Figure 3: Applications of Supercapacitor

Future Plan:

Explosive growth in electronic equipments and the urgent need for the electric and hybrid electric vehicle based green transportation demand for the high power and high energy storage devices. The super capacitors are very attracting energy storage device in this regards. They also have advantages over batteries and conventional capacitors by their high power density and longer shelf and cycle life. The projected development in the energy density should open new market for super capacitor if their price can also be significantly reduced. The price can in turn be reduced by using low cost electrode material. In future work is going on how to increase the energy density and power capability. This can be done by using carbon with higher specific capacitance and by reducing the cost of collector and binder which binds the carbon to the substrate. We can also increase the energy density by increasing the cell voltage but it can be done by changing the electrolyte. The power capability can also be increased by reducing the specific resistance of the cell. This can also be achieved by reducing the time constant. One such method by which we can reduce the time constant is to decrease the thickness of the electrode which also reduces the specific resistance.

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Uncharted Territories: Novel Raw Materials for Biofuel Exploration

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SUMMARY:

Biofuel production has traditionally relied on conventional raw materials such as crops, vegetable oils, and organic waste. However, to expand the sustainability and efficiency of biofuel production, researchers are now exploring novel and unconventional sources. This article provides an overview of these uncharted territories in biofuel exploration.

The article begins by highlighting the importance of biofuels in reducing greenhouse gas emissions and promoting sustainable energy practices. It emphasizes the need for diverse raw materials to minimize waste and maximize resource efficiency. Conventional raw materials like corn, soybean oil, and animal fats are discussed as crucial feedstocks for biofuel production.

The article then delves into innovative raw materials that have already shown promise in biofuel production. These include algae, cellulosic biomass, waste biomass, lignocellulosic sugars, municipal solid waste, waste carbon dioxide, and seaweed. Each raw material is described in terms of its growth characteristics, conversion processes, and environmental benefits.

Moreover, the article introduces exotic examples of raw materials that have demonstrated potential for biofuel production. These include camelina, jatropha, pongamia, tung tree, mahua, and sugar beet. The unique properties and adaptability of these raw materials make them valuable resources for sustainable biofuel production.

In addition, the article highlights raw materials that have not been extensively explored but show potential for future exploration. These include seawater-grown crops, aquatic microorganisms, invasive plant species, agricultural residues from specialty crops, microalgae consortia, waste from insect farming, and microbial electrosynthesis. These untapped resources offer new opportunities to expand the biofuel feedstock options.

Furthermore, the article presents other rare raw materials that have the potential for biofuel production. These include carbon dioxide from air capture, industrial emissions from steel or cement production, plastic waste, algal blooms, atmospheric nitrogen, volatile organic compounds, and even extra-terrestrial

resources such as lunar regolith or Martian soil. While these materials require further research and development, they offer innovative possibilities for biofuel production and environmental sustainability.

BACKGROUND: Biofuels, including ethanol, biodiesel, and biomethane, are derived from a variety of organic raw materials. Ethanol is produced through the fermentation of sugars found in crops like corn or sugarcane. Biodiesel is derived from vegetable oils, such as soybean oil or rapeseed oil, as well as animal fats like tallow or poultry fat. Biomethane, on the other hand, is generated through the anaerobic digestion of organic waste materials like agricultural residues, food scraps, and sewage sludge.

These raw materials serve as crucial feedstocks for biofuel production. By utilizing crops, vegetable oils, animal fats, and organic waste, biofuels offer renewable alternatives to fossil fuels. They enable the efficient conversion of organic matter into energy, reducing greenhouse gas emissions and promoting sustainable energy practices. Moreover, the use of these diverse raw materials helps to minimize waste and maximize resource efficiency.

Overall, biofuels demonstrate the potential to address environmental concerns, reduce dependence on finite resources, and contribute to a more sustainable and environmentally friendly energy landscape. This article attempts to break the boundaries and explore unconventional sources for sustainable biofuel production, apart from a peep into the conventional sources of biofuel production.

CONVENTIONAL RAW MATERIALS FOR MAKING BIOFUELS:

Here are some examples of conventional raw materials that have shown potential for biofuel production:

- 1. <u>Camelina</u>: Camelina sativa, also known as false flax or gold-of-pleasure, is an oilseed crop that has gained attention as a potential feedstock for biofuel production. It is a drought-tolerant plant that can grow in marginal lands with limited water and fertilizer requirements. Camelina seeds contain oil that can be processed into biodiesel, making it a promising alternative to conventional oilseed crops. [Ref: Valorization of camelina oil to biobased materials and biofuels for new industrial uses: a review by Muhammad Arshad a, Amar K. Mohanty, Rene Van Acker, Rachel Riddle, Jim Todd, Hamdy Khalil and Manjusri Misra, RSC Adv., 2022, 12, 27230-27245; Camelina sativa, a short gestation oilseed with biofuel potential: **Opportunities** for Indian Ankur Agarwal, Om Prakash, Madhu Bala, Oil Crop Science, Vol 6, Issue 3, July 2021, Pages 114-121]
- 2. <u>Jatropha</u>: Jatropha curcas is a tropical plant that produces oil-rich seeds suitable for biofuel production. It can thrive in poor soil conditions and is not a food crop, reducing concerns about competing with food production. Jatropha oil can be converted into biodiesel, and the plant's ability to grow in arid regions makes it an attractive option for biofuel production in dry climates.
- 3. <u>Pongamia</u>: Pongamia pinnata, also known as Indian beech, is a leguminous tree native to tropical and subtropical regions. Its seeds contain oil that can be processed into biodiesel. Pongamia trees can grow in various types of soils, including marginal lands, and they have nitrogen-fixing properties that

- improve soil fertility. The tree also produces non-edible oil, reducing concerns about diverting food resources for fuel production.
- 4. <u>Tung Tree</u>: The tung tree (Vernicia fordii) produces seeds rich in tung oil, which has been traditionally used in industrial applications. However, tung oil can also be processed into biodiesel. The tung tree is adaptable to different soil types and can tolerate drought conditions. Its cultivation for biofuel production can provide economic opportunities for regions where the tree is native or suitable for growth.
- 5. <u>Mahua</u>: Madhuca longifolia, commonly known as mahua, is a tree native to the Indian subcontinent. The seeds of the mahua tree contain oil that can be used for biofuel production. Mahua is a fast-growing tree that can tolerate a wide range of soil conditions. Its cultivation for biofuel purposes can also provide livelihood opportunities for rural communities in India.
- 6. <u>Sugar beet</u>: Sugar beet is primarily cultivated for sugar production, but it also has potential as a raw material for bioethanol production. The sugar-rich beets can be processed to extract sugars, which can then be fermented and converted into bioethanol. Utilizing sugar beet for biofuel production diversifies the feedstock options and reduces reliance on traditional crops like corn or sugarcane.
- 7. <u>Used Cooking Oil</u>: The utilization of used cooking oil as a raw material for biofuel production offers several benefits. Recycling waste cooking oil reduces landfill waste and promotes sustainable waste management. Biofuels derived from this oil are renewable energy sources, reducing greenhouse gas emissions and dependence on non-renewable resources. They also have a lower carbon footprint compared to fossil fuels. The economic advantages include job creation in the recycling sector and energy security by reducing reliance on imported fuels. This process aligns with the principles of a circular economy, closing the loop on waste and creating a valuable resource. Overall, using used cooking oil for biofuel production contributes to environmental sustainability, energy efficiency, and a greener future.

These examples showcase the diversity of potential raw materials for biofuel production. Exploring and harnessing the unique properties and adaptability of these materials have contributed to the sustainable production of biofuels worldwide.

INNOVATIVE RAW MATERIALS FOR MAKING BIOFUELS:

There are several innovative raw materials being explored and used for making biofuels. Here are some of the most notable ones:

- 1. <u>Algae</u>: Algae are microscopic organisms that can convert sunlight, carbon dioxide, and nutrients into lipids or oils, which can be used to produce biofuels such as biodiesel or bioethanol. Algae have high growth rates and can be cultivated in various types of water, including wastewater or seawater, making them a promising source of biofuels.
- 2. <u>Cellulosic biomass</u>: Cellulosic biomass refers to non-food plant materials, such as agricultural residues (corn stover, wheat straw), forestry residues (branches, bark), and dedicated energy crops (switchgrass, miscanthus). These materials contain cellulose, hemicellulose, and lignin, which can be converted into biofuels through processes like biochemical conversion or thermochemical conversion.

- 3. <u>Waste biomass</u>: Various types of waste biomass can be utilized for biofuel production. This includes food waste, animal manure, sewage sludge, and other organic waste materials. Anaerobic digestion and fermentation processes can convert these wastes into biogas or bioethanol, providing a sustainable way to manage and utilize organic waste.
- 4. <u>Lignocellulosic sugars</u>: Lignocellulosic sugars are derived from the breakdown of lignocellulosic biomass, such as agricultural residues and dedicated energy crops. These sugars can be converted into biofuels through processes like fermentation or chemical conversion. Advances in pre-treatment technologies have made the extraction of lignocellulosic sugars more efficient and cost-effective.
- 5. <u>Municipal solid waste (MSW)</u>: MSW is the waste generated from households, businesses, and institutions. It contains organic materials that can be converted into biofuels through processes like anaerobic digestion or gasification. MSW can serve as a renewable feedstock to produce biogas, bioethanol, or bio-oil.
- 6. Waste carbon dioxide (CO₂): Carbon dioxide emitted from industrial processes can be captured and used as a raw material for biofuel production. By utilizing microorganisms or chemical catalysts, CO₂ can be converted into biofuels like methane or methanol. This approach helps reduce greenhouse gas emissions while producing valuable energy carriers.
- 7. <u>Seaweed</u>: Seaweed, also known as macroalgae, can be cultivated in oceans or coastal areas, and used for biofuel production. It grows rapidly and does not compete with food crops for land or freshwater resources. Seaweed can be processed into biofuels such as biogas, bioethanol, or bio-oil, and it has the additional benefit of absorbing carbon dioxide during growth.

These are just a few examples of the innovative raw materials being explored for biofuel production. Continued research and development in this field are likely to uncover even more sustainable and efficient sources of biofuels in the future.

RAW MATERIALS WHICH ARE NOT SO FAR MUCH EXPLOITED FOR MAKING BIOFUELS:

Here are some raw materials that have not been extensively exploited for biofuel production but show potential:

- Industrial waste streams: Various industrial processes generate waste streams that contain organic
 materials. These waste streams, such as food processing waste, brewery waste, or agricultural
 processing residues, can be explored as potential feedstocks for biofuel production. By converting
 these waste streams into biofuels, industries can achieve both waste management and renewable
 energy goals.
- 2. <u>Microorganisms</u>: Microorganisms other than algae can be harnessed for biofuel production. For example, bacteria and fungi with unique metabolic capabilities can be engineered or optimized to convert specific organic substrates into biofuels. These include bacteria that produce bioethanol from lignocellulosic sugars or fungi that generate biodiesel precursors from agricultural residues.

- 3. <u>Carbon-rich waste gases</u>: In addition to waste CO₂, other carbon-rich waste gases can be utilized for biofuel production. For instance, methane emitted from landfills or anaerobic digesters can be captured and upgraded to biomethane, a renewable natural gas. Similarly, carbon monoxide or syngas produced from industrial processes or biomass gasification can be converted into liquid fuels through chemical catalysis.
- 4. Aquatic plants: Apart from algae and seaweed, various aquatic plants, such as water hyacinth or duckweed, have the potential to be explored as biofuel feedstocks. These plants have high growth rates and can be cultivated in freshwater bodies or wastewater treatment systems. They can be converted into biofuels through similar processes used for terrestrial biomass, such as fermentation or pyrolysis.
- 5. Organic waste from urban areas: Organic waste generated in urban areas, including food waste from households, restaurants, or supermarkets, has the potential to be utilized for biofuel production. Effective waste management strategies, such as anaerobic digestion or composting, can convert this waste into biogas or bioethanol. Implementing such systems at the community or city level can provide a sustainable solution for waste management while producing renewable energy.
- 6. Woody biomass: While woody biomass is a known feedstock for bioenergy, there are unexplored sources within this category. For example, invasive tree species or forestry residues with limited commercial value can be used for biofuel production. These materials can be sourced sustainably, providing an additional economic incentive for managing invasive species and promoting healthy forest ecosystems.

These raw materials offer untapped potential for biofuel production. Continued research, technological advancements, and the development of efficient conversion processes will determine their viability and commercial feasibility in the future.

RAW MATERIALS THAT ARE NOT YET EXTENSIVELY EXPLORED FOR MAKING BIOFUELS BUT HAVE POTENTIAL TO BE EXPLORED:

Here are some materials that have not been extensively explored for biofuel production but hold potential for future exploration:

- 1. <u>Seawater-grown crops</u>: Researchers are exploring the cultivation of salt-tolerant crops using seawater irrigation. By growing crops like saltwater rice or salt-tolerant varieties of sugarcane using seawater, it could be possible to produce biofuels without using freshwater resources. This approach has the potential to reduce the strain on freshwater supplies and open up new possibilities for biofuel feedstocks.
- 2. <u>Aquatic microorganisms</u>: While algae are extensively studied for biofuel production, there are many other types of aquatic microorganisms that could be explored. For example, diatoms, cyanobacteria, or certain types of protozoa may possess unique characteristics and lipid content suitable for biofuel production. Research efforts in this area could uncover new and efficient biofuel sources from aquatic environments.

