Advancing Sustainability: Biodegradable Electronics and New Materials through AI and Machine Learning

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Abstract:

Artificial Intelligence (AI) and machine learning (ML) are revolutionizing science and engineering by enabling researchers to analyze vast amounts of data, uncover patterns, and make predictions with unprecedented accuracy. The integration of AI and ML techniques are driving innovation across disciplines, paving the way for groundbreaking discoveries and technological advancements. On another corner, sustainability in core engineering disciplines is taking hold. Much work has been done on transient technologies, with a particular emphasis on transient electronics. The research in this domain explores the new materials, architectures, and functionalities of devices with a time-bound lifetime. We present a whole landscape view of the field with a focus on the most recent developments, focusing mainly on transitory materials such as metals, polymers, and semiconducting materials. The development and optimization of commercially viable materials are being accelerated by the rapid integration of AI and molecular design tools for high-throughput experimentation. There is a discussion of the difficulties in expanding data-driven technologies from small molecules to polymers, highlighting the importance of AI in finding new molecular designs and revamping existing molecules for innovative applications. The paper emphasizes how crucial it is to define and standardize polymer systems for ML models to generate a cohesive data collection system for AI and automation improvements. It also highlights the need for improvements in ML methods to fully utilize the advantages of data-driven polymer chemistry, highlighting the significance of reliable and varied datasets for predictive models in the synthesis of polymers. The article's conclusion addresses the necessity of fundamental studies in polymer classification and standardization to fully capitalize on the potential of polymer development.

1. Introduction

Sustainable development is a way of utilizing resources that strives to fulfill the needs of humans, while also protecting the environment so that they can be addressed not only at present but also potentially for future generations.[1] The rise of electronics as an omnipresent aspect of modern society has brought difficulties in managing electronic waste (e-waste). Addressing the necessity for zero-waste consumable electronics, research has been geared towards transient electronics, developing electronic devices based on biodegradable materials.[2] Transient electronics is a burgeoning technology that has the unique ability to physically dissolve in controlled ways within physiological contexts.[3] However, to develop biodegradable electronics, it is necessary to explore new material class with biodegradable substrates, insulators, conductors, and semiconductors, which together make up the basic components of devices.[4]

Traditionally, materials discovery and synthesis has been based on trial-and error methods, which rely on researcher's insight, knowledge, and experience; wherein the researchers would spend significant time and resources conducting experiments and simulations based on their intuition and existing knowledge. However, this approach often resulted in lengthy trial-and-error cycles and missed opportunities for innovation. With AI, researchers can harness the power of ML and data analytics to accelerate the discovery process. By analyzing large dataset of materials properties, chemical compositions, and synthesis methods, AI can identify patterns and relationships that might elude human intuition alone. Furthermore, AI enables the exploration of vast design spaces and optimization of materials properties through virtual simulations and predictive modeling. This not only accelerates the discovery of new materials but also allows researchers to tailor materials properties for specific applications with greater precision and efficiency. In this review, we consolidate the landscape of the AI and ML-based materials discovery focusing on four categories of representative materials including natural polymers, synthetic polymers, metals, and semiconductors, which form the cornerstone of any electronic device.

2. Transient Electronics

The Global e-waste Monitor 2020, released by the Global e-waste Statistics Partnership (GESP), provides a thorough overview of the global e-waste problem. In 2019, a total of 53.6 million metric tons (Mt) of e-waste, which refers to discarded electronic items that contain a battery or plug, such as computers and mobile phones, was generated globally. Merely 17.4 % of e-waste was officially recorded as being properly gathered and recycled in 2019. The new

analysis forecasts that global e-waste will reach 74 million metric tons by 2030. This increase is driven by escalating rates of electric and electronic consumption, shorter product lifespan, and constrained alternatives for repair. In 2019, valuable components such as iron, copper, and gold, which are estimated to be worth around US 57 billion dollars, were predominantly discarded or incinerated instead of being collected for processing and reuse. In this regard, reusing and recycling valuable materials found in e-waste can facilitate a circular economy by promoting the usage of secondary materials.[5] However, the analysis shows that recycling and reuse alone may not be able to keep up with the e-waste figures and therefore the best alternative solution to this issue lies in the context of transient technology.

Transient technology is an emerging area that necessitates the development of materials, technologies, and systems to have the ability to disappear without leaving behind any noticeable or traceable remnants after a period of steady operation. Electronics possessing the ability to disintegrate or vanish after consistent functioning are emerging as a captivating area of study and have garnered growing interest. Recently, there has been a noticeable expansion of transience technology into areas like intelligence applications such as bioelectronics, environmental monitoring systems, energy harvesters, and storage.[4] For example, a soft, skin-interfaced microfluidic system capable of monitoring sweat loss, sweat rate, pH, and chloride concentration using thermoplastic copolyester elastomer (TPC) as a microfluidic layer and a cellulose film as a sealing layer has been combined to demonstrate applications in sweat biomarkers. Here, the fabricated devices have been shown to fully degrade in natural soil or composting facilities to organic compounds that can act as plant nutrients, thereby eliminating environmental stresses from discarded devices.[6] On the other hand, polylactic acid (PLA) has been reported in many of medical applications including drug carriers,[7] scaffolds for tumor applications,[8] dental implants,[9] etc. The PLA with magnesium composite demonstrates osteogenic properties and promotes bone cell ingress.[10]