- 3. <u>Invasive plant species</u>: Invasive plant species, which have a negative impact on ecosystems, could be explored as potential biofuel feedstocks. Species like water hyacinth, giant reed, or kudzu grow rapidly and in abundance. By converting these invasive plants into biofuels, it would help control their spread while producing renewable energy.
- 4. <u>Agricultural residues from specialty crops</u>: Specialty crops such as coffee, cocoa, or tea generate significant amounts of agricultural residues that are currently underutilized. By exploring the potential for converting these residues into biofuels, it could enhance the sustainability of these industries and provide additional value streams.
- 5. <u>Microalgae consortia</u>: Instead of focusing on individual algae strains, researchers are beginning to explore the potential of microalgae consortia or communities. These communities consist of different algae species that work synergistically, enhancing productivity, nutrient uptake, and overall stability. By harnessing the unique characteristics of these microalgae consortia, it may be possible to achieve higher yields and optimize the production of biofuels.
- 6. Waste from insect farming: Insect farming for animal feed or food production generates significant amounts of organic waste. This waste, such as insect frass (excreta) or discarded insect parts, can be explored as a potential feedstock for biofuel production. Processes like anaerobic digestion or insect-based bioconversion could be used to convert this waste into biogas, bioethanol, or other biofuels.
- 7. <u>Microbial electrosynthesis</u>: Microbial electrosynthesis is a process where microorganisms use electricity as an energy source to convert carbon dioxide into biofuels or other value-added chemicals. This emerging technology has the potential to utilize renewable energy sources like solar or wind power to drive the production of biofuels from carbon dioxide emissions.

These materials represent promising avenues for future exploration in the field of biofuel production. As research and technology continue to advance, these untapped resources may offer sustainable and efficient alternatives for biofuel feedstocks.

OTHER RARE RAW MATERIALS FOR BIOFUEL PRODUCTION:

There are materials that have not traditionally been considered as raw materials for biofuel production but could potentially be explored in the future. While their feasibility as biofuel feedstocks would require extensive research and development, here are a few examples:

- 1. <u>Carbon dioxide (CO₂) from air capture</u>: Rather than focusing solely on waste CO₂ from industrial processes, capturing carbon dioxide directly from the atmosphere (air capture) is an emerging concept. By utilizing advanced technologies and catalysts, it might be possible to convert captured CO₂ into biofuels, effectively recycling atmospheric carbon and reducing greenhouse gas emissions.
- 2. <u>Industrial emissions from steel or cement production</u>: Industries such as steel or cement production release significant amounts of carbon dioxide during their processes. While these emissions are typically considered pollutants, exploring methods to capture and convert these industrial emissions into biofuels could offer a novel approach to both carbon mitigation and biofuel production.

- 3. <u>Plastic waste</u>: Plastic waste is a global environmental challenge, but it contains carbon-rich molecules that can potentially be transformed into biofuels. Technologies like pyrolysis or gasification can break down plastic waste into smaller hydrocarbon molecules, which can then be processed into biofuels. This approach could provide a dual benefit of plastic waste management and renewable energy production.
- 4. <u>Algal blooms</u>: Algal blooms, which are excessive growths of algae in bodies of water, are often considered harmful due to their negative impacts on aquatic ecosystems. However, exploring methods to harness and convert these algal blooms into biofuels could help mitigate their environmental effects while simultaneously producing renewable energy.
- 5. Atmospheric nitrogen (N₂): Nitrogen gas (N₂) makes up the majority of Earth's atmosphere, and capturing and utilizing this nitrogen as a raw material for biofuel production is a relatively unexplored concept. Nitrogen-fixing bacteria or other innovative technologies could be employed to convert atmospheric nitrogen into biofuels, potentially reducing the need for nitrogen fertilizers in conventional biofuel feedstock cultivation.
- 6. <u>Volatile organic compounds (VOCs)</u>: VOCs are organic chemicals emitted as gases from various sources, including industrial processes, landfills, or wastewater treatment plants. These VOCs could be captured and used as potential precursors for biofuel production. Advanced catalytic processes might enable the conversion of VOCs into useful biofuels, providing a means of valorizing these otherwise harmful emissions.

It's important to note that while these materials hold potential, their viability as biofuel feedstocks would require extensive research, technological advancements, and consideration of economic, environmental, and sustainability factors.

LESSER-KNOWN RAW MATERIALS FOR POSSIBLE BIOFUEL PRODUCTION:

Here is a list of some of the lesser-known raw materials that have potential for biofuel production:

- 1. <u>Coffee grounds</u>: Coffee waste, such as used coffee grounds, has the potential to be converted into biofuels. The high oil content in coffee grounds can be extracted and processed into biodiesel, offering a unique and sustainable source for biofuel production.
- 2. <u>Pine resin</u>: Pine trees produce resin, which contains a mix of hydrocarbons. Extracting and processing pine resin into biofuel could be an unconventional source, particularly in regions with abundant pine forests.
- 3. <u>Cactus plants</u>: Certain species of cactus plants, such as Opuntia ficus-indica (prickly pear), have high sugar content in their fruits. These sugars can be converted into bioethanol, making cactus plants a unique and potentially sustainable biofuel feedstock.
- 4. <u>Invasive water hyacinth</u>: Water hyacinth, an invasive aquatic plant, can rapidly multiply and cover large bodies of water, disrupting ecosystems. However, this plant can also be utilized as a raw material for biofuel production, potentially helping to control its spread while generating renewable energy.

- 5. <u>Insects and insect waste</u>: Insect-based biofuel production is an emerging field. Insects, such as black soldier flies, can be reared and processed to obtain oils or fats that can be converted into biofuels. Additionally, insect waste, such as larvae excreta or discarded parts, can be used for biofuel production.
- 6. <u>Agave plants</u>: Agave plants, commonly known for their use in tequila production, have high sugar content in their juice. This sugar can be fermented and processed into bioethanol, presenting a unique and potentially valuable biofuel feedstock.
- 7. <u>Seaweed species</u>: In addition to commonly known seaweed varieties, various lesser-known species of seaweed can be explored for biofuel production. These include species like kelp, dulse, or sea lettuce, which have high growth rates and can be cultivated in coastal areas or open ocean farms.
- 8. Glycerol waste from biodiesel production: Biodiesel production generates a by-product called glycerol. While glycerol has various applications, it can also be converted into biofuels through processes like gasification or fermentation, offering a way to utilize this waste stream more efficiently.
- 9. <u>Rice husks</u>: Rice husks are the outer protective layers of rice grains. These husks contain high levels of cellulose, which can be converted into biofuels using advanced technologies like pyrolysis or biochemical processes.
- 10. <u>Microorganisms from extreme environments:</u> Microorganisms that thrive in extreme environments, such as volcanic springs or deep-sea hydrothermal vents, might possess unique metabolic capabilities for producing biofuels. Exploring and harnessing the potential of these extremophile microorganisms could unlock new avenues for biofuel production.

It's important to note that while these materials have potential, their commercial viability as biofuel feedstocks would require further research, development, and optimization

NOVEL NON-CARBON SOURCE FOR MAKING BIOFUELS:

Currently, most biofuels are derived from carbon-based sources such as biomass, algae, or waste materials. However, there is ongoing research and exploration into novel non-carbon sources for biofuel production. While these approaches are still in the early stages of development, here are a few examples:

- 1. <u>Solar fuel</u>: Solar fuels, also known as solar-to-fuel conversion, involve using sunlight to directly convert water and carbon dioxide into hydrogen or other energy-rich molecules. These solar fuels can serve as alternative energy carriers and potentially be used as biofuels. However, significant advancements are required to make solar fuel technologies commercially viable for large-scale biofuel production.
- 2. <u>Electricity-driven conversion</u>: Electro fuels, or electro synthetic fuels, involve using renewable electricity to power the conversion of carbon dioxide or nitrogen into liquid fuels through electrochemical processes. This approach can potentially provide a carbon-neutral pathway for biofuel production, bypassing the need for biomass or carbon-based feedstocks.

- 3. <u>Hydrogen-based biofuels</u>: Hydrogen can be produced through various methods, including electrolysis of water using renewable electricity. Hydrogen gas can then be used directly as a fuel or converted into liquid fuels like hydrogenated vegetable oil (HVO) or ammonia. Hydrogen-based biofuels offer high energy density and cleaner combustion compared to traditional carbon-based fuels.
- 4. <u>Bio electrochemical systems</u>: Bio electrochemical systems, such as microbial fuel cells or microbial electrolysis cells, utilize microorganisms to convert organic matter into electricity or hydrogen gas. These systems can potentially be integrated with other biofuel production processes or used as a stand-alone approach for generating renewable biofuels.
- 5. Synthetic biology approaches: Synthetic biology techniques involve engineering or designing microorganisms to produce specific biofuels or biofuel precursors directly from non-carbon sources. Researchers are exploring the use of non-carbon feedstocks such as nitrogen, sulfur, or metals to produce biofuels through synthetic biology approaches.

It's important to note that while these non-carbon sources show promise, they are still in the research and development stage. Overcoming technical challenges, optimizing efficiency, and ensuring economic viability are critical steps towards the commercialization of novel non-carbon biofuel sources.

"OUT-OF-THE-WORLD" EXAMPLES OF RAW MATERIALS FOR BIOFUEL PRODUCTION:

Here are few "out of the world" examples of a potential non-carbon source for biofuel production:

1. Martian resources: As space exploration advances, there has been speculation about utilizing resources on other planets for various purposes. In the context of biofuels, there have been conceptual discussions about the possibility of utilizing resources found on Mars, such as carbon dioxide from the Martian atmosphere and water from ice deposits, to produce biofuels for potential future human missions or colonization efforts. The idea involves using advanced technologies to convert Martian resources into biofuels, providing a means of sustainable energy production in a resource-limited extra-terrestrial environment.

It's important to note that this example is purely speculative and highly theoretical at this point. The feasibility and practicality of utilizing extra-terrestrial resources for biofuel production would require significant advancements in space exploration, resource extraction, and biofuel production technologies.

[Ref: Resource Utilization on Mars by Cole C. Pazar, Colorado School of Mines Center for Space Resources, Golden, CO, 80401, https://www.researchgate.net/publication/344326060]

2. <u>Lunar Regolith</u>: The utilization of extra-terrestrial resources for various applications has been a subject of interest and research in recent years. One particularly intriguing area is the potential use of lunar regolith, the layer of loose soil and rock on the Moon's surface, as a raw material for biofuel production.

Lunar regolith consists of various elements and compounds that could potentially serve as valuable feedstocks for biofuel production. These include minerals rich in metals like iron and titanium, as well as abundant oxygen and hydrogen. Researchers are exploring ways to extract and process these resources to derive biofuels that could contribute to sustainable energy practices, both on Earth and potentially in space missions.

The concept of utilizing lunar regolith as a raw material for biofuel production presents several advantages. Firstly, it offers a unique opportunity to tap into a virtually untouched resource, opening new avenues for resource exploration and utilization. Secondly, the extraction and utilization of lunar regolith for biofuel production could potentially reduce the dependence on traditional terrestrial resources and mitigate environmental impacts associated with their extraction.

However, there are several challenges associated with harnessing lunar regolith for biofuel production. The extraction process would require innovative and efficient technologies capable of handling the extreme conditions present on the Moon. Additionally, transportation logistics and cost considerations would need to be addressed to ensure the feasibility and viability of such ventures.

Despite these challenges, the potential benefits of utilizing extra-terrestrial resources like lunar regolith for biofuel production are significant. They include diversifying the range of raw materials available for biofuel production, reducing environmental impacts, and promoting sustainable energy practices. Furthermore, research in this field contributes to our understanding of extra-terrestrial resource utilization and expands our knowledge for potential future space exploration and colonization.

In conclusion, while the utilization of lunar regolith as a raw material for biofuel production is still in the realm of exploration and research, it holds immense potential. Further studies and technological advancements are necessary to overcome the challenges and unlock the possibilities presented by extraterrestrial resources. Continued exploration of these resources not only expands our understanding of the universe but also offers prospects for sustainable energy solutions on Earth and beyond.

[Ref: https://ntrs.nasa.gov/api/citations/20090010050/downloads/20090010050.pdf]

Here's another exotic example of a potential non-carbon source for biofuel production:

3. <u>Deep-sea methane hydrates</u>: Methane hydrates are ice-like structures that contain trapped methane gas. While methane is a carbon-based compound, deep-sea methane hydrates offer an unconventional and relatively untapped source of this gas. These methane hydrates exist in vast quantities in deep-sea sediments and could potentially be harnessed and processed to produce methane-based biofuels. However, extracting and utilizing methane hydrates pose significant technical and environmental challenges, and their commercial viability is still being explored.

It's important to note that deep-sea methane hydrates are a complex and controversial area of research due to concerns about the release of methane, a potent greenhouse gas, during extraction. The potential

use of deep-sea methane hydrates for biofuel production would require careful consideration of environmental impacts and technological feasibility.

[Ref: hydrates/]

CONCLUSION:

In conclusion, the exploration of unconventional raw materials presents a promising avenue for advancing sustainable biofuel production. Continued research, technological advancements, and the development of efficient conversion processes will determine the viability and commercial feasibility of these raw materials in the future. By expanding the range of raw materials, biofuel production can become even more environmentally friendly, reduce dependence on finite resources, and contribute to a sustainable energy landscape, both on Earth and potentially beyond.

Water Electrolyser Technologies for Green Hydrogen Production

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The world is undergoing a dramatic change in the way energy is produced, transformed, stored and used in its various forms. People are becoming increasingly conscious of the need to move towards a society where energy stops contributing to climate change and local pollution, replacing fossil fuels with renewable energy. As the deployment of renewable energy sources increases all over the globe in the power sector, solutions that leverage renewable electricity to decarbonise end-use sectors using power-to-gas strategies, or to convert electricity into high-value chemicals or fuels, need to be quickly introduced. However, there is still a need to decarbonise applications for which direct electrification is more challenging (the so called "hard-to-abate" sectors).

Green hydrogen (*i.e.* hydrogen produced from renewable electricity) is gaining importance world over as one of the important tool to achieve Net Zero Emission goals and decarbonize hard to abate sectors. The potential for green hydrogen is much higher than fossil fuels, since it is linked to solar and wind potential, which far exceeds global energy demand today and in any future scenario. Green hydrogen is the only zero-carbon option for hydrogen production.

While there are multiple pathways to produce green/clean hydrogen, this article focus on water electrolyser technologies for green hydrogen production.

Green Hydrogen Production using Water Electrolysis

The hydrogen value chain begins with production, generating hydrogen from various feedstocks and natural resources.

Water electrolysis is the process of splitting water into hydrogen and oxygen through the application of electrical energy. When the source of electricity is Renewable (Solar, Wind, Hydro), the hydrogen so produced is termed as Green Hydrogen. Electrolysis of water is an oxidation-reduction reaction that does not occur spontaneously. Since the heat in the form of electricity is supplied to the electrolytic cell in the electrolysis of water, the reaction is endothermic.