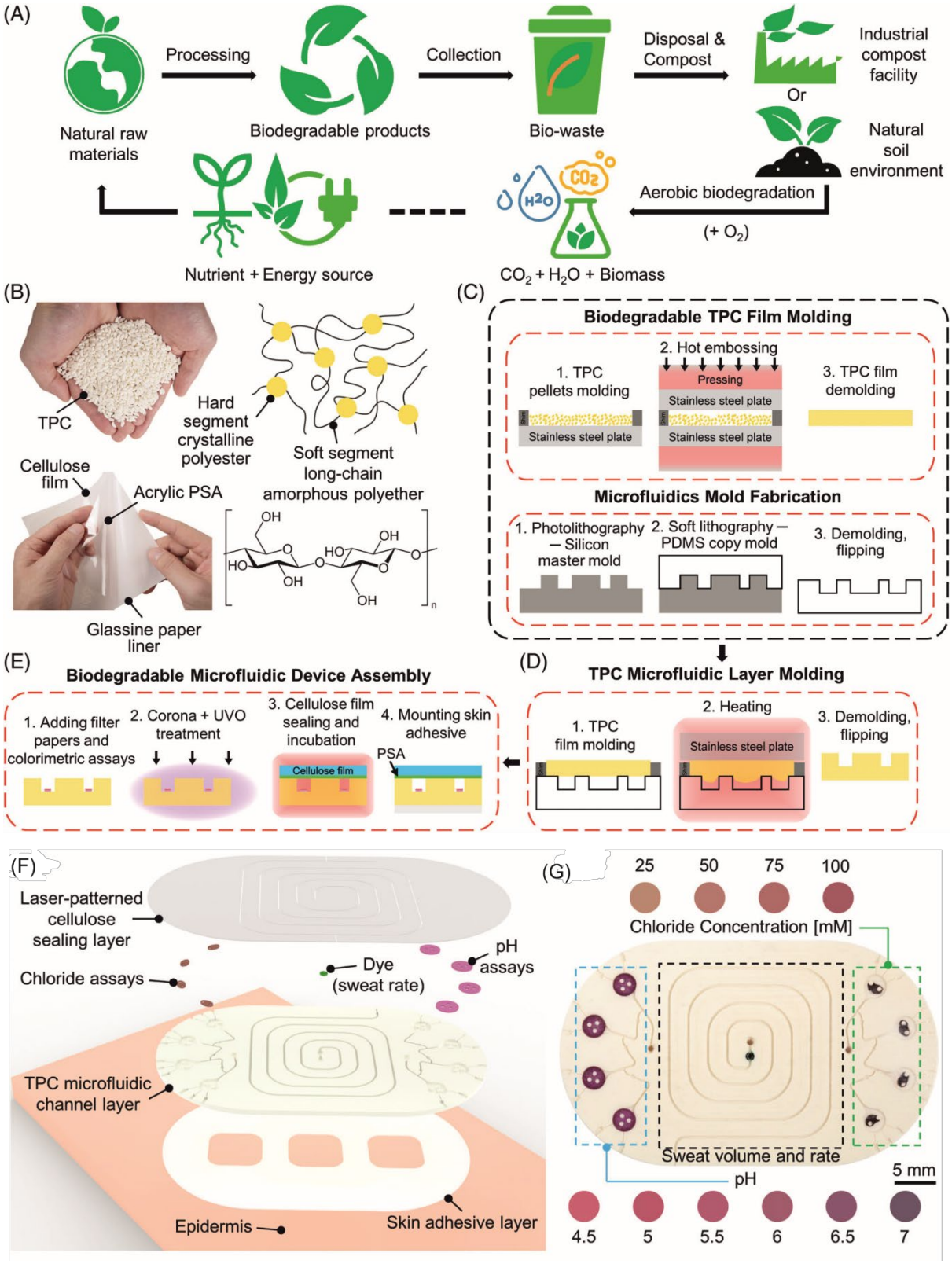

Figure 1: (A) Schematic illustrating the biodegradation process of biodegradable materials in natural soil environments, or in industrial compost facilities. (B) Chemical structures and pictures of a biodegradable thermoplastic copolyester elastomer (TPC) as a microfluidic layer and a cellulose film with an acrylic pressure-sensitive adhesive (PSA) for the sealing layer. (C–

E) Step-by-step procedure of the device fabrication (C) Fabrication of a silicon master mold, a PDMS replica mold, and a molded TPC film; (D) Fabrication of a TPC microfluidic layer; (E) assembly of a device by adding filter papers and colorimetric assays to the TPC microfluidic layer, bonding the cellulose sealing layer on top, and mounting onto a skin-compatible adhesive on the bottom. (F) Schematic illustration of the microfluidic device showing the different layers and components. (G) Optical image of a device that includes a microfluidic channel for sweat volume and rate measurement, and reservoirs with colorimetric assays for pH and chloride analysis. The color evolution of both assays occurs over physiologically relevant ranges of chloride and pH in human sweat. Reproduced with permission.[6]

4. Functional Biodegradable Materials

Transient materials are able to consistently keep their complete functionality and capabilities under regular usage, ensuring reliable performance, while finally degrading at the end of life without leaving any potential harmful residues. Upon the introduction of a solution trigger, the materials will undergo either complete physical or chemical dissolution in a controlled fashion, either partially or entirely. This review focuses on discussing recent research on such transient materials including metals, polymers, and semiconductor materials.

4.1 Metals

Conductive materials in electronics function as electrodes and connectors. Conventional metals are attractive in comparison to conductive polymers due to their low resistance, stable characteristics, and well-established functions in commercial products. Currently, researchers have been investigating the use of magnesium (Mg), zinc (Zn), iron (Fe), tungsten (W), and molybdenum (Mo) as soluble metals in the field of transient electronics. Each of these metals plays a crucial role in biological processes and has the potential to be utilized in biomedical implants.[11,12] Typically, Mg and Zn exhibit fast transient behavior in DI water and biological solutions, while W and Mo display gradual but foreseeable rates of degradation. These behaviors offer diverse alternatives to fulfill the demands of degradation spans for varied applications. W and Mo can be employed for slow transient applications, such as medical devices that need metals to directly interact with biological tissues for signal detection, because of their purposeful and controlled rates of degradation. Mg and Zn can be considered for applications requiring temporary functionality due to their rapid degradation, such as secure electronics that need to be disappeared within a defined limited time frame.[4]

4.2 Polymers

Two categories of biodegradable polymers are distinguished based on their origin: natural polymers, derived from renewable and natural resources, and synthetic polymers, which are produced from petroleum oil.

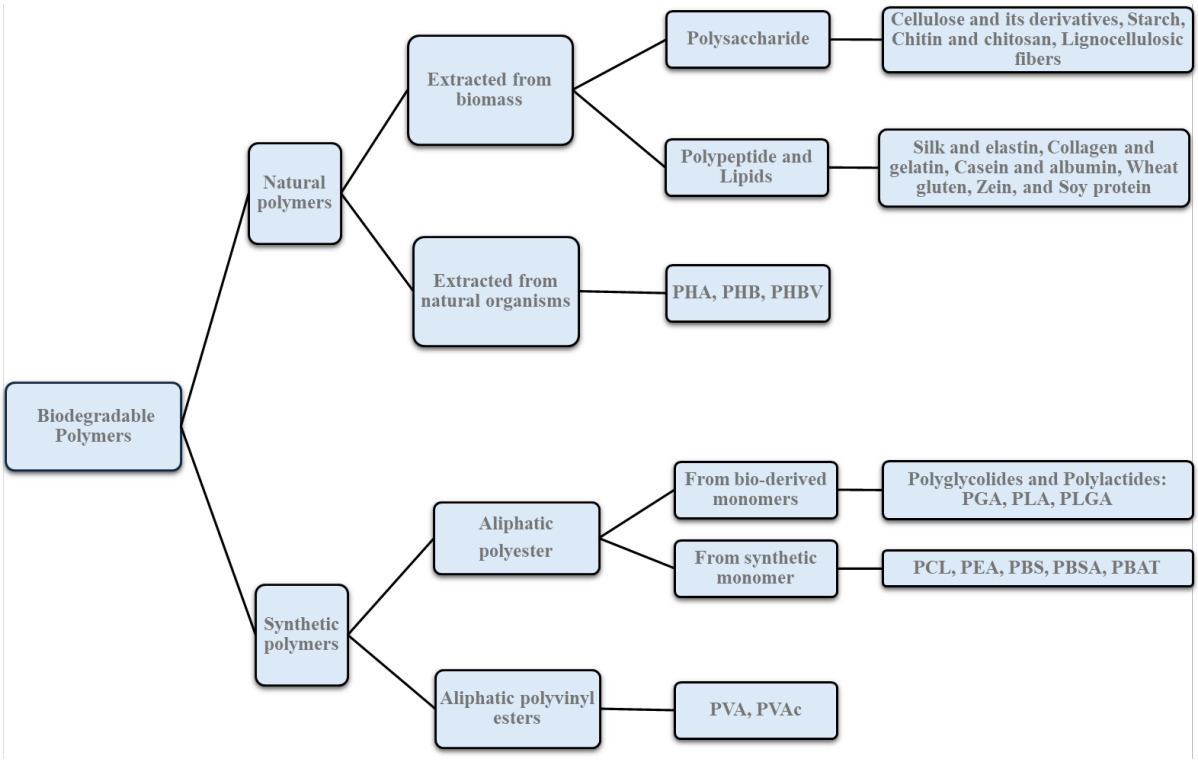

Figure 2: Categorization of biodegradable polymeric materials, both natural and synthetic.

4.2.1 Natural polymers

Cellulose and silk as natural polymers demonstrate significant potential as non-toxic and biodegradable substances for transitory electronics. Cellulose-based materials, in particular, exhibit exceptional degrading capabilities, favorable biocompatibility, superior performance, and cost-effectiveness, hence showcasing significant prospects for environmentally sustainable mass production of electronics.[13] Starch as a polysaccharide with a granular form has the advantages of affordability, abundance, and renewable, which renders it a desirable material for manufacturing biodegradable polymers. For application in the future of flexible disposable organic electronics, a study by Jeong et al. developed an environmentally friendly biodegradable starch paper with excellent mechanical strength (tensile strength and Elongation at break values of 39.8 MPa and 1.13 mm, respectively) without the need for a planarization polymer layer.[14] Gelatin is another natural polymer typically used in the food industry processes due to its good functional qualities. It is a denatured fibrous protein extracted by

thermal hydrolyzing of collagen. Nonetheless, gelatin-based composite films have certain drawbacks like weak water vapor barrier characteristics and are relatively moisture sensitive. On the other hand, the mechanical properties, water resistance, thermal stability, light, and oxygen barrier properties of gelatin-based films have been improved by a variety of modification strategies, including the addition of plant-extracted phenolic compounds, enzymes, proteins, aldehydes, and nanomaterials.[15]

4.2.2 Synthetic polymers

In addition to green polymers discussed above, synthetic polymeric materials have also been reported as a promising candidate demonstrating non-toxic and biodegradability for transitory electronics. Biodegradable polymers enable the production of flexible substrates. These polymers are substituted or incorporated by adding hydrophilic groups to their backbone, allowing them to disperse, swell, or dissolve in water.[12] The hydrolytically degradable polymers that have been extensively studied comprise poly (glycolic acid) (PGA), poly (lactic acid) (PLA), poly-lactic-co-glycolic acid (PLGA), poly(ε-Caprolactone), poly(vinyl alcohol) (PVA), and which has been shown in Figure 1.[16–18] PGA is one of the most promising biodegradable polymers available today. It has similar chemical structure to PLA, however the lack of methyl side group enables the polymer chains to pack tightly and yields a high gas barrier, high mechanical strength, high thermal stability, and high degree of crystallinity. While, PGA has a biodegradation profile similar to cellulose and is completely compostable. Besides, their high processing temperature, it's difficult to melt mix them with other commercial biopolymers including PCL, PBS, and PHB as well as biomass-based polymers like cellulose and starch.[19] The next well studied polymer in transient electronics is PLGA, which is a hydrophilic polymer with a high degree of biocompatibility and when it dissolves, it emits byproducts that are toxicology benign. It is composed of PLA and PGA that can be controllably degraded by tailoring the molecular weight and the ratio of its components.[16] Next is the PCL polymer, which is a linear polyester synthetic with almost 50% crystallinity that is composed of 6-hydroxyhexanoates. The PCL-degrading micro-organisms are among the most significant variables affecting PCL biodegradation that generate various forms of PCL hydrolases.[20] Kim and collaborators, created a biocompatible and biodegradable fiber electrode using PCL and Mo microparticles. The fiber electrode's intact PCL core and Mo/PCL conductive layer allowed for high electrical conductivity (≈43.5 $\boldsymbol{\Omega}$ cm^{-1}), mechanical robustness, bending stability, and durability over more than 4000 bending cycles.[21] Yet another polymer is PVA, holding several benefits, such as non-toxicity, non-carcinogenic nature, and its ability to dissolve in various

solvents. These characteristics make it an excellent choice for transient electronic devices used in biomedical applications.[4] The solubility of PVA in water is primarily determined by the degree of polymerization and the temperature of the solution. A noteworthy report demonstrated the tailoring of PVA dissolution rate by altering the composite structure. Both computational and experimental studies reveal that the transiency of a PVA polymer matrix can be controlled either by increasing or decreasing the addition of gelatin or sucrose.[22]

4.3 Semiconductors

The performance of electronic devices heavily relies on quality and characteristics of the semiconducting materials, making them a crucial element in the field of electronics. Notably, the ever-decreasing demand in degradable electronics has motivated several research endeavours to study the degradability of different electronic components in material perspective including Si-based, metal oxides, organic semiconductors, and dielectrics.