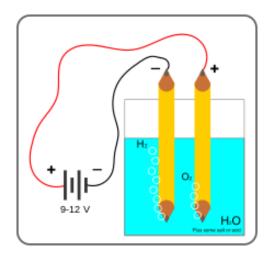


Fig 1: Simple schematic of water electrolyser

A DC electrical power source is connected to **two electrodes** (typically made from an inert metal such as platinum or iridium) that are placed in the water. Water dissociates into hydrogen (H⁺) and hydroxide (OH⁻) ions and moves to the opposite electrodes. Hydrogen appears at the **cathode** (where electrons enter the water), and oxygen at the **anode.**

However, due to limited self-ionization of water, there is no conductivity due to lack of ions. *Hence, an ELECTROLYTE is required such as; a Salt, an Acid, or a Base, along with eletro-catalyst to increase the efficiency & facilitates the continuous flow of electricity.*

In pure water, at the negatively charged cathode, a reduction reaction takes place, with electrons (e⁻) from the cathode being given to hydrogen cations to form hydrogen gas. At the positively charged anode, an oxidation reaction occurs, generating oxygen gas and giving electrons to the anode to complete the circuit. The two half-reactions, reduction and oxidation, are coupled to form a balanced system. *In order to balance each half-reaction, the water needs to be acidic or basic.*

In the presence of **acid**, the equations depicting two-half cells are shown below:

Cathode:
$$4H^+ + 4e^- \rightarrow 2H_2$$
, $E^\circ = 0.0 \text{ V}$
Anode: $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$, $E^\circ = +1.23 \text{ V}$

Combining either half reaction pair yields the same overall decomposition of water into oxygen and hydrogen:

$$2 H_2O(I) \rightarrow 2 H_2(g) + O_2(g)$$

Thus, the standard potential of the water electrolysis cell:

$$E^{o}_{cell} = E^{o}_{cathode} - E^{o}_{anode}$$
 is -1.229 V at 25 °C at pH 0 ([H⁺]

So, theoretically, Water electrolysis requires a minimum potential difference of 1.23 volts. However, water decomposition requires overpotential. In an electrolytic cell, the existence of overpotential implies that the cell requires more energy than thermodynamically expected to drive a reaction. It requires more energy than thermodynamically expected to drive a reaction because of many complex side reactions. Therefore, though water electrolysis requires a minimum potential difference of 1.23 volts, at that voltage, some external heat is also required and hence typically 1.5 volts is required. However, for continuous generation of H₂ typically, 2 volts is required (additional energy for gas liberation, pushing the reaction to forward direction etc).

Types of Water Electrolysers

There are mainly 4-types of water electrolysers:

- 1. Proton Exchange Membrane (PEM) Electrolyzer
- 2. Alkaline Electrolyzer (AE)
- 3. Solid Oxide Electrolysis Cell (SOEC)
- 4. Anion Exchange Membrane (AEM) Electrolyzer

The name of the electrolyser is based on the type of electrolyte and the membrane used to separate the electrodes, as you will see on the next page. The membrane separates the products, provides electrical insulation between electrodes, and conducts ions.

i) Proton Exchange Membrane (PEM) Electrolyzer

- In PEM water electrolysis, water is electrochemically split into hydrogen and oxygen at their respective electrodes such as hydrogen at the cathode and oxygen at the anode.
- PEM water electrolysis is accrued by pumping of water to the anode where it is spilt into oxygen (O₂), protons (H⁺) and electrons (e⁻). The anode side of the cell, which is positively charged, attracts electrons to initiate the reaction.
- These protons traveled via proton conducting membrane to the cathode side. As the polymeric membrane (Nafion) allows only protons to pass thru, this technology is terms as Proton Exchange Membrane (PEM) electrolyser. This selective permeability of the membrane is critical because it prevents oxygen and hydrogen gases from mixing, reducing the risk of explosions and enhancing purity.
- The electrons exit from the anode through the external power circuit, which provides the driving force (cell voltage) for the reaction.
- At the cathode side, the protons and electrons re-combine to produce the hydrogen.

PEM electrolysis uses expensive platinum-group metals (PGMs) such as; Platinum (at Cathode for Hydrogen Evolution Reaction (HER), and Iridium/ruthenium (at Anode for Oxygen Evolution Reaction (OER) as a catalyst.

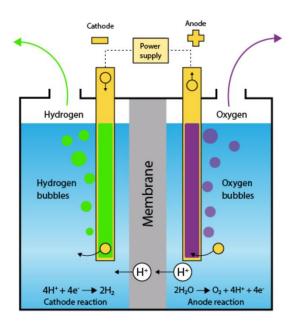


Fig 2: Schematic of a PEM Electrolyser

PEM technology has its roots in the space program. Initially, the Proton Exchange Membrane (or Polymer Electrolyte Membrane) was developed in the 1960s by NASA as a method for fuel cells (reverse of water electrolysis process) to generate power and clean water on spacecraft.

Pros of PEM Electrolysers

- **High Efficiency**: PEM electrolysers achieve high efficiency, making them suitable for applications requiring optimized energy use.
- **Fast Response Time**: Their rapid startup and load adjustment capabilities make them well-suited for use with intermittent renewable energy sources.
- Compact and Lightweight Design: Small size allows for installation in limited spaces, which can be advantageous for certain projects.
- **High-Purity Hydrogen Production**: PEM technology produces high-purity hydrogen, minimizing the need for additional purification.
- **Lower Operational Temperatures**: Lower temperatures reduce the degradation rate of materials, potentially extending equipment lifespan.

Cons of PEM Electrolysers

While PEM electrolysers offer some benefits, they also come with significant limitations that need to be carefully considered:

• **High Initial Cost**: The complex materials needed, including precious metal catalysts (platinum and iridium), drive up the cost of PEM electrolysers, making them a larger investment than alkaline systems.

- **Limited Lifespan**: Despite lower operational temperatures, PEM membranes and electrodes are more prone to wear and tear over time. This can result in a shorter operational life compared to alkaline electrolysers.
- **Expensive and Complex Maintenance**: The intricate design of PEM electrolysers requires specialized knowledge for repairs and maintenance, often increasing long-term costs.
- **Dependence on Precious Metals**: PEM electrolysers rely on platinum and iridium as catalysts, which are both costly and subject to market fluctuations. This can make scaling up PEM production financially challenging.
- **Limited Scalability**: Scaling PEM electrolysers for large, industrial applications can be complex and expensive due to material costs and technical constraints. This restricts their suitability for high-volume hydrogen production.
- Membrane Degradation Under Stress: While PEM electrolysers respond quickly to variable loads, the constant adjustment can accelerate membrane degradation, impacting lifespan and overall cost-effectiveness.

ii) Alkaline Electrolyzer (AE):

- The basic components in an alkaline electrolyser are the same like Anode, Cathode, an electrolyte and a separating membrane.
- In an Alkaline electrolyser, a dilute aqueous sodium or potassium hydroxide is used as the electrolyte.
- Typical electrolyte used is 20-47% KOH, which is preferred due to higher conductivity.
- The electrodes are separated by a **diaphragm**, separating the product gases and *transporting the hydroxide ions* (*OH*⁻) from one electrode to the other.
- The diaphragm material is Zirfon (a composite material of zirconia and Polysulfone) or NiO

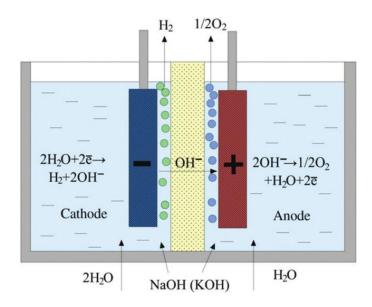


Fig 3: Schematic of an Alkaline Electrolyser along with anode, cathode reactions

The catalyst material on the cathode are typically Ni/Co/Fe based and on the anode is Ni/C-Pt

Pros of Alkaline Electrolysers

- **Lower Production Costs**: Due to simpler materials and designs, production costs for alkaline electrolysers are lower, making them more accessible.
- **Durability**: Alkaline electrolysers are known for their longevity and consistent performance over time.
- **Proven Technology**: Trusted in industrial hydrogen production, alkaline electrolysers are a well-known solution with a long operational history.
- **Ease of Maintenance**: With fewer complex components, maintenance is simpler and requires less specialized expertise.
- Scalability for Large-Scale Production: Alkaline electrolysers are well-suited to large setups where costs need to be controlled, allowing for efficient, steady hydrogen output.

Cons of Alkaline Electrolysers

- **Lower Efficiency**: Alkaline technology in some cases has lower energy efficiency, particularly at high current densities.
- Longer Startup and Shutdown Times: Alkaline electrolysers are slower to start and adjust their output, which can limit their effectiveness in applications with variable energy sources.
- **Lower Hydrogen Purity**: Compared to PEM electrolysers, alkaline electrolyser provide lower hydrogen purity. Additional purification steps may be required, especially for applications needing very high-purity hydrogen, adding to operational costs.

Comparison Table – PEM Electrolysers vs. Alkaline Electrolysers

Feature	Alkaline	PEM
Cost	Lower	Higher
Efficiency	Good	Better
Startup Time	Longer	Fast
Response to Load Changes	Slower	Rapid
Hydrogen Purity	Good	Better
Durability	High	Moderate

Scalability	Suitable for large scale	Limited
Operating Temperature	60–80°C	50–70°C
Maintenance Complexity	Simple	Complex
Material Cost	Lower	Higher

iii) Solid Oxide Electrolyzer Cell (SOEC)

- In SOEC, the Electrolyte is solid Ceramic oxide, which separates the electrodes. Hence is the name as Solid Oxide electrolyser.
- At the cathode, water is reduced to hydrogen and oxide ions.
- The oxide ions pass through the ceramic oxide membrane to the anode to become oxygen gas.
- It operates at high temperatures of 700 to 800°C -High operating temperatures provide a greater overall efficiency than other technologies.

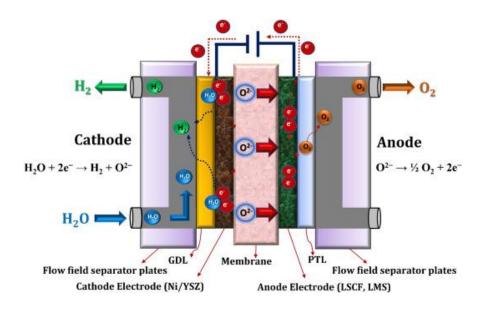


Fig 4: Schematic of a Solid Oxide Electrolyser along with anode, cathode reactions

The most common **electrolyte**, is a dense ionic conductor consisting of ZrO₂ doped with 8 mol-% Y₂O₃ (also known as YSZ, ytrium-stabilized zirconia). Anode and cathode are made from special inks that coat the electrolyte and facilitate an electrochemical pathway to produce hydrogen from renewable electricity.

Cathode: Ni doped YSZ or Perovskite-type lanthanum strontium manganese (LSM)

Anode: LSM, Gd-doped CeO₂

Pros: Superior efficiency thanks to heat reuse, making them ideal for industrial applications with access to excess heat.

Cons: The high temperatures involved result in faster degradation of materials, increasing maintenance needs and limiting lifespan.

Being a high temperature electrolyser, SOEC provides a greater overall efficiency than other technologies and electricity required to produce 1Kg of hydrogen is much lower compared to PEM and Alkaline Electrolysers.

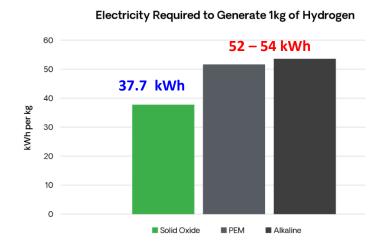


Fig 5: Bar chart showing amount of electricity required to generate 1Kg of Hydrogen using different types of electrolysers

Anion Exchange Membrane (AEM) Electrolyser

- Anion exchange membrane (AEM) electrolysis is the electrolysis of water that utilises a semipermeable membrane that conducts hydroxide ions (OH-), and hence called an "anion exchange membrane".
- Like a PEM, the membrane separates the products, provides electrical insulation between electrodes, and conducts ions.
- Unlike PEM, AEM conducts hydroxide ions.
- AEM electrolysis combines the advantages of alkaline water electrolysis (AWE) and PEM electrolysis
- **Membrane:** Polymer backbone with quaternary ammonium (QA) headgroups

- The major advantage of AEM water electrolysis is that a high-cost noble metal catalyst is not required, low-cost transition metal catalyst; Ni, Fe, Co, Mn, Cu, etc can be used instead.
- Hydrogen can be discharged at High pressure
- AEM is yet to be commercialized, as Membrane life is the main bottleneck.

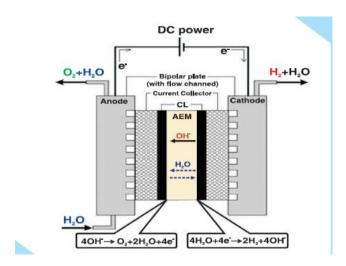


Fig 6: Schematic of an Anion Exchange membrane (AEM) electrolyser

Technology Comparison:

The following table gives a high level technology comparison of three major types of waste electrolysers.