4.3.1 Silicon based

The remarkable progress in silicon technology has spurred extensive research into degradability studies, with findings highlighting the degradability of Si nanomembrane (30-300 nm), polycrystalline silicon (poly-Si), amorphous silicon (a-Si), germanium (Ge), and silicon germanium alloys (SiGe) dissolvability in physiological aqueous solutions.[23–26] Typically, the electronic components degradability studies have been conducted in de-ionized (DI) water or in simulated bio-fluids such as phosphate buffered saline, and phosphate buffered solutions. Notably, the dissolution rate in Si nanomembrane and amorphous silicon is controlled by several factors such as solution concentration,[27] temperature,[26] pH,[25] and the presence of surrounding environment[28] in the solution. Elevated temperature and pH levels accelerate the dissolution rates of Si nanomembranes (Si NMs), whereas the high doping concentrations (10^{20} cm^3) significantly decreases the dissolution rate.[25,27] In fact, the different deposition techniques (electron-beam deposition, plasma-enhanced chemical vapor deposition (PECVD), low-pressure chemical vapor deposition) has found to demonstrate different dissolution rate in SiO_2 films of 100 nm thick. The mechanism behind the silicon dissolution behaviour has been revealed using Density functional theory (DFT) and molecular dynamics (MD) simulation tools; wherein silicon dissolution proceeds through the nucleophilic attack of silicon surface bonds, which significantly weakens the interior bonds of surface silicon atoms (backbonds) and thereby increases their susceptibility to further ion attack. Similarly,

dissolution rates of poly-Si, Ge, and SiGe are greatly affected by pH, temperatures, proteins and types of ions.[3]

4.3.2 Metal Oxides

Beyond Si technology, conventional semiconductor electronics have predominantly been governed by inorganic oxide semiconductors. Among the available enormous oxide systems (Gallium oxide (Ga_2O_3), tin oxide (SnO_2), indium oxide (In_2O_3), tin doped indium oxide (ITO) and fluorine doped indium oxide (IFO)), only few oxides have found to demonstrate good biodegradability which includes iron oxide (Fe_2O_3), zinc oxide (ZnO), titanium oxide (TiO_2), tungsten oxide and magnesium oxide (MgO); wherein, ZnO has been widely exploited in various health monitoring device applications owing to its ease of synthesis, varied solution processability, stability, and efficient charge transfer properties. Moreover, the primary outcome of the degradation pathway is a metabolite that can be processed by the body, namely zinc hydroxide ($Zn(OH)_2$). Besides ZnO, the next attractive oxide which holds excellent biocompatibility is TiO_2 and widely used in biosensing, drug delivery, antibacterial activity, and implant applications. Notably, the addition of inorganic particles (TiO_2) to a polymer matrix (aliphatic polyester/clay, poly (L-lactide), poly (vinyl chloride)) improves the biodegradability, and a high dispersion of inorganic nanoparticles in a polymer is a key factor for enhancing the performance.[29] Along the same line, TiO_2 nanoparticles have been added in different kind of polymer matrix to improve their degradability. Instead of the parameters mentioned earlier, such as those associated with silicon nanomembranes, the degradability of oxide film is primarily influenced by the thickness of the deposited film, playing a crucial role in regulating the degradation rate. Similarly, the other biodegradable oxides such as iron oxide (Fe_2O_3), tungsten oxide and magnesium oxide (MgO) consisting of few tens of nanometres thickness slowly dissolves in deionized water resulting with a byproduct of hydroxide and a water.

4.3.4 Organic semiconductors

Various organic semiconductors (OS) such as polythiophenes, polypyrrole (PPy), polyaniline (PANI), and poly (phenylene vinylene), have been employed as active materials in numerous electronic devices to date. Their usage as active material imparts improved mechanical conformability and better biological interface, which are crucial for biomedical applications, in addition to bringing added advantages of synthetic tunability and low-cost processing.[30] The conductivity in these OS materials is offered by the delocalization of electrons along the π-

conjugated backbone. However, these polymers demonstrate less resistant to degradation owing to their strong C-C bond. Nevertheless, one of the easy ways to impart biodegradability in these polymers is to blend them with the nonconducting polymers and thus eventually making them disintegrable. In this process, a dual advantage of having good conductivity as well as degradability can be achieved. There have been several reports demonstrating such blending/grafting of conducting polymers like PPy with polylactic acid,[31] PPy with poly (L-lactideco-glycolide - PLGA),[32] poly (3-thiophene methyl acetate) with biodegradable polyester,[33] poly(3,4-ethylenedioxythiopene)-poly(styrene sulfonate) with polylactic acid composite,[34] P3HT- poly(3-hexylthiophene) with PLGA,[35] P3HT blended with PCL - poly (Ɛ-caprolactone),[36] etc., to improve the composite degradability. Apart from blending/grafting approach, the biodegradability can also be imparted by synthetically modifying the structure of these functional polymers; wherein the desirable electrical and mechanical properties can be easily tuned.[37] Such reported strategies include polymerization of modified monomers, introducing hydrolysable linkages into conjugated polymer backbone and co-polymerization of conducting oligomers with biodegradable polymers.[38–42] In general, the small OS molecules can be completely biodegradable since they can easily pass through the digestive system.[43] However, the degradation rate of the molecules in various environments depends on their chemical structure. As a thumb rule, the resistance to biodegradation of a particular molecule increases when the solution contains of strong electron withdrawing substituents like chlorine.[44] Similarly, the presence of extensive branching found to reduce the susceptibility to biodegradation. Nevertheless, the solution condition and the environment of the molecule plays a critical role in determining its biodegradability.

The degradation mechanism of organic moieties occurs by the cleavage of chemical bonds at the molecules resulting in non-toxic by-products. Generally, the degradation process consists of three main mechanisms including 1. Hydrolytic degradation where the breakage of chemical bond happens by water. 2. Enzymatic degradation – bond breakage governed by the enzyme catalyst. 3. Oxidative degradation – the oxygen molecules help in breaking the macromolecules by forming free radicals. The other factors which affect the biodegradation rates of the OS materials are molecular weight, temperature, pH of the medium, surface area of the material and cross-links absence.[45]

4.4 Dielectric materials

Dielectric materials are electrical insulators which exhibits polarization when subjected to an electric field. Upon application of electric field, dipole moments alignment takes place and

thereby resulting in an internal electric field that decreases the overall field contained in the dielectric material. Owing to this phenomenon dielectric materials are widespread their applications in field-effect transistors (FETs) and capacitive sensing devices which further lead to the realization in medical diagnostics and structural health monitoring devices. Typically, they are classified into organic and inorganic dielectrics.[46]

4.4.1 In-organic dielectric materials

Magnesium oxide (MgO), silicon dioxide (SiO_2), silicon nitride (Si_3N_4), and spin-on-glass (SOG) are the available potential choices of inorganic dielectric materials capable of utilizing as gate or interlayer dielectrics, passivation coatings, and the encapsulation layers of biodegradable electronic devices.[47,48] Among these, SiO_2 and Si_3N_4 are the two most widely used dielectric material in the fabrication of field effect transistors.[49] A completely biodegradable electronic implant consists of *n*-channel FETs have been developed on a silk substrate using SiO_2 and Si_3N_4 as a dielectric and encapsulation layer respectively. Herein, a complete degradation of the fabricated devices has been observed in deionized water in less than 5 minutes.[46] Notably, MgO has also been used as an inorganic dielectric material in numerous applications.[50]

4.4.2 Organic dielectrics

The commonly available organic polymers such as PLA, PVA, PMMA, PVP, PPC, PDMS, and PU have been extensively studied as a dielectric material in biodegradable organic electronic devices owing to their commercial availability and ease of processability.[51–53] The presence of alcohol or acid groups in these polymers can be polarized under an applied electric field which makes them a potential candidate as dielectric materials.[54] The synthetic polymer PPC[55] and PVA have demonstrated to show high dielectric constant and utilized in the organic field effect transistors and circuits wherein the former shown to degrade quickly via enzymatic degradation and the later by hydrolysis process respectively.[56–58] Both the synthetic polymers exhibit excellent degradability and as a result, their composites have been developed for a variety of applications which can be found elsewhere.[59,60] Besides, synthetic, and elastomeric polymers, natural polymers such as cellulose,[61] silk fibroin,[62] keratin,[63] jute[64] and bamboo[65] exhibits high k values and used in organic TFTs. In addition to organic dielectric materials, new and innovative electrolytes are constantly being tested for application in biodegradable organic transistors. Incorporating biodegradable electrolyte materials into organic transistors

introduces a novel range of biological capabilities, enhancing their applicability in upcoming wearable, implantable, and electronic skin applications.[66–68]

5. Design and Fabrication Requirements

In the twenty-first century, the most pressing objective for a material scientist is to figure out how to balance performance with sustainability in polymers. In general, the function and life cycles of materials in the defined environment dictate the material design. For instance, in applications of integrating electronics in the biological context, the materials' biocompatibility, the method of implanting the device, and its integrative design need to be considered.[69] Molecular design is a technique to accomplish desired functionality. The main variables in polymer chemistry that impact the functions are topology (such as branching, regioregularity, and tacticity) and composition (such as monomer sequence, chain length, dispersity, end functionality, side chain type, and backbone).[70] The relationship between polymer composition and topology lies in many different chemical scales, from the molecular to the macromolecular. The molecular structure and polymer composition determines their mechanical, optical, and electrical characteristics. The following examples illustrate how slight adjustments in the composition of polymers can directly affect the characteristics of macromolecules, especially their flexibility and water solubility. After examining a collection of 51 low-band-gap polymers, Roth et al. identified some major trends in the stiffness (tensile modulus) and ductility (crack-onset strain); wherein the presence of fused rings along the backbone tend to reduce ductility and increase the modulus. While, the opposite impact is experienced by branched side chains.

The side chains can act as solubilizing agents despite the rigidity of the molecular structure by introducing functional groups or interfering with crystallization. Consequently, the most flexible films can be remarkably ductile (crack-onset strain ≤68%) and compliant (modulus > 150 MPa).[71] Additionally, there have been reports adjusting the polymer's physical characteristics, such as absorption, emission, energy level, molecular packing, and charge transfer by engineering the side-chain. Conjugated polymers are typically insoluble in organic solvents owing to their lacking side chains which makes them highly challenging to process into thin films. To improve solubility in nonpolar liquids, branched alkyl chains are frequently utilized instead of their linear analogs, since their bulkiness might impede interchain interactions. Even adding ionic side chains can make them more soluble in water and polar organic.[72] Besides, structure-dependent characteristics can be fundamentally understood by

examining polymer architecture, as it affects intra- and intermolecular interactions in melts and solutions. Block copolymer structural characterization is an intriguing and still-developing field of study with great potential for advancement in both science and technology. Controlling the morphology at the nanoscale can result from selecting the right blocks in terms of chemistry, composition, and architecture.[73] Numerous structures, including linear, branched (such as star),[74] bottlebrush,[75] cyclic,[73] and network,[76] are potential topologies for polymers. The following examples are elaborating the dependency of polymer characteristics on architectural structure.

It has been demonstrated that living polymerization techniques are highly effective in producing asymmetric star polymers. These materials contain stars with varying molecular weights, chemical compositions, or topologies in their arms. As majority of these products are well-defined and homogenous in terms of both composition, and molecular structure, it is possible to relate their characteristics to the molecular structure. Numerous attempts to forecast the characteristics of the asymmetric stars. Nevertheless, in most circumstances, these hypotheses cannot be evaluated by experimental evidence. For this objective, novel architectures and partially deuterated Miktoarm stars must be devised.[77]

A class of grafted polymers known as bottlebrush polymers (BBPs) have attracted great interest owing to their exciting new applications. As molecular experimental investigation of BBPs can be problematic, a variety of computational and theoretical techniques have been effectively used to examine BBPs. By adjusting architectural characteristics such as the grafting density and the degree of polymerization of the side chains and backbone, it is possible to readily adjust the properties of these grafted polymers. Furthermore, the conformations and consequently the characteristics of BBPs can be greatly influenced by variables such as pH, temperature, and solvent quality. As a result, enormous computational and experimental investigations have been carried out to investigate the conformations of BBPs in different situations. In order to explore BBPs, computational techniques such as particle-based and field-theory-based methods have been frequently used in recent decades.[78] Numerous investigations have been done on particle-based models of BBP with side chains or a rigid backbone,[79,80] The inherent flexibility of polymers plays a crucial role when evaluating the conformations of BBPs, a precisely transferable models of BBPs are required to adequately represent the flexibility of the side chains as well as the backbone in both solvent- and solvent-free conditions. A new area of study that can be exploited to comprehend and/or forecast BBP behaviors is the utilization of ML techniques in conjunction with theoretical and computational techniques. For instance, data-

driven models can be trained to predict the conformational and mechanical properties of simulated BBPs and their self-assembled architectures using the massive amounts of data produced by molecular simulations. The innate architecture of BBPs can be investigated via deep learning (DL) techniques, which are difficult to accomplish by traditional analysis.[81] Sidky et al. reported using data-driven ML/DL-based trajectory forecasting algorithms to reduce the computational load of simulating these complicated structures. To comprehend the underlying relationship between the complex architecture and the characteristics of grafted polymers, ML techniques coupled with simulations can potentially be useful.[82]