Parameter	Alkaline Electrolyzer	PEM Electrolyzer	Solid Oxide Electrolyzer
Electrolyte	KOH (20-30%)	Polymer Nafion	Yitria stabilized zirconia
Current Density (A/m²)	2000-4000	10000-20000	6000
Operating temperature(°C)	60-90	50-80	500-1000
Operating pressure (bar)	1-30	30-80	1
Efficiency (%)	59-70	65-82	Up to 90%
Specific energy cons. (kWh/Nm³)	4.5-7.0	4.5-7.5	2.5-3.5
Lifetime stack (hr)	<90000 (10-years)	<60000 (4-5 years)	<40000
Cold start-up time, minutes	15	<15	>60
Maturity	Commercial	Commercial	Demonstration
Dynamic operation (frequent start ups & varying power input)	Limited	Quick	Limited
CapEx (USD/kWe)	900-1500	1100-1700	2800-5600
Footprint area	Big	Small	-

Major global manufacturers of commercial water electrolysers are depicted below:

Pictures of Some Commercial Electrolysers:

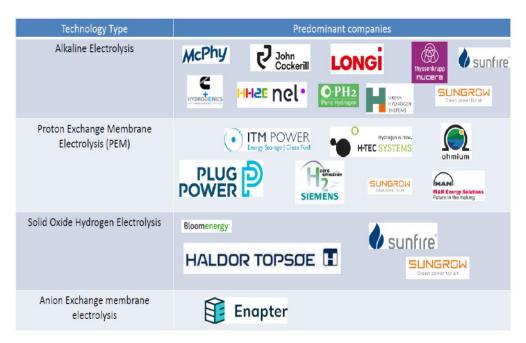




Fig. 7: Some commercial PEM electrolysers

- Tokyama plant 25 MW - 12 t/d



Akzo Nobel/Nouryon, Norway - Chemicals - 1.940Nm3/h - 9.2MW



Fig. 8: Some commercial Alkaline electrolysers

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Textile Waste and Management

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Abstract

Due to the widespread use of toxic chemicals and the creation of toxic waste across the clothing value chain, the textile industry, in particular, has a considerable negative influence on the environment. 10% or so of global CO₂ emissions come from the textile industry. In terms of market size, employment, and product value, the textile industry ranks among the top industries in the world. India's domestic apparel and fashion industry makes vital contributions to the economy, with a 5% contribution to the country's GDP, 7% value added from the same within the modern economy, and 12% of total national earnings from exports. There are some particular challenges related to textile waste management that affect India's textile industry. These challenges include different types of fabrics produced in many different forms, large sections of the industry being unorganized, and a lack of sufficient waste treatment facilities. It is clear that the textile sector needs to continue to develop recycling strategies. A workable, environmentally friendly circular economy idea should enable quantitative and "green" recycling of all material components without producing extra waste streams or increasing energy use due to complicated processing stages.

1. Introduction

Environmental pollution has become a major issue with a serious impact on the Earth's ecosystem. The rise of modern industries is important for the economic growth of developing countries, such as India. But along with this modern industrial growth there is growth in pollution or by-products of industrialization [1]. Since fast fashion has attempted to accommodate the desires of a rapidly growing population, there has been a significant increase in global waste pollution [2]. The textile industry produces large quantities of wastewater, which contains unwanted byproducts from the various process units of the textile industry having possible complex chemical compounds. Verma et al. (2012) states that these chemical compounds are released with Textiles Company's wastewater from their processing industries. Some companies, with no wastewater treatment plant, sometimes dispose of their untreated wastewater into the environment. Negative environmental changes occur as a result of the improper disposal of untreated waste water, which has an effect on ecological status [3]. The textiles industry produces, manufactures, and disposes over 1.2 billion tonnes of CO₂ emissions annually, or 8% of global emissions [4].. Hazardous colours varied pigments, oil, surfactants, heavy metals, sulphates, and chlorides were identified in the effluent of the textile industry. All of these pollutants adversely affect the water quality and aquatic life [5]. For the textile industry and other problems like solid waste and resource water management, wastewater is a major ecological barrier [6]. Many methods can be used for

textile wastewater treatment, encompassing physical, chemical, and biological methodologies. Though the by-products of these treatment processes may be toxic and disposal of them can be hazardous. It is therefore essential to develop and implement a textile waste water treatment process that is sustainable and environmentally sustainable [5]. Within this framework, the purpose of this study is to illustrate the current situation related to the environmental issues associated with textile productions, and the alternative practices for limiting the creation of solid textile waste meant to be disposed of.

1.1 Fashion Sustainability

The modern textile industry in India began in the 1850's when the first cotton textile mill was opened in Bombay in 1854. Currently, it is the second-biggest employment provider in the Indian economy after agriculture and a significant industry in the Indian economy. The textile sector is a major contributor to international trade, making up around 13% of India's total exports. The textile sector is one of the oldest and fastest-growing industries in India, dating back to the Indus Valley Civilization, when people wore garments made of homespun cotton. India generates around 1 million tonnes of textile waste annually [7]. The textile sector is one of the oldest and fastest-growing industries in India, dating back to the Indus Valley Civilization, when people wore garments made of homespun cotton. India generates around 1 million tonnes of textile waste annually. Although the sector brings a sizeable economic value to our societies, it also brings certain unique challenge [8]. The production of one T-shirt alone requires 2700 L of water, which contextualizes the 2015 fashion industry's use of 79 billion cubic of water. Because of the characteristics of fast fashion and increasing overconsumption (Jin & Shin, 2021), clothing is seen as disposable, and fast fashion also causes a considerable amount of waste, waste-related emissions, and toxicity (Rossi et al., 2020, Stål & Corvellec, 2018) [8]. It is now possible to make clothing for everincreasingly lower prices, so low in fact, many people regard this clothing as disposable. Some people call this "fast fashion," the fast food of fashion. Technology advancements that allow businesses to replicate more products place an enormous burden on our natural resources and are increasing our willingness to throw things away. This makes it a double-edged sword; it improves the economy, but also causes an increasing burden for garment and textile disposal. Regardless, the recycling industry has to deal with everything produced by the fashion industry [9]. Accordingly, fashion-oriented products increase consumption beyond what is necessary. The problem of what to do with remaining waste textile materials for the home and clothing will continue to grow as long as consumers keep on buying.

2. Types of textile waste

2.1 Pre - Consumer textile waste

In today's exciting fashion environment, rapid fashion cycles have emerged due to the short life spans of clothing. A large proportion of Indian consumers, especially urban ones, repeatedly purchase clothing, and this behavior has led to large amounts of post-consumer textile waste (PCTW), often in the form of second-hand clothing (SHC) or used clothing [11]. The amount of pre-consumer industrial textile waste has expanded along with the growth of the fashion sector. According to estimates 10–20% of the fabrics used to make clothes are wasted. Reusing pre-consumer textile waste in the fashion supply chain has many environmental benefits, such as: Moving waste away from landfills and incinerators, resource conservation and addressing the current shortages of virgin fibers and natural resources, providing

inexpensive raw materials for fashion products, delivering a lower financial and environmental processing cost than virgin fibers [12]. Businesses either organize their own trash disposal services or use services that are controlled by the council, and they pay landfill fees based on how much is disposed off [9].

2.2 Post-consumer textile waste

Since 1960, the amount of post-consumer textile waste (PCTW) generated in the United States has been rising steadily - approximately tripling on an annual basis - to more than 34 billion pounds in 2018. The amounts of PCTW in the current context stem largely from the changes in textile production and consumption that have focused on a fast fashion system [13]. Most of the garments in this category are typically exported to developing countries at least of fair to good quality. As used clothing, it can be reclaimed and recycled by another user. Clothing that is very unlikely to be worn again can be shredded into fiber and used to make products similar to pre-consumer textile waste [9].

2.3 Industrial textile waste

Industrial textile waste arises from both commercial and industrial uses of textiles, including carpet and curtain, waste from households, waste from hospitals, and industrial uses such as filtering products and conveyor belting, and others. As a general rule, "dirty waste" denotes industrial textile waste. This category has had the most difficult path for recovery due to collection methods and chemical contamination. Most of these end-of-life products go to incineration or landfill. However, there are some companies (e.g., the carpet sector), that are undertakes studies to learn more about utilizing this resource [9]. Shoddy the textile recycling industry in Panipat, known as the global textile recycling capital, stands out for India's most enduring and efficient practices. Annually, it processes approximately 144,000 tonnes of Second Hand Clothing (SHC) discarded by developed nations. This substantial volume of textile waste, primarily SHC, serves as a crucial raw material for the production of various low-quality goods such as blankets, shawls, and carpets. Notably, about 3 tonnes of fabric yield approximately 1.5 tonnes of shoddy yarns, highlighting the industry's significant role in sustainable resource utilization and economic activity within the region [11].

3. Textile recycling

In general, textile reuse and recycling can have advantageous environmental effects since they may help reduce the production of virgin textile fiber and end the process of degrading the textile product later in its lifecycle. Furthermore, textile recycling and reuse is less environmentally damaging than incineration or land filling. Nevertheless, reuse is seen as superior to recycling, especially if the reuse process is prolonged. Textile reuse refers to a variety of ways to extend the usable service life of textile products from the initial owner to another owner. Commonly, this occurs through rental, trading, swapping, borrowing, and inheritance facilitated by thrift stores, garage sales, flea markets, online marketplaces, and charitable organizations.

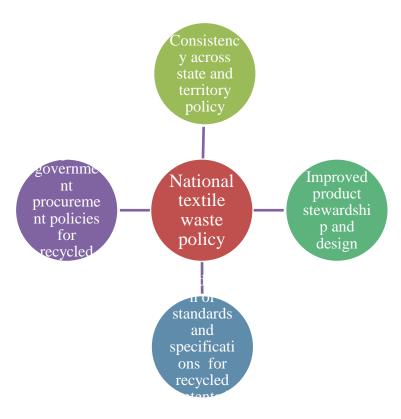


Figure 1 Focuses of national textile waste policy

More than 90% of textile waste can be reprocessed into new products or seen as raw material [14].



Figure 2 Textile and apparel waste management hierarchy model

4. Options for Recycling Textile Waste

4.1 Composting

With the use of effective microorganisms, one can utilize fortification as well as enrichment, to enhance the nutrient value of the medium for the soil, plants, and bodies of water. Natural fibers are very easily broken down when chopped up and thrown away. This is a very popular process particularly in the interior design and automobile industries where the use of natural fibers would offer the bonus of reducing the weight of the automobile, resulting in better mileage for the vehicle. It is now a priority of the package textiles to make their own biodegradable bags, basically focusing on research and the possible economic benefits of using eco-friendly textile materials.

4.2. Non-woven engineering

Non-woven refers to producing textiles through the use of short threads to fasten them with heat, glue, chemicals, or ironing to produce a product that is similar to textiles, non-woven lends a lot of creativity with respect to materials since systematic fiber length and fabric construction may not be possible due to the heterogeneity of recycled fibers. The vast array of textiles for agricultural, construction, geo, acoustic and filtration industries can greatly benefit from composites that combine fiber and matrix made of polymer that is glued together under heat and pressure. Composite technology is also innovating with the advent of FRP (fiber reinforced polymers) based on a fiber of a recycled resource. For the manufacturing of recycled fibers, for the most part, polymer thermoplastics like polyester and polyamide will be melted down and ground to granules. In addition, you can use natural fibers to formulate composites. For example, pineapple fibers are used for reinforcement purposes. Some of the novel or nontraditional fiber options that are making their way into the marketplace like coir, basalt, kenaf, hemp, bamboo, flax, jute, sisal, arecanut and banana. If your company is involved with exporting, sustainability is key in today's economies. In the past, waste fabrics a couple of years ago were disposed of recognized as a resource [15].

5. Circular economy

The raised prominence of the circular economy concept in international and national policy relates to the interest in increasing reuse and recycling of textiles; and for example, sees 2015 EU Circular Economy Action Plan (EC, 2017). Consequently, the circular economy has built up momentum in the corporate sector [16]. The circular economy notion is creating a new textile economy. Circular in the fashion sector means promoting the extended life of garments, and textile and clothing items, and their recycling/repurposing for further round of production, and using sustainable and eco-important inputs. On the basis of this position, the European Union has enacted the suggested Action Plan for Circular Economy, which implements horizontal and vertical actions with better regulation principles, including an impact assessment when necessary [17]. The Ellen MacArthur Foundation's 2017 proposal for a new textiles economy contains four primary goals that align with the ideas of the circular economy .By rethinking the current textile industry and seizing chances that its current linear nature has missed, these goals seek to contribute to the creation of a new textile economy [18].

1. Keep out chemicals of concern and discharge of microfibers.

- 2. To overcome the fact that clothing is becoming more and more disposable, change the way it is made, marketed, and worn.
- 3. Change the way that clothing is designed, collected, and reprocessed to drastically increase recycling.
- 4. Use resources wisely and switch to renewable inputs.

Circularity refers to the desire to reduce waste and keep textile products in a cycle of use during the design, production, and consumption processes until they are securely returned to the biosphere once they have reached the end of their useful lives (Brismar, 2017; Niinimäki, 2017) [19].

Four essential measures need to be taken in order to implement circular economy in the T&C sector [20].

- (i) Phase out the use of hazardous materials and microfiber spills. This calls for creative production and design techniques;
- (ii) Modifying the conception, promotion, and use of clothing;
- (iii) Creating items that can be recycled by employing products that can be recovered;
- (iv) Developing effective resource utilization and switching to the use of renewable materials.
- (v) To promote sustainable practices, these need for a significant shift in consumer behavior and product designs.

Classification of textile reuse and recycling routes

6.1. Upcycling

An increasing number of fashion designers are utilizing the idea of upcycling. In the last 10 years, the term "upcycling" has been invented and added to the lexicon of sustainability initiatives. In the book Cradle to Cradle by William McDonough one sees "upcycling" for the first time (McDonough & Braungart, 2002). As companies and fashion houses look to minimize the impacts of the business with socially and environmentally responsible options, many are becoming aware of the practice and utilizing it [19]. Upcycling involves repurposing, repairing, upgrading, and remanufacturing materials and products that have gone or are about to go to waste, in a way that increases their value. Concerning this, textile wastewater can also be lethal to many marine life forms due to the presence of metal particles and chlorine in the synthetic dyes. Thus, textile wastewater must be treated before it can be released [21]. This integration of combination has the added benefit of lower chemical costs, moderate running times, and less process control issues. As a result, the combination was recommended for the treatment of textile wastewaters [22].

6.2. Aerobic/Anaerobic Biological Methods of Color Removal

While some facultative organisms have demonstrated their capacity to reduce colours, there are relatively few accounts of bacteria degrading azo dyes. Pseudomonas aeruginosa was able to decolorize Navitan Fast Blue SSR, a commercial tannery and textile dye. The bacterium was also decolorizing other azo dyes used in textiles. Azo dyes can be broken down by Aeromonas hydrophila and Bacillus sp. It was challenging to isolate these microbes for the purpose of degrading dyes. Anaerobic environments allow dyes to easily split via a four-electron at cleavage producing aromatic amines, a persistent

metabolic byproduct. Under methanogenic conditions, an organic carbon/energy source is necessary for dye decolorization. The microbes totally mineralized the amines that had produced during aeration. Sandhya et al. demonstrated how facultative bacteria are used in microaerophilic—aerobic conditions to reduce and destroy the quantity of dyes. Anaerobic—aerobic treatment can be administered concurrently or sequentially [23].

Conclusion

Currently, there are numerous efforts underway to lessen the harm the textile industry has historically caused to the environment. Notably, some leading brands endorsed initiatives focused on using recycled materials, limiting solid waste, and avoiding wasting raw materials; non-profit organizations were established to certify companies that, in producing their goods, utilize pre- or post-consumer waste; and finally, science has investigated the options for returning textile waste to the ecosystem as a multifunctional material by lessening exploitation of resources through the circular economy.

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AI in Chemistry: A Decade of Revolution

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Abstract

The last decade (2015 to 2025) has witnessed an unprecedented revolution in the execution of Artificial Intelligence (AI) across the chemical sciences. Urged by advancements in machine learning algorithms, computational power, deep learning architectures, and the cumulative availability of large chemical datasets, AI has transitioned from a niche tool to a ubiquitous partner in chemical research and development. This manuscript delivers a wide-ranging synopsis of transformative impact of AI in chemistry in the last decade, covering its profound influence on data analysis, molecular design, reaction prediction and optimization, materials discovery, and drug development. The key methodologies, significant breakthroughs, challenges and future outlook were discussed for this rapidly evolving interdisciplinary field.

1. Introduction

Chemistry, a foundational science, has historically relied on a combination of theoretical insights, experimental ingenuity, and serendipitous discovery. However, the sheer complexity of chemical space, the vast number of possible molecular structures and reactions, and the intricate relationships between structure and properties have long posed significant bottlenecks. The advent of high-throughput experimental techniques and sophisticated computational methods has generated an explosion of data, simultaneously offering new opportunities and demanding more powerful tools for analysis and interpretation.

The use of AI in chemistry date back decades, the period from mid-2015 to mid-2025 marks a critical inflection point. This decade has seen the evolution of powerful AI algorithms, the development of specialized chemical informatics tools, and a shift towards more autonomous and data-driven chemical discovery. This article aims to summarize the most significant advancements during this transformative period, illustrating how AI has fundamentally reshaped chemical research.

2. Data-Driven Chemistry and Predictive Modeling

The foundation of AI in chemistry is grounded on its propensity to learn from and generalize across cosmic chemical datasets. The last decade has seen significant revolutions in data curation, representation, and the application of sophisticated predictive AI models.

2.1. Enhanced Data Representation and Feature Engineering: A crucial advancement has been the development and widespread adoption of more effective molecular representations for AI models.

Beyond traditional descriptors (e.g., physicochemical properties, fingerprints), graph-based representations (e.g., molecular graphs, SMILES, SELFIES) have become prevalent. Graph neural networks (GNNs), which directly operate on molecular graphs, have revolutionized property prediction by intrinsically capturing local and global molecular topology. Advancements in featurization techniques, including learned embeddings from large chemical datasets, have also significantly improved model performance.

2.2. Robust Predictive Models for Properties and Activities: The application of ML algorithms, particularly support vector machines, random forests, gradient boosting machines (XGBoost, LightGBM), and neural networks, has become standard practice for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) modeling. Over the past decade, these models have moved beyond simple regression to address more complex tasks, including multi-target prediction, uncertainty quantification, and transfer learning, enabling more reliable predictions of solubility, toxicity, bioavailability, and catalytic activity for a wide range of compounds.

3. Revolutionizing Molecular Design and Synthesis

AI has profoundly impacted the design and synthesis of new molecules, moving beyond simple prediction to active generation and intelligent planning.

- **3.1. Generative Molecular Design:** One of the most exciting breakthroughs in AI has been developed in *de novo* molecular design. Generative models, notably Variational Autoencoders (VAEs), Generative Adversarial Networks (GANs), and more recently, transformer-based architectures, are now capable of generating novel chemical structures with desired properties. These models can explore vast chemical spaces intelligently, navigating design constraints and generating molecules with high synthetic accessibility. This capability has accelerated lead optimization in drug discovery and the design of novel materials.
- **3.2. Retrosynthesis and Reaction Prediction:** AI has made significant strides in automating and improving retrosynthesis and forward reaction prediction. Deep learning models, often based on sequence-to-sequence architectures or graph transformations, can now predict reaction outcomes with high accuracy and suggest plausible synthetic routes for complex target molecules. Platforms leveraging these AI algorithms have emerged, offering chemists powerful tools to navigate synthetic challenges, reduce experimental trial-and-error, and optimize reaction conditions. The integration of reaction databases (e.g., Reaxys, SciFinder) with AI models has been crucial here.
- **3.3. Autonomous Synthesis and Robotics:** The last 10 years have seen the rise of "self-driving" laboratories where AI controls robotic platforms to autonomously design, execute, and learn from experiments. These systems can optimize reaction conditions, discover new reaction pathways, and synthesize novel compounds with minimal human intervention. These systems can design experiments, execute them, analyze the results, and refine their strategies, accelerating the discovery of new catalysts,

polymers, and other functional materials. This integration of AI, robotics, and automation promises to dramatically accelerate the pace of chemical discovery and development.

4. Impact on Materials Science and Drug Discovery

The advancements in AI in chemistry have had a particularly profound impact on two critical application areas: materials science and drug discovery.

4.1. Accelerating Materials Discovery and Optimization: AI has become indispensable in the search for novel materials with customized characteristics. Machine learning models are used to forecast the properties of hypothetical materials, screen vast databases of existing materials, and guide the synthesis of new compounds. This includes applications in catalysis, energy storage (e.g., battery materials), superconductivity, and polymers. Data-driven approaches are also being used for inverse design – designing materials with desired properties from the outset. Furthermore, AI is crucial for analyzing complex experimental data from materials characterization techniques, accelerating insights into structure-property relationships.

4.2. Transforming Drug Discovery and Development: AI has revolutionized nearly every stage of the drug discovery pipeline as:

Target Identification and Validation: AI-powered bioinformatics tools and graph-based approaches are aiding in identifying novel drug targets by analyzing omics data and biological networks. The breakthrough in protein structure prediction (e.g., AlphaFold) has fundamentally transformed structure-based drug design.

Virtual Screening and Lead Prioritization: AI-powered virtual screening platforms like advanced docking algorithms and predictive ADMET (Absorption, Distribution, Metabolism, Ex Excretion, Toxicity) models, rapidly screen billions of compounds, identifying potential drug candidates with unprecedented efficiency. Deep docking techniques, for instance, can effectively screen massive ligand libraries, greatly reducing the size of libraries requiring further experimental evaluation. AI also plays a crucial role in prioritizing promising "lead" compounds for further evaluation, offering a more advanced method compared to traditional ranking techniques. Generative models are designing novel scaffolds and optimizing existing leads for improved potency, selectivity, and pharmacokinetic profiles.

Clinical Trials and Repurposing: AI is increasingly used to analyze clinical trial data, identify patient subgroups for personalized medicine, and predict trial outcomes. Furthermore, AI has become a powerful tool for drug reprofiling, which analyses copious quantities of clinical data and biomedical literature to identify novel therapeutic applications for already-approved medications.

5. Spectroscopy and Analytical Chemistry

AI, in particular deep learning and machine learning is used for enhanced interpretation of complex spectroscopic data, improving compound identification, and optimizing analytical techniques. The sheer volume and complexity of data generated by modern analytical instruments necessitate advanced computational approaches, and AI provides powerful tools to address these challenges. The key roles of AI in spectroscopy and analytical chemistry are as follows:

5.1. Enhanced Data Processing and Interpretation

Automated Preprocessing: AI algorithms can automate tedious and error-prone data preprocessing steps like noise reduction, baseline correction, and peak alignment, saving time and minimizing human error.

5.1.1. Spectral Analysis and Interpretation

Peak Assignment and Identification: AI improves the accuracy of peak assignment in techniques like NMR and Mass Spectrometry, aiding in metabolite and compound identification.

Molecular Structure Prediction: Machine learning models can predict molecular structures directly from spectral data (e.g., IR, Raman).

Feature Extraction: Deep learning algorithms can automatically extract pertinent parameters from complex spectral data, eliminating the prerequisite of labor-intensive data preprocessing or feature engineering.

Quantitative and Qualitative Analysis: AI-powered chemometric tools enhance multivariate data analysis, leading to more accurate quantification and classification of substances.

Real-time Analysis: AI algorithms offer spectroscopic data analysis in real-time, enabling quicker decision-making in applications like drug detection, food safety, and environmental monitoring. This is particularly valuable for portable analytical devices.

5.2. Method Development and Optimization

Experimental Design: AI can assist in designing experiments, optimizing instrument measurement conditions and parameters, and creating more efficient experimental workflows.

Chromatographic Optimization: AI can optimize retention times in chromatographic techniques (e.g., HPLC, GC), thereby reducing analysis time and solvent consumption. Predictive models help in peak deconvolution, improving compound identification accuracy.

Robotics and Automation: AI-guided robots can perform high-throughput screening and self-optimizing systems can adjust experimental conditions in real-time, greatly accelerating research and development.

5.3. Predictive Capabilities

Predicting Chemical Properties and Behavior: Relying on prevailing spectroscopic data, Machine learning models can be proficient to anticipate the conclusions of material behaviors, chemical reactions, and even the bioactivity of new drugs using QSAR models.

Material Discovery: AI scrutinizes complex datasets of spectroscopic statistics to diagnose propitious new materials with desired properties, streamlining the material discovery process.

Process Analytical Technology: AI enables real-time monitoring and control in industrial manufacturing (e.g., pharmaceuticals, food safety), allowing for early detection of contaminants, degradation, or anomalies.

5.4. Addressing Data Challenges

Handling Large and Complex Datasets: Modern analytical instruments generate immense volumes of high-dimensional data. AI is adept at processing and extracting meaningful insights from such complex datasets that are often beyond traditional human interpretation.

Dealing with Scarce Data: While deep learning often thrives on large datasets, new AI approaches are being developed to perform well even with limited spectroscopic data, overcoming a common challenge in the field.

6. Challenges and Future Outlook

Although the advancements in AI in chemistry over the last decade have been extraordinary, still several challenges remain as:

- **6.1. Data Availability and Quality:** Despite increasing data, truly comprehensive, high-quality, and standardized datasets across all chemical domains remain a bottleneck. The "garbage in, garbage out (GIGO)" principle still applies, emphasizing the need for robust data curation and sharing initiatives.
- **6.2. Interpretability and Trustworthiness:** Most of the cutting-edge AI models, especially deep learning architectures, maneuver as "black boxes," are unfathomable to explain the reasoning behind their predictions. For critical applications like drug discovery, model interpretability and the quantification of uncertainty are crucial for gaining user trust and regulatory acceptance. Explainable AI is an active area of research addressing this.
- **6.3. Integration and Adoption:** While AI tools are becoming more accessible, seamless integration into existing chemical workflows and widespread adoption by the broader chemistry community still require efforts in education, training, and user-friendly software development.
- **6.4. Ethical Considerations:** As AI-driven discovery accelerates, ethical considerations related to responsible innovation, intellectual property, and potential misuse of powerful generative models become increasingly important.
- **6.5. Future Outlook:** The next decade promises even more profound advancements. The following points can be anticipated as:

Hybrid AI Models: The synergistic combination of other domain based models with data-driven AI, leading to more robust and generalizable predictions.

Autonomous Discovery Platforms: Fully integrated, closed-loop AI-driven labs capable of independent hypothesis generation, experimentation, and discovery.

Quantum-AI Synergy: The emerging field of quantum computing offering new paradigms for simulating complex chemical systems, potentially enhancing AI capabilities for molecular design and their property prediction.

Broader Accessibility: Democratization of AI tools and methodologies, making them accessible to a wider range of researchers and laboratories.

6. Conclusion

The last decade has fundamentally reshaped the landscape of chemical research through the transformative power of Artificial Intelligence. From accelerating data interpretation and revolutionizing molecular design to driving drug discovery and materials innovation, AI has moved from a promising concept to an indispensable tool. While challenges remain, the rapid pace of innovation suggests that AI will continue to be a cornerstone of chemical discovery, enabling unprecedented efficiencies, fostering deeper scientific understanding, and ultimately contributing to solutions for pressing global challenges in health, energy, and sustainability.

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Conducting Polymers, Biocomposites, and Applications: A Review

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Abstract

Conducting polymer-based Biocomposites represent one of the most promising compounds for various applications such as sensing, deposition, and deposition of metal ions due to a unique combination of Biocompatibility, electrical conductivity, and mechanical flexibility. Furthermore, polypyrrole offers good electrical properties suitable for biosensors, drug delivery, tissue engineering and bioelectronics. Conducting polymers combined with synthetic and natural biopolymers (Sodium Alginate, chitin, chitosan, etc.) enhance the biodegradability, structure integrity, and biocompatibility.

This review aims to provide a detailed analysis of conducting polymer-based Biocomposites and their derivatives, highlighting recent advancements, material innovations, and strategies to overcome these challenges. Overall, PPy-based Biocomposites represent a multifunctional material bridging the gap between electronics and biology, with great potential for next-generation chemical applications.

Introduction

The increasing demand for advanced biomaterials with multifunctional capabilities has led to exploring conductive polymers such as polypyrrole (PPy) and polyaniline (PANI) in the Biocomposites strategy. Pani and PPy, known for their good electrical conductivity, chemical stability, and ease of synthesis, are increasingly relevant in sensing[1], dye degradation[2], and biomedical fields. However, its integral brittleness and partial biodegradability have required its combination with biopolymers like sodium alginate[3], chitosan[4], gelatine, chitin[5], cellulose[6], and polylactic acid, resulting in Biocomposites with improved mechanical strength, biocompatibility, and degradability. Conducting polymer-based Biocomposites bridge the gap between conventional bio-inert polymers and smart biomaterials capable of different applications. This review aims to provide a comprehensive overview of the current state of research on PPy-based Biocomposites, focusing on their fabrication strategies, properties, applications, and future potential in the chemical field.