Many properties of polymer networks are determined by their topology, however, due to their amorphous nature, they are challenging to control. Various methods can be employed to manipulate structural features of polymer networks at the molecular level. These techniques include programming topological information into network precursors or biassing of polymerization kinetics.[83] Meanwhile, elasticity is a crucial characteristic of polymer networks; nevertheless, it is not clear how elastically deficient loops affect bulk elasticity. Therefore, theories designed to predict elastic modulus from the molecular scale have proven challenging to validate experimentally.[84]. In a recent effort to enhance our comprehension of the relationship between topology and elasticity, Zhong and colleagues conducted a study. They evaluated the elasticity of classical phantom and affine network theories by examining the shear elastic modulus and quantifying topological "loop" defects of various orders in a range of polymer hydrogels. This investigation utilized techniques such as rheology, disassembly spectrometry, and simulations to gain insights into the interplay between topology and elasticity in these materials. The effects of loop defects on the elasticity of polymer networks are explained by the real elastic network theory (RENT), which is a modified version of the phantom network model.[76,83,85] RENT considers the anticipated effects of loops of different orders on network elasticity and provides estimates of shear elastic modulus that align with experimental results. On the other hand, there were also reports employing kinetic Monte Carlo simulation to characterize growth kinetics and network structure at the same time.[85] The effectiveness of this theory in predicting mechanical properties emphasizes the value of molecular knowledge to comprehend the chemical basis of polymer network architecture.[83] The subject area will proceed to take control of the topology of polymer networks to a greater extent. By employing advanced characterization techniques and synthesis methods, researchers aim to better understand how network topology influences the overall properties of materials.

This understanding could pave the way for the development of new materials possessing unique mechanical qualities and functionalities that were previously considered improbable.[83]

A large range of biodegradable polymers are used in many products with short lifespans. Every biodegradable polymer comprises of hydrolyzable or oxidable bonds. Due to this, the material is susceptible to mechanical stress, heat, light, and moisture. The various forms of polymer degradation—photo, thermal, mechanical, and chemical—can occur singly or in combination, contributing to the degradation. When water molecules are present, the macromolecular chemical bonds may hydrolyze, which can result in chain scissions. These scissions happen at the ester groups in the case of aliphatic polyesters.[86] Nonetheless, a key challenge here is to understand the mechanical behavior of biodegradable materials throughout their degradation. Vieira et al. examined hyper elastic constitutive models, including the Neo-Hookean, the Mooney-Rivlin modified, and the second reduced order. For example, a forecast model is utilized to read the mechanical properties in a composite of polycaprolactone (PCL) and polylactic acid (PLA). Here, a numerical method using ABAQUS® is provided, in which a User Material subroutine (UMAT) automatically updates the material properties of the proposed model in accordance with the degradation time. This model is claimed to be applied to other thermoplastic biodegradable materials that exhibit hyperelastic behavior.[87] Yet another report by Jiang et al. aimed to develop ML-based models to predict primary and ultimate biodegradation rates of organic chemicals, crucial for environmental risk assessment. The survey offers valuable tools for predicting biodegradation rates and insights into underlying mechanisms (Figure 3a).[88]