Operating model of conducting polymers-based Biocomposites

Conducting polymers-based Biocomposites work on the cooperative effect of electrical conductivity and biocompatibility. Its conductivity is due to the delocalized π -electron system of polypyrrole within the polymer[17]. It is doped with counterions like as Cl⁻¹, COO⁻¹ or SO₄⁻², so polypyrrole

is electrically conductive[18], which allows for charge transfer in biosensors. Composite functionality increases when biopolymers combine with PANI, and PPy which improves biodegradability, mechanical strength and structural support.

Table 1: Conducting polymer-based composite and their application.

Sr. No.	Polypyrrole-based Biocomposite	Advantage	References	
1.	PPy thin film	Glucose sensor	[7]	
2.	PPy grafted ZnO Nps	Xanthine oxidase	[8]	
3.	PPy/Hydrogel Membrane	Cholesterol Sensor	[9]	
4.	PPy/Cu nanowire	H ₂ O ₂ Sensor	[10]	
5.	PPy/walnut sawdust	MB dye absorption	[11]	
6.	PPy/Chitosan/Graphene oxide	Ponceau 4R absorption	[12]	
7.	PPy/Chitosan/Lignosulfonate	Congo red	[13]	
8.	PANI/Wheat shells	Orange G	[14]	
9.	PANI/Rice Husk	Acid Red 18	[15]	
10.	PANI/Prosopis Juli flora	Disperse 23	[16]	

Key Challenges in Conducting Polymers-Based Biocomposites and Their Derivatives

Despite the potential of conducting polymers-based Biocomposites in chemical and microelectronic applications, several **challenges** limit their broader adoption and long-term performance. These challenges are the duration of **material synthesis**, **biocompatibility**, **mechanical stability**, **scalability**, inconsistent electrical conductivity, complex synthesis and processing, and lack of standardisation[19].

Recent Advances in Conducting Polymers-Based Biocomposites

In past years, conducting polymers-based Biocomposites have observed important advancements in their functionality, biocompatibility, and applicability in chemical and electronic domains. Innovations

have attentive on **material design**, **fabrication techniques**, **and multifunctionality**, primarily for a new generation of smart, responsive, and sustainable Biocomposites.

1. Nano-structuring and Morphological Control

- **Advance**: Development of PPy nanostructures—nanotubes, nanowires, nanoparticles, and hollow spheres.
- **Example**: PPy-coated electrospun nanofibers for neural scaffolds and energy-harvesting devices[20].

2. Green and Bio-Inspired Synthesis

- **Advance**: Use of plant extracts, microorganisms, or biocompatible dopants (e.g., phytic acid, amino acids) for the green synthesis of PPy.
- **Example**: PPy synthesised using Aloe vera or tea extracts combined with chitosan or cellulose matrices [21].

3. Hybrid Composites with Other Conductive Nanomaterials

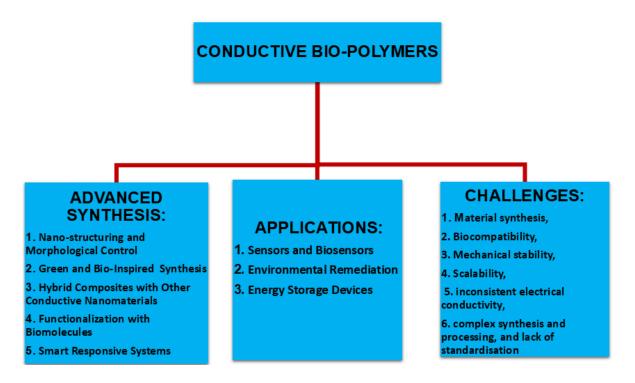
- **Advance**: Combination of PPy with graphene, MXenes, carbon nanotubes (CNTs), or metallic nanoparticles.
- Example: PPy–graphene oxide composites for supercapacitors or PPy–CNT scaffolds for nerve regeneration[19], Acacia Leucophloea Wood Sawdust-Based Activated Carbon and ZnCo₂O₄@PPy Composite[18].

4. Functionalization with Biomolecules

- Advance: Surface modification of PPy with peptides, growth factors, antibodies, or drugs.
- Example: PPy-chitosan composites functionalized for metal ion sensing[22]

5. Smart Responsive Systems

- **Advance**: Development of stimuli-responsive PPy Biocomposites that respond to pH, temperature, light, or magnetic fields.
- **Example:** PPy/TiO₂/Ti₃C₂TX nanocomposite film[23]



Application:

1. Sensors and Biosensors:

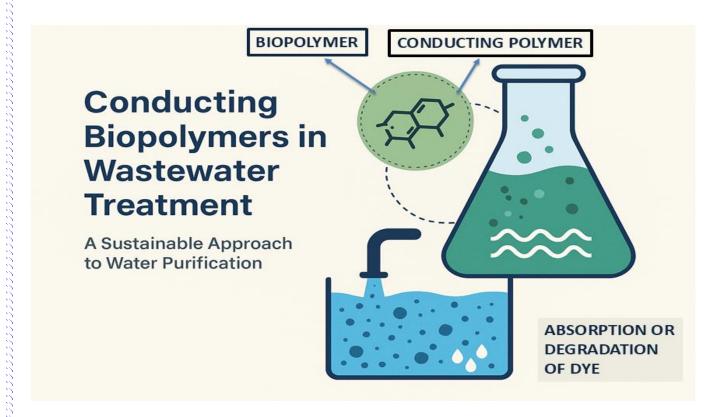
Polyaniline and Polypyrrole's electrochemical sensitivity make them perfect materials for Bio and chemical sensing. PPy-grafted nanoparticles and PPy-grafted biopolymers can detect Heavy metal ions[24], Xanthine oxidase, and glucose[7] with good sensitivity and selectivity. The sensor is cheap, flexible, lightweight, portable, and suitable for advanced technology[25].

2. Environmental Remediation:

Conducting polymer-based Biocomposites are developed for the removal of contaminants such as dyes, heavy metal ions[24], and oil from wastewater[26,27], due to their adsorption and redox capabilities. They are prepared using green synthesis processes with natural polymers to support eco-friendly water treatment technologies.

3. Energy Storage Devices:

Conducting polymer-based Biocomposites have greatly contributed to the development of batteries and supercapacitors. Due to their high surface area, mechanical flexibility and pseudocapacitive nature[27]. They make them compatible with energy storage devices. In addition to carbon-based materials like Graphene and carbon nanotubes (CNT)[28] improve cycle stability[29] and energy density.



Future Directions and Applications of Conducting Polymer-Based Biocomposites

Conducting polymer-based Biocomposites have garnered important attention due to their biocompatibility, ease of functionalization, and intrinsic conductivity. As research continues, several capable directions and applications are developing, such as Biomedical Applications, Environmental Remediation, energy storage and conversion, smart textiles and wearables, and Sustainable and green materials.

Conclusion

Conducting polymers-based Biocomposites and their derivatives have been developed as an up-and-coming class of functional materials due to their unique combination of electrical conductivity, biocompatibility, and mechanical tunability. Their flexibility has enabled large applications in chemical engineering, heavy metal sensing, environmental remediation (like dyes), and elastic electronics. By mixing polyaniline, polypyrrole with natural or synthetic polymers and nanoparticles, these Biocomposites offer various properties that can be adapted for specific end uses, particularly in smart scaffolds like heavy metal adsorption.

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Biochemical Method of Combating Malaria Vector

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Introduction:

Malaria is a leading cause of morbidity and mortality in tropical and subtropical regions caused by *Plasmodium* parasites, which are primarily transmitted to humans through the bites of infected female *Anopheles* mosquitoes (Fig. 1). It persists as a significant global health burden, despite decades of control efforts. The main intervention strategies include Insecticide-Treated NetsorLong-lasting insecticidal nets (ITNs/LLINs), Indoor Residual Spraying (IRS), larviciding, and the use of biocides. However, the effectiveness of these control measures is threatened by the increasing spread of resistance among malaria vectors. The impact of these insecticides on the environment and their safety concerns towards human and non-target species have increased complications [1]. To combat this, there has been a shift towards the development of novel and sustainable control strategies to combat malaria transmission.

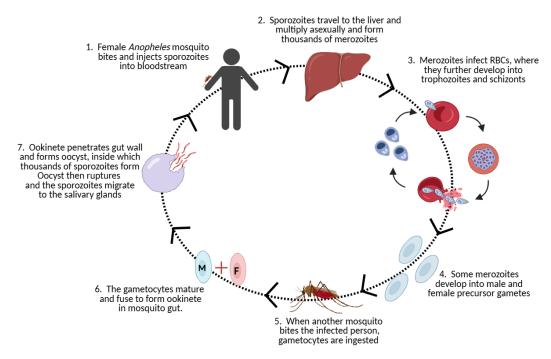


Fig. 1: Life Cycle of the Malaria Parasite - 1. Sporozoite injection into a human 2. Liver invasion by sporozoites and production of merozoites through schizonts asexually 3. Merozoites infect RBCs and undergo multiple stages, including the ring, trophozoite, and schizont stages, which then rupture, releasing merozoites that infect more RBCs. Some merozoites develop into gametocytes 5. These are taken up by mosquitoes during a blood meal 6. Gametocytes mature into gametes and fuse to form a

zygote. 7. Zygote develops into motile ookinete, penetrates the gut wall and forms oocyst, which mature and rupture, releasing sporozoites, which migrate to salivary glands until the mosquito's next blood meal.[3]

Global Impact of Malaria:

An estimate of 263 million cases was reported from malaria globally in 2023, with the African Region accounting for 94% of the global burden. Approximately 597,000 deaths due to malaria occurred worldwide, with Africa accounting for 95% of fatalities due to poor health infrastructure, poverty, and climatic conditions. Children under five and pregnant women are especially vulnerable [1]. India remains the most affected country in the Southeast Asia Region, although not as severely impacted as sub-Saharan Africa, particularly in several states, including Odisha, Chhattisgarh, Jharkhand, West Bengal, Maharashtra, Tripura, and Mizoram [2]. There was a significant decrease in the cases and deaths over the recent years due to increased control measures, resulting in India's exit from the High Burden to High Impact (HBHI) group in 2024 [1], marking a significant milestone towards the elimination of malaria.

Commonly Used Insecticides for Malaria:

Chemical insecticides play a pivotal role in mitigating malaria. Major classes of insecticides used for the control of malaria include pyrethroids, organophosphates, carbamates, and, to a lesser extent today, organochlorines such as Dichloro-diphenyl-trichloroethane (DDT) (Fig. 2). The mode of action of these classes is shown in Fig. 3, and the examples, applications, and limitations are summarized in Table 1. Pyrethroids are used widely in prevention interventions LLINs and IRS, because they have long residual activity and are highly effective in killing or repelling mosquitoes, without being toxic to humans and mammals at recommended doses (Lambda-cyhalothrin: 0.02-0.03 g/m², DDT: 1-2 g/m²) [4, 5]. They are also cost-effective for large-scale action. This is the only insecticide class that is used in LLINs because of their favorable safety profile, durability, and efficacy against mosquitoes, unlike other classes like organophosphates and carbamates, which are more toxic and unstable for LLIN treatment [4]. Organophosphates and carbamates play a crucial role in control measures and serve as alternatives to regions with pyrethroid resistance. They are both used in the IRS. Both these classes are generally safe to humans when used at operational doses (Malathion: 2 g/m², Bendiocarb: 0.4 g/m²) due to controlled application and less sensitivity of mosquitoes towards these insecticides [4, 5, 8]. DDT from the organochlorines was one of the earliest chemical insecticides that were used to control malaria due to its effectiveness in reducing malaria transmission, and residual activity as an IRS. However, its use has been restricted due to the development of resistance, environmental and health impacts [4, 7].

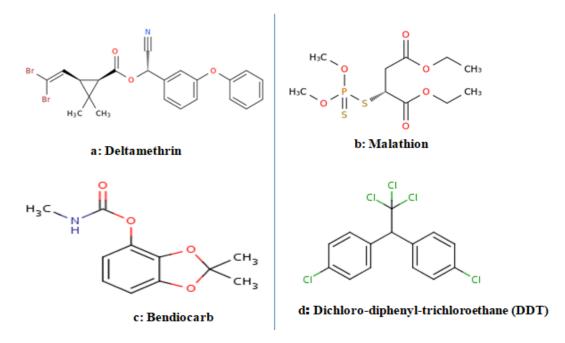


Fig. 2: Structures of some of chemical insecticides used for malaria vector control [6]

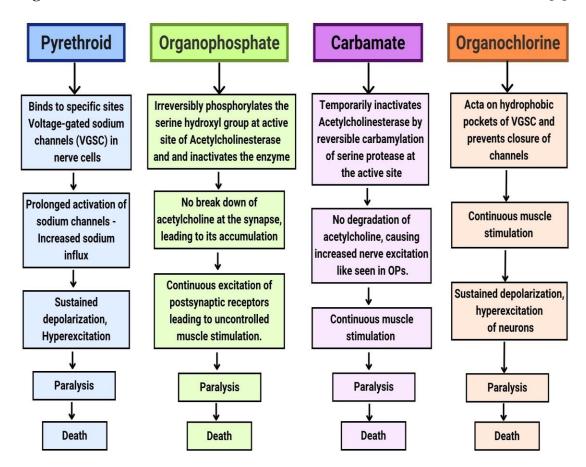


Fig. 3: Mode of action of the insecticide classes

Table 1: Comparison of key insecticide classes with their resistance mechanism and limitations

S.N o	Insecticide Class	Examples	Applicati ons	Limitations	Resistance Mechanisms	Referen ces
1.	Pyrethroids	Deltamethr in, Permethrin , Lambda- cyhalothrin	LLINs, IRS	Widespread resistance (kdr gene mutation); Reduced efficacy in many regions	kdr gene mutation: L1014F, L1014S, V1016G, F1534C, S989P, etc (VGSC) Overexpression of cytochrome P450s, GSTs Up-regulation of cuticle protein genes	[4, 12, 13, 14, 17]
2.	Organophosph ates	Malathion, Fenitrothio n, Pirimiphos - methyl	IRS	Increasing resistance (ace-1 gene mutation); Potentially toxic to humans and non-target species	ace-1 gene mutation: G119S Increased carboxylesterase activity	[4, 13, 15, 16, 17]
3.	Carbamates	Bendiocar b, Propoxur	IRS	Emerging resistance: Possibly toxic to humans and non-target species	ace-1 gene mutation: G119S - Increased carboxylesterase activity	[4, 13, 15, 17]
4.	Organochlorid es (restricted use)	DDT	IRS	Its use has been restricted due to environmental persistence, bioaccumulati on; Developed	kdr gene mutations: L1014F, L1014S (VGSC) Overexpression of GSTs, cytochrome P450s.	[4, 12, 17]

		resistance;	
		Harmful	
		effects on	
		health	

The Rising Limitations:

Despite their important role in vector control, all 4 major classes of chemical insecticides are facing increased limitations that are affecting their effectiveness and sustainability. The most prevalent reason is the growing resistance of mosquito vectors towards these insecticides (Table 1). The resistance towards pyrethroids and DDT is widespread, and towards organophosphates and carbamates is increasing rapidly [9]. This is due to the genetic mutations in the malaria vectors, like kdr mutations in voltage-gated sodium channels for pyrethroids and DDT, and mutations in the acetylcholinesterase gene (ace-1) for organophosphates and carbamates [8, 9]. Also, the increased resistance due to altered metabolic pathways, where there is an over expression of detoxifying enzymes, mainly glutathione S-transferases (GSTs) and cytochrome P450s. The over expression of enzymes can also confer cross-resistance to multiple insecticide classes. Modification or thickening of the cuticle confers cuticular resistance, reducing insecticide resistance (Fig. 4). This can make the management efforts more challenging [9]. To combat this, the use of combination approaches to overcome resistance, such as using pyrethroid nets and non-pyrethroid IRS; pyrethroid and second active agent (such as chlorfenapyr, piperonyl butoxide, or pirimiphos-methyl); alternating pyrethroid and carbamate IRS; has been successful to manage insecticide resistance, still their effectiveness relies on the local context and they require careful planning and monitoring [10, 11]. This deepens the need for novel approaches and new control agents for malaria transmission.

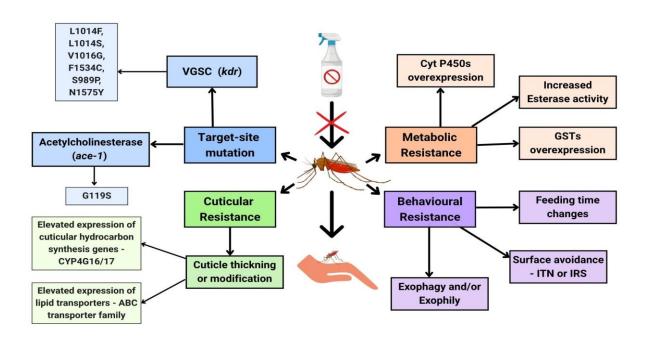


Fig. 4: Resistance mechanisms of malaria vectors: Malaria vectors develop resistance to insecticides primarily through target-site mutations (kdr for pyrethroids/DDT and ace-1 for organophosphates/carbamates), metabolic alteration mechanisms (increased enzyme detoxification by P450S and GSTs) these are coupled with cuticular and behavioral resistance. [13, 15, 17]

Bioinsecticides: The New Approach

The potential of bioinsecticides has been highlighted in recent research. They are a type of biopesticide that is derived from natural materials, organisms as plants, bacteria, fungi, protozoa, and viruses. Research has shown that the biopesticide efficiently kills both conventional and chemical insecticide-resistant mosquitoes at standard doses. This is beneficial because the resistance mechanisms developed against synthetic insecticides, like target-site mutation, metabolic resistance, high-affinity binding, cuticular resistance, and behavioral resistance, do not confer cross-resistance to bioinsecticides. They are safer and potentially more sustainable compared to the synthetic insecticides. Different types of bioinsecticides include bacterial, fungal, plant-based, and combined approaches (Fig.5) [9, 18, 19].

Bacterial Bioinsecticides like Bacillus thuringiensis israelensis (Bti), Bacillus sphaericus (Bs), and Lysinibacillussphaericus(Ls) are widely used for larval control. They are highly specific to mosquito larvae. The applications stretch to small-scale and large-scale operations are still limited. They are commonly formulated as larvicides and are applied to the breeding sites of mosquitoes [19, 20]. Another biological agent, Chromobacterium sp. Panama (Csp_P) has been observed to kill both insecticidesusceptible and insecticide-resistant Anopheles mosquitoes experimentally [21, 22]. Fungal Bioinsecticides include Beauveria bassiana, which can infect both larvae mosquitoes. Metarhiziumanisopliae and Isariafumosorose areduce mosquito survival effectively. These insecticides can be applied as spores. Conditions like temperature and humidity affect their efficacy, and the production and formulation of the fungal agents remain a challenge [19, 23]. Plant bioinsecticides are plant-derived compounds such as including neem, essential oils, citronella, lemongrass, pyrethrum, and alkaloids, etc. which act as insect growth regulators, repellents, larvicides, or neurotoxins, disrupting the development and behaviour of mosquitoes [24]. Other emerging approaches include the combination of bioinsecticidal agents, resulting in a synergistic effect, which can enhance the overall efficacy and minimize the risk of resistance development. One of the examples of this includes the formulation of Bti with fungal pathogens [25]. Each combination can be tailored according to the ecological conditions and associated factors.

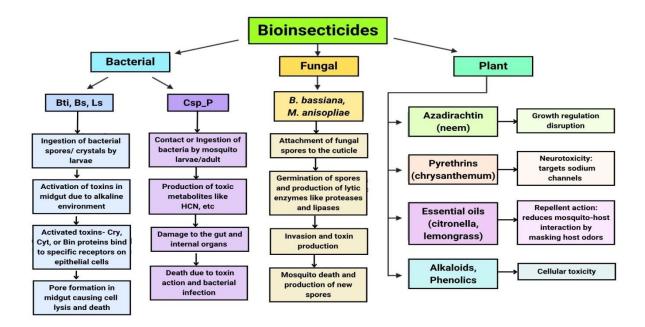


Fig.5: Classification of Bioinsecticides: Bacterial insecticides kill by producing toxins or toxic metabolites that damage mosquito organs, Fungal insecticides kill by infecting cuticle and producing enzymes, Plant-based insecticides act by disrupting growth, targeting nerves, cell toxicity and repellent action. [19, 21, 24]

Discussion:

Malaria continues to be a global health threat, specifically in regions with limited resources and high transmission rates. Chemical insecticides have been crucial agents in combating malaria incidence, but their effectiveness is threatened by increasing resistance mechanisms in malaria vectors, leading to their ineffectiveness. Problems also arose due to the impacts on the environment and safety concerns over their effects on human and non-target organisms [1, 4]. This has urged the search for alternatives and sustainable measures to control vectors. Bioinsecticides, which are derived from natural sources like bacteria, fungi, and plants, stand as a promising solution. This is due to their ability to be effective against susceptible and resistant vectors and their lower risk of resistance development and environmental effects. They are safe and non-toxic to humans and non-target organisms, which makes them more suitable for use in affected regions to control malaria [18]. However, problems arise regarding their large-scale production, formulation, implementation, and integration into the current control strategies. And biological methods alone may not provide sufficient control. Interventions combining both chemical and biological strategies can counter the problems, making the control programs more adaptable, sustainable, and tailored to the target region.

Conclusion:

The most important step to combat malaria spread at present is to overcome increasing resistance and environmental challenges. Biological insecticides show great promise in controlling malaria effectively. Drawbacks arise in their production and implementation, but they can be countered by continued research on the betterment of these strategies, and also investments towards the implementation of these measures.

Future research is needed to investigate the use of integrated insecticides combining both chemical and physical agents to overcome resistance and ensure sustainability. By embracing innovative and environmentally friendly solutions and tailoring strategies according to the local needs, malaria control and elimination can be achieved.

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Innovations and shortcomings in Electro-Chemical Energy Storage Devices

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Abstract

Owing to modern-day state-of-the-art material fabrication and characterization tools, significant achievements have been made in supercapacitor electrode materials. Recent advancements in supercapacitor electrode materials, which enable quick charging and discharging in a matter of seconds, have brought attention to the crucial roles that cycle stability and extended operating life play in enhancing device reliability. Researchers have investigated a variety of materials, including metal oxides, carbon-based nanomaterials, conductive polymers, and their composites, using their unique characteristics to improve supercapacitor performance. The development of electrochromic, self-healing, thermally chargeable, and micro-supercapacitors are noteworthy innovations that demonstrate the rapid progress in this field. Additionally, a lot of research has been done on improving electrolytes to reach higher power and energy densities, which will increase overall performance and dependability. This review provides a thorough and unique overview of the major advancements, new materials, and technological advancements in supercapacitor electrodes during the previous five years.

Introduction

Due to human-caused climate change, there is an urgent need for every country to reduce its carbon footprint. To reduce the carbon footprint, conventional fossil fuels must be replaced with clean and regenerative sources of energy viz. solar, wind, and tidal energy. However, the scope of practical application is largely limited due to the spasmodic behavior of these sources of energy. To fulfill the contemporary energy demand there is a need to develop a powerful source of energy [1]. Supercapacitors are a powerful energy source in hybrid energy storage systems because of their remarkable energy storage mechanism [2], which is characterized by high power density (2–10 kW/kg), high efficiency, ultra-long cycle life (10,000 cycles), environmental sustainability, safety standards, high-rate stability, and quick charge and discharge kinetics [3].

Mechanism

Based on the charge-discharge mechanism supercapacitors are classified into 3 types (i) Carbon material with electric double-layer capacitors (EDLCs) type behavior, which stores charge non-faradically by absorption and desorption of ions at the interphase between the electrolyte and electrode surface [4] (ii) conductive polymers and metal nitride/oxide/hydroxide with Pseudo-capacitive behavior, stores energy faradically by reversible redox reactions at the electrode-electrolyte interface and (iii) Hybrid SCs, bridge the gap between batteries and supercapacitors, by using a capacitive type electrode and a Faradic electrode. Due to the lack of translational charge transfer between electrolyte and active electrode [5], EDLCs have low specific energy density. Pseudocapacitors, which include redox reactions at the electrode-electrolyte interface offer relatively large capacitance and energy density at the expense of

decreased cycle stability and structural instability [6]. Due to the above-mentioned shortfall of both EDLCs and pseudo-capacitors, it is necessary to hybridize transition metal oxides with carbonaceous material, which may be employed efficiently to increase the electrochemical performance [7]. These issues are overcome by synthesizing nanostructured redox-active materials and combining them with conductive substrates or matrixes to produce nanohybrids [8]. Electrochemical capacitors (ECCs) employing hybrid electrode materials provide better energy density due to the combination of both faradaic and non-faradaic charge storage mechanisms. These devices are referred to as hybrid capacitors.

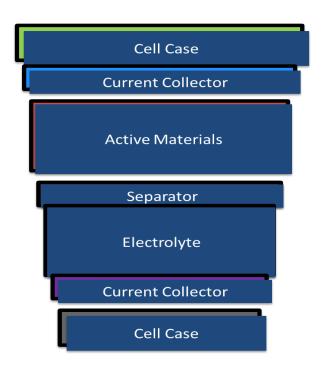


Fig 1. Schematic representation of internal layout of a supercapacitor structure

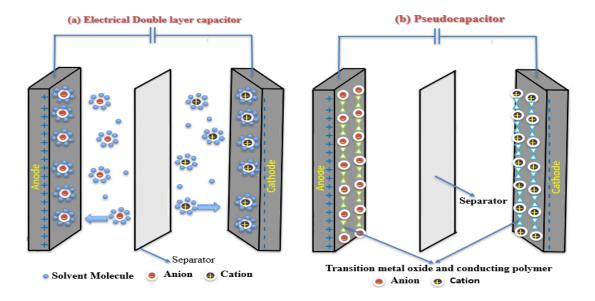


Fig 2. The characteristic representation of conventional supercapacitors (SCs) (a) electrical double-layer capacitors (EDLCs) (b) Pseudocapacitors.

Recent Advances in Supercapacitor Technology [9]

S. No.	Startup	Type	Specification			
1	nanoCaps	Supercapacitor Electrodes	 produces high surface-area-to- volume ratio supercapacitor electrodes for outstanding electron conductivity and fast ion diffusion. 			
2	Novac	Solid State Electrolyte Supercapacitors	 EV performance and efficiency are improved. Low risk of explosion, evaporation, and leaks due to the absence of liquid. 			
3	enyGy	Graphene-based Supercapacitors	• improved energy storage capacity utilizing graphene-based materials.			
4	Carbon-ion	Turbo-charged Supercapacitors	 Compared to traditional supercapacitors, carbon-ion, or Cion, cells offer superior power characteristics. Supporting fast charging, quick energy storage, and sustainable end-of-life recycling methods, thus extending the cell's operational lifetime. 			
5	florrent	Pure-carbon Electrode Energy Storage Medium	• use an active material, Contoured Carbon (domestically sourced hemp fibers), to enhance the energy density of its symmetric EDL capacitors.			
6	Innovasion Labs PINC	Nano-manufactured Supercapacitors	 platform improves electrical characteristics and outperforms existing energy storage capabilities by connecting functional nano-scale components in parallel. Increases the surface area by using its nano-assembly method, which 			

			improves the flow of ions and electrons.
7	Hyper- er_objects	Pressure Energy Recovery System (PERS)	 an energy recovery system, from pressurized liquids and stores it in high-power input supercapacitors.
8	Carbon Lite System	Biomass-derived Graphene Supercapacitors	 converts waste biomass into graphene to develop supercapacitors. Offers excellent electrical conductivity, mechanical strength, and surface area when utilized as an electrode material in supercapacitors.
9	Ecocitor	Nanotech-based Supercapacitors	 Using recycled components and carbon-based nanomaterials, these supercapacitors charge faster and are more cost-effective. Have longer lifespans, avoid leakages or swelling, and are compact.