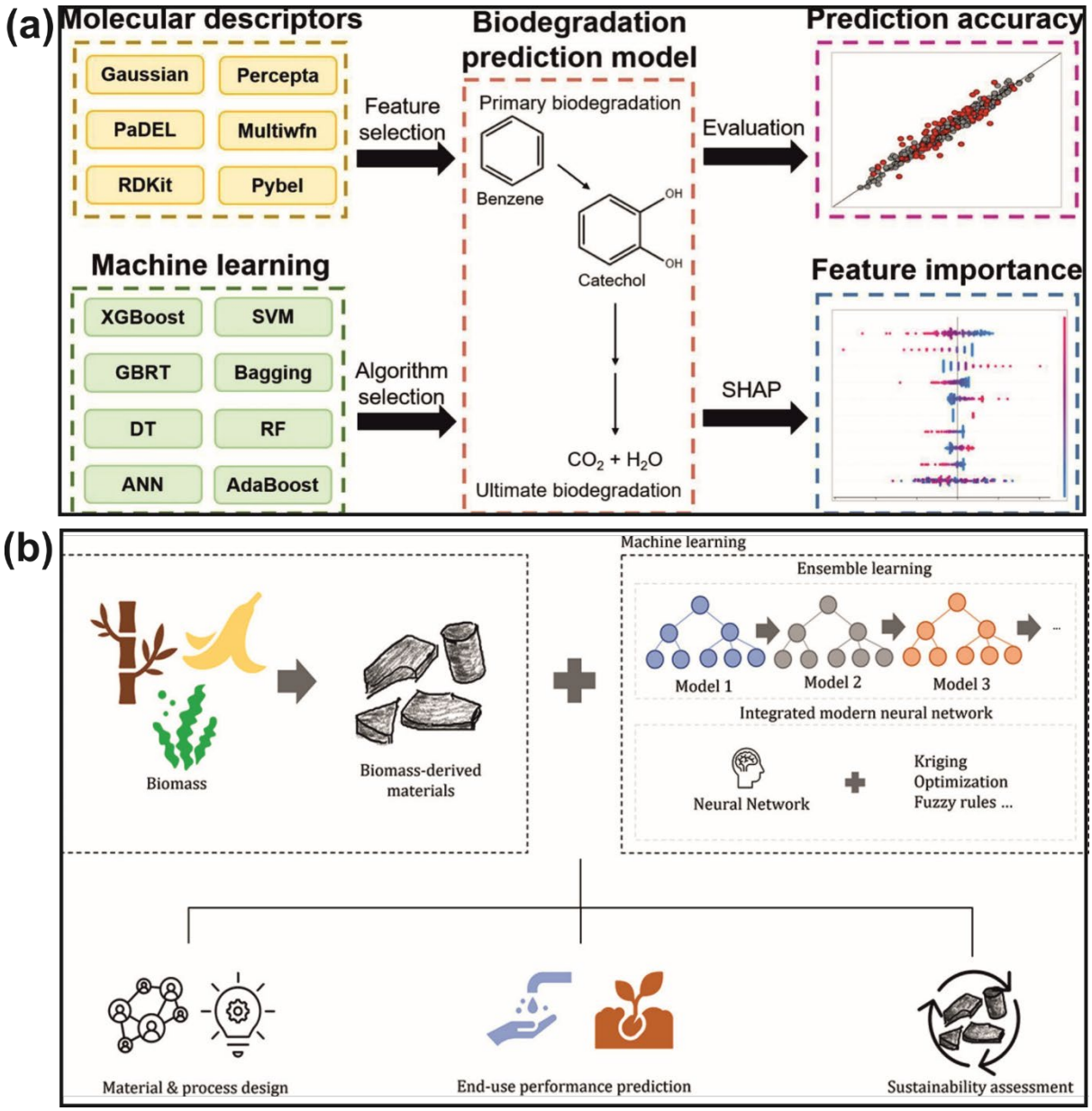

Figure 3: a) Schematic showing the utilization of ML-based models to predict and understand the biodegradation rate. Reproduced with permission.[88] b) The symbiosis of ensemble learning, integrated modern neural networks, and Kriging optimization fuzzy rules for material and process design in the realm of biomass and biomass-derived materials with a focus on end-use performance prediction in water and agricultural systems. Reproduced with permission.[89]

Figure 3b shows the application of ML in the context of biomass-derived materials for water and agricultural systems has been highlighted. Spanning 53 papers from 2008 onwards, they categorized ML applications into material and process design, end-use performance prediction, and sustainability assessment.[89]

The environmental fate of polymers, particularly biodegradable ones, has become a focal point across academic, industrial, and regulatory sectors. Albright III et al. examined test procedures often used to assess polymer biodegradation and identified important areas for improvement by reviewing the literature on the subject that was produced over the last decade. Key considerations include the physical form of the test material, appropriate reference materials, test system selection, the advantages and limitations of analytical methods (Refer Figure 4a). The authors identify crucial knowledge gaps and propose four recommendations for advancing polymer biodegradation studies: (1) establish standardized guidelines for various environmental matrices, (2) devise accelerated biodegradation and predictive methods for polymers, (3) adopt an integrated analytical approach using simple and effective methods, and (4) develop new frameworks for assessing overall polymer persistence accepted by the scientific community.[90]

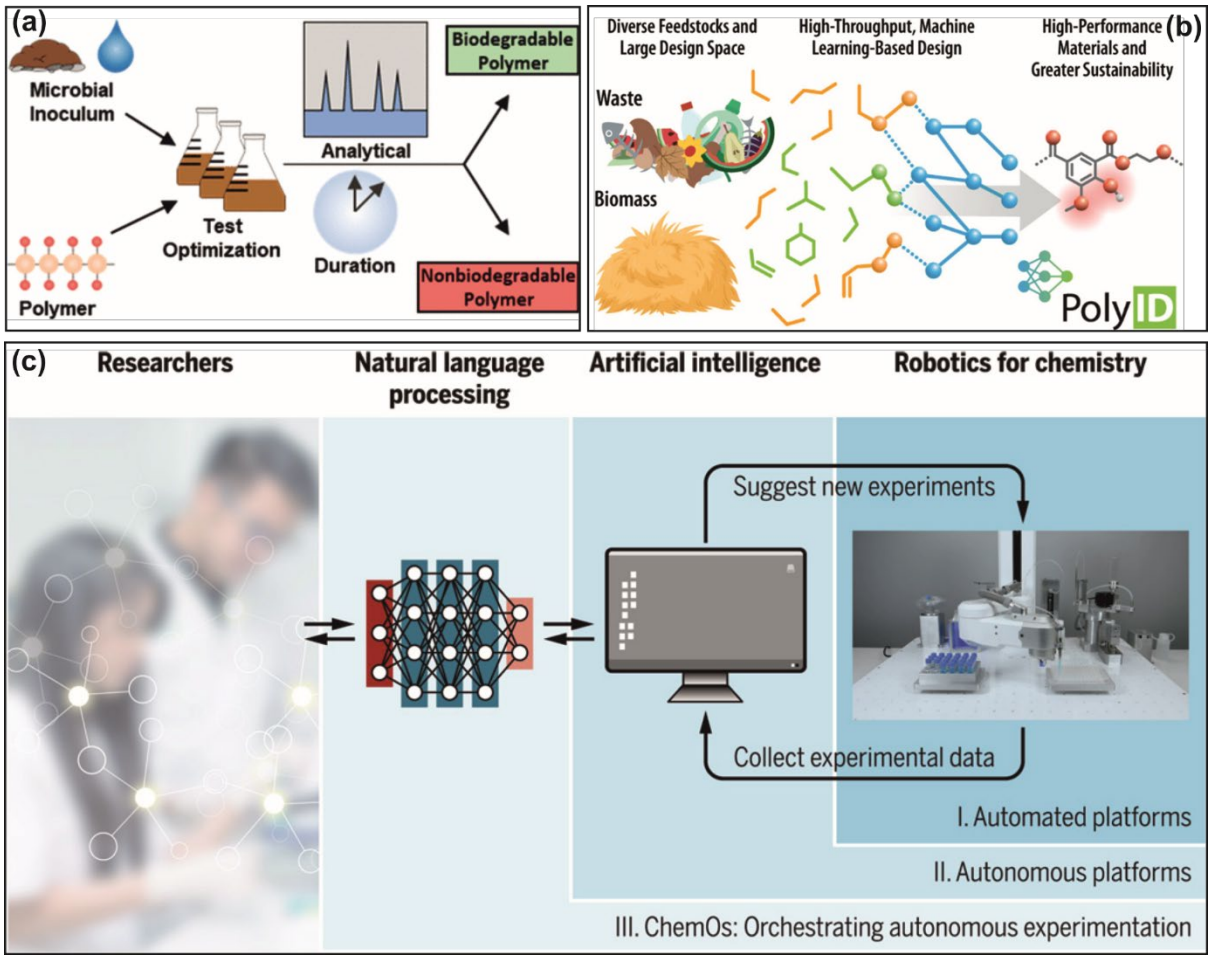

Figure 4: (a) Identification of crucial knowledge gap and proposing methods to determine polymer degradability. The data is Reproduced with permission.[90] b) Schematic illustrating ML-based tool PolyID, to reduce the design space of renewable feedstocks to enable efficient discovery of performance-advantaged, biobased polymers. Reproduced with permission.[91] c)