Recent Innovations in Supercapacitor Technology

• Concrete Supercapacitors

- Developed by MIT researchers
- Made from concrete and carbon black
- inexpensive and widely available materials.
- The breakthrough stems from the concrete's inner framework: it's infused with a densely intertwined network of conductive material, giving it an exceptionally large surface area. By mixing carbon black into the cement, researchers create filament-like structures throughout the solidified material. Once these are immersed in a conventional electrolyte such as potassium chloride the concrete transforms into a high-performance supercapacitor. Integration of supercapacitor into building foundation leads to 10 kWh of energy storage in a 3.5-meter-wide concrete cube which is sufficient for average household [10].

• Pi-Pop E-Bike Based on Supercapacitors

- A group of entrepreneurs in France created an e-bike that stores energy using supercapacitors rather than lithium batteries.
- ➤ Pi-Pop's supercapacitors are constructed of carbon, conducting polymer, aluminum foils, and pulp all of which are abundant and recyclable.

- ➤ Pi-Pop's supercapacitors have a lifespan of 10-15 years substantially outlasting the 5 to 6 years of a standard lithium battery.
- ➤ This breakthrough addresses the environmental challenges associated with lithium batteries and provides a quick, efficient energy storage option that could change urban mobility [11].

• Ultra micro-Supercapacitor

- ➤ Researchers at the Indian Institute of Science in Bengaluru recently produced an ultra-microsupercapacitor with three orders of magnitude lower dimensions than prior microsupercapacitors.
- Researchers built a supercapacitor using two-dimensional materials graphene and MoS₂ for its electrodes. Each electrode is composed of a few layers of MoS₂ flakes topped by graphene flakes, all assembled on a silicon dioxide base and immersed in a gel electrolyte.
- ➤ 2D materials as field-effect transistors: The MoS₂/graphene electrodes act like field-effect transistors, which greatly enhance the electrical characteristics of the device.
- ➤ Gate-voltage-boosted capacitance: When a gate voltage is applied, an electric double-layer forms not only at the electrode-electrolyte boundary but also between the stacked 2D layers. This effect increases the areal capacitance dramatically from 1.8 mF/cm² to about 54 mF/cm² [12].

• Solar-Powered Smart Supercapacitor

- ➤ Developed by researchers from Clemson University and the Indian Institute of Science.
- ➤ Researchers have developed a single, compact supercapacitor that both harvests solar energy and stores it electrochemically by using a unique stacked layer of vanadium pentoxide (V₂O₅) and zinc oxide (ZnO).
- > Simplified design: This "all-in-one" device eliminates the need for separate solar panels and storage units, making the system much less bulky compared to conventional setups.
- > Strong performance: It shows excellent electrochemical characteristics and maintains stability through over 5,000 charge-discharge cycles
- Future applications: The technology could lead to self-charging electronics like wearable health monitors and offer a compact alternative to traditional solar cells for capturing sunlight [13].

• Seaweed-Based Paper Supercapacitor

- > Developed by Researchers at the Gujarat Energy Research and Management Institute.
- Researchers claimed it world's thinnest, lightest, and most fully biodegradable supercapacitor using cellulose nanofibers extracted from seaweed. They grew reduced graphene oxide—zinc oxide (rGO–ZnO) nanowires atop the seaweed-derived fibers, forming a flexible "anodic paper." This device can fully charge in just 10 seconds, boasts high tensile strength, and maintains stable performance across 6,000 charge-discharge cycles without any degradation.
- Energy density: 9.5 Wh/kg
 Series resistance: 120 Ω

- ➤ Cost-effective and scalable: Fabricated using a simple, hands-on process well-suited for large-scale production
- ➤ This innovation a seaweed-based, paper-like supercapacitor is biodegradable, inexpensive, and delivers exceptional performance, making it a promising candidate for sustainable, flexible energy storage solutions [14].

• Structural Supercapacitors

- > Developed by Engineers at the University of California San Diego.
- > It combines mechanical support with energy storage capabilities.
- Researchers developed a structural, fabric-based supercapacitor by weaving carbon fibers into a cloth, which is then coated with a hybrid layer of conductive polymer and reduced graphene oxide (rGO). This composite structure enhances mechanical durability while boosting ion transport and energy storage capacity.
- The device uses a solid-state electrolyte made from epoxy resin blended with polyethylene oxide (PEO). Uniquely, the electrolyte is engineered to have a concentration gradient with higher PEO levels and salt content near the electrodes optimizing ion mobility close to the active material while preserving the overall structural integrity.
- ➤ By integrating strong, conductive electrodes with a gradient-based solid electrolyte, the design delivers both enhanced power performance and load-bearing capability offering a lightweight energy storage solution ideal for electronics and vehicle components that don't sacrifice strength for capacity [15].

Current limitations of supercapacitors

• Limited Energy Density

Supercapacitors can charge and discharge rapidly, but they store far less energy per unit mass or volume than lithium-ion batteries. This gap typically under 20 Wh/kg versus batteries' 30–200 Wh/kg limits their suitability for long-term energy supply, often relegating them to secondary or hybrid roles [16].

• High Material & Manufacturing Costs

Premium electrode materials like graphene, carbon nanotubes, and activated carbon offer superior performance but come with high synthesis costs and energy consumption. For instance, processes such as chemical vapor deposition require temperatures over 1,000 °C and clean-room standards, driving up production expenses [17].

• Scale-Up & Quality Consistency

Scaling lab-scale breakthroughs like graphene, MXenes, or MOFs to mass production remains difficult. Manufacturing at scale often leads to yield losses (e.g., 15–20% reduction for graphene) and batch inconsistency with capacitance varying by 30% between units undermining commercial reliability [18].

• Raw-Material and Supply-Chain Vulnerabilities

Many essential materials such as high-purity graphite, rare-earth oxides, and specialized electrolytes are sourced from limited regions, exposing the supply chain to export controls, geopolitical risks, and price volatility. Graphite export restrictions in 2023, for example, caused spikes in graphene prices [19].

Absence of Industry Standards & Testing Protocols

With no universal benchmarks for performance metrics such as cycle life, safety, or durability, products vary widely. This inconsistency hampers adoption in sensitive sectors like automotive and aerospace, where rigorous standards are essential [20].

• Safety, Thermal & Voltage Management

Thermal runaway, electrolyte breakdown, and risks from overcharging/over-discharging pose safety challenges especially in high-power systems. Incorporating robust thermal management, voltage monitoring, and protection circuitry raises both complexity and cost [21].

• Battery Competition & Market Positioning

Lithium-ion batteries and emerging solid-state alternatives remain dominant due to their higher energy density and established ecosystem. Supercapacitors, though unmatched in power delivery speed or cycle life, are often confined to niche applications [20].

• Regulatory & Environmental Constraints

Environmental regulations such as EU bans on solvents like NMP and nanoparticle controls under REACH complicate production processes and can reduce device performance. Additionally, carbon emission tariffs (e.g., EU's CBAM) penalize energy-intensive manufacturing, further increasing costs [22].

Conclusion

In short, supercapacitors deliver lightning-fast charging, power densities between 2 and 10 kW/kg, and lifespan beyond 10,000 cycles, so they slot in nicely beside conventional batteries. Still, commercialization faces roadblocks-high costs, uneven scaling, fragile supply chains, spotty standards, tricky thermal control, stiff battery rivalry, and wary regulators-yet recent breakthroughs keep hope alive. Startups such as nanoCaps, Novac, and Carbon-ion are rethinking electrodes and electrolytes, while lab work on concrete cells, seaweed-paper devices, graphene-MoS2 chips, and energy-harvesting fabric widens the horizon. For these ideas to hit the street, prices must fall, factories must ramp up, standards must firm up, and clever hybrid designs must emerge.

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Seeing Beneath the Soil: Advances in Radiological Survey Techniques for Archaeological Excavations

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Abstract

Radiological techniques have transformed archaeological research by enabling non-invasive exploration and analysis of subsurface features, artifacts, and human remains. This review highlights the major radiological methods currently employed in archaeological excavations, including Ground Penetrating Radar (GPR), X-ray Radiography, Computed Tomography (CT), Neutron Radiography, Gamma Radiography, Portable X-ray Fluorescence (pXRF), and Synchrotron Radiation Techniques. Each method offers unique advantages in visualizing internal compositions and buried structures while preserving the integrity of the archaeological record. The integration of these technologies has significantly advanced documentation, conservation, and interpretation in archaeological science, providing a multidimensional view of the past.

Keywords: Archaeometry, Non-destructive techniques, Ground Penetrating Radar, Computed Tomography, Cultural heritage imaging

Introduction

Archaeology has long relied on excavation and manual documentation to uncover and interpret remnants of past civilizations. However, these traditional methods are often invasive and can risk damaging fragile cultural materials. In recent decades, radiological techniques have emerged as essential tools in archaeological research, offering non-destructive, high-resolution insights into both buried structures and the internal composition of artifacts. Techniques such as Ground Penetrating Radar (GPR), X-ray Radiography, and Computed Tomography (CT) scanning allow researchers to examine features hidden beneath the soil or within artifacts without altering their context or form. Additionally, advanced methods like Neutron Radiography and Synchrotron Radiation provide unparalleled detail at the molecular level, enhancing material characterization, provenance studies, and conservation planning. This article explores the application and impact of these radiological techniques in modern archaeology, emphasizing their role in transforming how sites are surveyed, analyzed, and interpreted. Following are radiological techniques:

- 1. Ground Penetrating Radar (GPR) is a non-invasive geophysical method that uses high-frequency electromagnetic waves to detect and map subsurface structures. It is widely employed in archaeological excavations to locate buried walls, graves, voids, and artifacts without disturbing the site. GPR transmits radar pulses into the ground and records reflected signals from different materials, generating high-resolution images of underground features. Its effectiveness depends on soil composition, moisture content, and target depth. GPR has significantly advanced archaeological prospecting by enabling rapid, accurate site assessments (Conyers, 2013; Goodman & Piro, 2013).
- 2. X-ray Radiography is a widely used non-destructive imaging technique in archaeology for examining the internal structure of artifacts and human remains. By passing X-rays through objects, it reveals hidden features such as manufacturing methods, repairs, and inscriptions. This technique is particularly valuable for analyzing metals, ceramics, and organic materials embedded within other substances. In bioarchaeology, it aids in the assessment of skeletal pathologies and trauma without disturbing remains. Its high resolution and ability to visualize internal details make it essential in conservation, research, and documentation (Beckett & Conlogue, 2020; Lang & Middleton, 2005).
- 3. Computed Tomography (CT) Scanning is a high-resolution, non-invasive imaging technique that generates cross-sectional and 3D images of objects by combining multiple X-ray projections. In archaeology, CT scanning is invaluable for analyzing mummies, skeletal remains, and complex artifacts without physical damage. It enables detailed visualization of internal structures, pathologies, and manufacturing techniques. CT has revolutionized bioarchaeological and conservation studies by offering insights into health, trauma, and artifact composition. Its precision makes it ideal for digitally preserving and reconstructing fragile heritage materials (Beckett & Conlogue, 2020; Panzer et al., 2017; Roberts & Manchester, 2007).

- **4. Neutron Radiography** is a non-destructive imaging technique that uses neutrons to penetrate materials and produce detailed internal images, especially effective for visualizing light elements like hydrogen. In archaeology, it is particularly useful for detecting organic materials such as wood, leather, or resins enclosed within metal or stone artifacts. Unlike X-rays, neutrons can easily pass through dense metals while highlighting low atomic number substances, offering a complementary view for artifact analysis. It has proven valuable in conservation, restoration, and provenance studies (Lehmann et al., 2005; Kardjilov et al., 2010).
- 5. Portable X-ray Fluorescence (pXRF) is a non-destructive analytical technique widely used in archaeology to determine the elemental composition of artifacts directly in the field. It allows for rapid, in situ analysis of materials such as ceramics, metals, pigments, and soils without the need for sampling or laboratory preparation. pXRF is particularly valuable in provenance studies, helping to trace the geographic origins of raw materials. Its portability, speed, and ease of use have made it an essential tool for archaeological surveys, conservation, and cultural heritage studies (Shackley, 2011; Frahm, 2014; Goodale et al., 2012).
- **6. Gamma Radiography** is a non-destructive imaging technique that uses gamma rays, typically from isotopes like Iridium-192 or Cobalt-60, to visualize the internal structure of dense archaeological materials. It is particularly effective for examining thick metal or stone artifacts

that are less penetrable by X-rays. In archaeology, gamma radiography helps detect hidden features, structural weaknesses, or inclusions within large or corroded objects. This technique plays a critical role in artifact conservation, restoration planning, and structural assessment, especially when traditional radiography is limited (Schreiner et al., 2004; Vontobel et al., 2005; Csikai, 2012).

7. Synchrotron Radiation Techniques utilize high-intensity X-rays produced in particle accelerators to investigate materials at micro to nano scales. In archaeology, these methods—such as X-ray fluorescence (XRF), X-ray absorption spectroscopy (XAS), and phase-contrast imaging—are invaluable for analyzing the composition, structure, and degradation processes of artifacts. Synchrotron radiation allows for non-destructive, high-resolution analysis of pigments, corrosion layers, organic residues, and ancient inks, providing insights into manufacturing techniques and provenance. Its ability to detect trace elements and map chemical distributions makes it a powerful tool for cultural heritage science (Cotte et al., 2010; Bertrand et al., 2012; Janssens et al., 2010).

Conclusion

Radiological techniques have become indispensable in archaeological investigations, offering non-invasive alternatives to traditional excavation and analysis. From GPR's ability to map buried structures to the atomic-scale resolution of synchrotron imaging, these methods enable comprehensive, detailed, and context-sensitive exploration of cultural heritage. Their application not only enhances artifact preservation and site integrity but also broadens our interpretive capacities by uncovering information invisible to the naked eye. As technology continues to advance, the integration of radiological methods with digital modeling and artificial intelligence promises even more precise reconstructions and deeper understanding of archaeological contexts. Ultimately, these innovations are reshaping archaeological practice and expanding the boundaries of discovery.

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