The set of instructions provided to ChemOS by researchers is interpreted through a natural language processing module. New experiments to be assessed on the automated robotics platforms are suggested by the AI algorithm. The outcomes of the experiments are gathered and employed to enhance the AI model of the ongoing experiment in a closed-loop approach. Reproduced with permission.[92]

As shown in Figure 4b, a ML-based tool called PolyID has been developed to facilitate the transition from fossil-derived plastics to biobased polymers for a sustainable economy. PolyID is a multioutput, graph neural network, significantly narrows down the design space of renewable feedstocks, streamlining the discovery process of high-performance, biobased polymers. The tool incorporates a novel domain-of-validity method, addressing gaps in training data to enhance accuracy. The tool not only provides accurate predictions but also offers explainability through the analysis of individual bond importance, aiding biobased polymer practitioners in discovering sustainable materials with enhanced performance.[91]

In addition, AI algorithms are used with automated robotics platforms to create autonomous labs to conduct experiments independently. AI designs and recommends experiments, validated by robotics platforms. The AI analyzes results to enhance experimental strategies and propose better hypotheses for subsequent experiments, all achieved without human intervention (Figure 4c).[92]

6. AI assisted Materials Discovery

AI has the potential to be a transforming and groundbreaking power that will accelerate advancement in a wide range of scientific and technical fields, including chemistry, materials science, and engineering.[93] It is an effective instrument for increasing productivity and accelerating research, innovation, and discovery in sustainable chemical techniques while substantially minimizing time, energy, and resources used. In several sectors, the ability of AI to extract insights from complex systems has shown to boost productivity, lower capital costs, and improve product quality and user satisfaction. However, AI's actual worth may be found in its ability to advance scientific discoveries and provide answers to difficult worldwide issues related to the global environment, economy, and society.[94] Bringing together specialists in the green and sustainable domains, the AI experts expediate the development of circular economy. The synergy between ML algorithms and material science is revolutionizing the discovery and development of new materials. As a result, through simulated screening, researchers may evaluate new materials more effectively, resulting in a reduction in the need for experimental

and computing resources. AI algorithms are employed with automated robotics platforms to create autonomous laboratory settings based on a human-defined goal. In autonomous labs, AI algorithms design and recommend experiments, and these suggestions are verified on automated robotics platforms. The AI algorithms evaluate the results of this validation to improve experimental tactics and, as a result, to make more accurate predictions about the experiment that should be conducted next. Compared with automated labs, where the researchers pre-define the experimental procedures, this so-called closed-loop approach is modified. As a result, autonomous labs might advance traditional trial-and-error methods, hastening the discovery of chemicals and materials.[95] Furthermore, they may reduce the conflict between the expense of human-driven testing, which may have peaked in terms of efficiency benefits, and the anticipated time to discovery.[95] Besides, AI-driven quantum mechanics and computing resources have the capability to revolutionize predictive toxicology, an underlying aspect of sustainability analysis.[96]

Through advanced algorithms and machine learning techniques, AI shifts through vast databases of existing materials, scientific literature, and experimental data to uncover hidden patterns, correlations, and potential breakthroughs. AI-driven approaches leverage vast amounts of data and advanced algorithms to streamline and enhance the process. Material discovery using AI is a many-stage task. It mainly involves four key stages: characterization, property prediction, synthesis, and theory paradigm discovery. The initial stage involving gathering information about a material, lays the foundation for subsequent discovery phases. The characterization stage encompasses imaging and instrument-related contexts, and creates vast high-dimensional data, which surpasses human processing capabilities. Thus, AI can assist by automating and enhancing the characterization process, reducing manual labour, enhancing data quality, and uncovering valuable insights from complex datasets. The imperative to revolutionize the approach to transient electronics stems from the critical need to mitigate environmental impact, paralleling the requirement for the development of eco-friendly chemicals to align with sustainability objectives and minimize the gap between technological advancement and ecological responsibility.

AI heavily depends on extensive, high-quality databases crucial for software learning. Overcoming roadblocks in chemical sustainability discovery acceleration involves addressing two key factors: securing access to relevant, large datasets in chemical research and promoting open data for fair and equitable AI development.[97,98] Efforts are underway to create an open-access framework and infrastructure for organizing and disseminating organic reaction data

through a centralized repository, a crucial step for advancing AI in the future.[94] In conclusion, the transformative capacity of AI extends to the realm of chemical engineering and chemistry, encompassing advancements in the exploration of innovative materials, optimization of processes, and enhancement of quality and safety standards.

7. Summary and perspective

We have accomplished a concise study of the recent advancements in transient technology, specifically in the context of transient electronics. Our focus was on analysing the materials, designs, and performances of these devices. A major part of this review focused on transient materials, encompassing metals, polymers, and semiconductor materials. Further research should target on enhancing the efficiency of the developed transitory devices, so that they can be on comparable levels with conventional devices. While there is a trade-off between the performance of a device and its transitory capabilities, it is crucial to achieve suitable balancing. The development of AI and robotics-based molecular design tools for autonomous high-throughput experimentation is accelerating. These technologies expedite the process of generating and optimizing commercially viable materials and equip chemists with tools for predicting molecular properties.[99] This versatile and data-driven approach is required in order to prevail upon the time-consuming and costly procedure brought on by the complications of the experiments. For large-scale bulk applications, it will be essential to be able to precisely and logically forecast how variations in molecular-level characteristics transfer to bulk properties.[100] Because of the higher degrees of variability and possible combinations of repeating units, extending data-driven technologies from optimization of small molecules to polymers unveils challenges for the effective identification of desirable options. As a result, the effective use of AI will pave the way for the discovery of novel molecular designs and the renovation of existing molecules for novel applications.[101] Building a cohesive and complete data collection of attributes is crucial for the advancement of AI and automation for the discovery of novel materials. This includes defining and standardizing systems representing polymers used in ML models. More advancements in ML techniques are required to realize the potential benefits of data-driven polymer chemistry, including discovery and chemical synthesis simplification. After structuring the data, it was necessary to compile comprehensive bio-composite data related to the planned behaviour from research publications and technical reports. The accuracy of the ML predictive model is contingent upon the diversity and the size of the investigated database. The last step is assigned to the evaluation of the accuracy of collected data.[102] To effectively realize the promise of polymer development, basic research on

polymer standardization and classification is needed. In summary, several AI techniques have been effectively used to the field of chemical research because of the growing multidisciplinary nature of research. In some sectors, using AI has even grown commonplace. AI has not yet had a significant influence on certain fields of growing research, such as sustainable technology. More interdisciplinary research and advancements in AI data training itself will assist these fields move forward efficiently.

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