

REVIEW ARTICLE

Advancing sustainability: Biodegradable electronics and materials discovery through artificial intelligence

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Abstract

The pressing need for sustainable materials and devices stems from growing environmental concerns and the imperative to mitigate climate change. Traditional materials and devices often rely on non-renewable resources and generate significant waste and pollution throughout their lifecycle. By prioritizing sustainability in material and device design, we can foster innovation, promote circular economies, and build a greener future for generations to come. Artificial intelligence (AI) and machine learning (ML) can analyze vast datasets to identify novel materials with desirable properties by reducing the experimental workload. In this paper, we explore the synergistic relationship between sustainable materials discovery and ML models. By leveraging advanced algorithms, researchers can efficiently explore vast chemical spaces to identify environmentally friendly materials with tailored properties. ML techniques, including predictive modeling and generative models, facilitate the rapid discovery and optimization of sustainable materials for various applications, ranging from renewable energy technologies to eco-friendly consumer products. We present a 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. Furthermore, classification and regression techniques to model the degradation behavior of polymers have been addressed, pointing to key challenges and proposing solutions for enhanced ML applications. The paper discusses the challenges of scaling up data-driven technologies from small molecules to polymers, underscoring AI's role in discovering new molecular designs and optimizing existing ones for novel applications. It emphasizes the importance of defining and standardizing polymer systems to enable ML models to create a unified data collection system for AI and automation enhancements. Furthermore, it stresses the necessity of refining ML methods to harness the benefits of data-driven polymer chemistry fully, emphasizing the importance of reliable and diverse datasets for predictive models in polymer synthesis.

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1. Introduction

Sustainable development is an approach 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 toward 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 classes with biodegradable substrates, insulators, conductors, and semiconductors, which together make up the basic components of devices.⁴

Conventionally, materials discovery and synthesis have been based on trial-and-error methods, which rely on the 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 artificial intelligence (AI), researchers can harness the power of machine learning (ML) and data analytics to accelerate the discovery process. By analyzing large datasets 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 the optimization of material 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 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 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, 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 focusing on the development of materials, technologies, and systems that would 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 transient technology into areas like intelligent 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 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 medical applications including drug carriers,⁷ scaffolds for tumor applications,⁸ and dental implants.⁹ The PLA with magnesium composite demonstrates osteogenic properties and promotes bone cell ingress (Figure 1).¹⁰

3. Functional biodegradable materials

Transient materials are able to consistently maintain their complete functionality and capabilities under regular usage, delivering reliable performance, while finally degrading at the end of life without leaving any potential harmful residues. On the introduction of a solution, 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, semiconductors, and dielectric materials.

3.1. Metals

Conductive materials in electronics function as electrodes and connectors. Conventional metals are attractive in

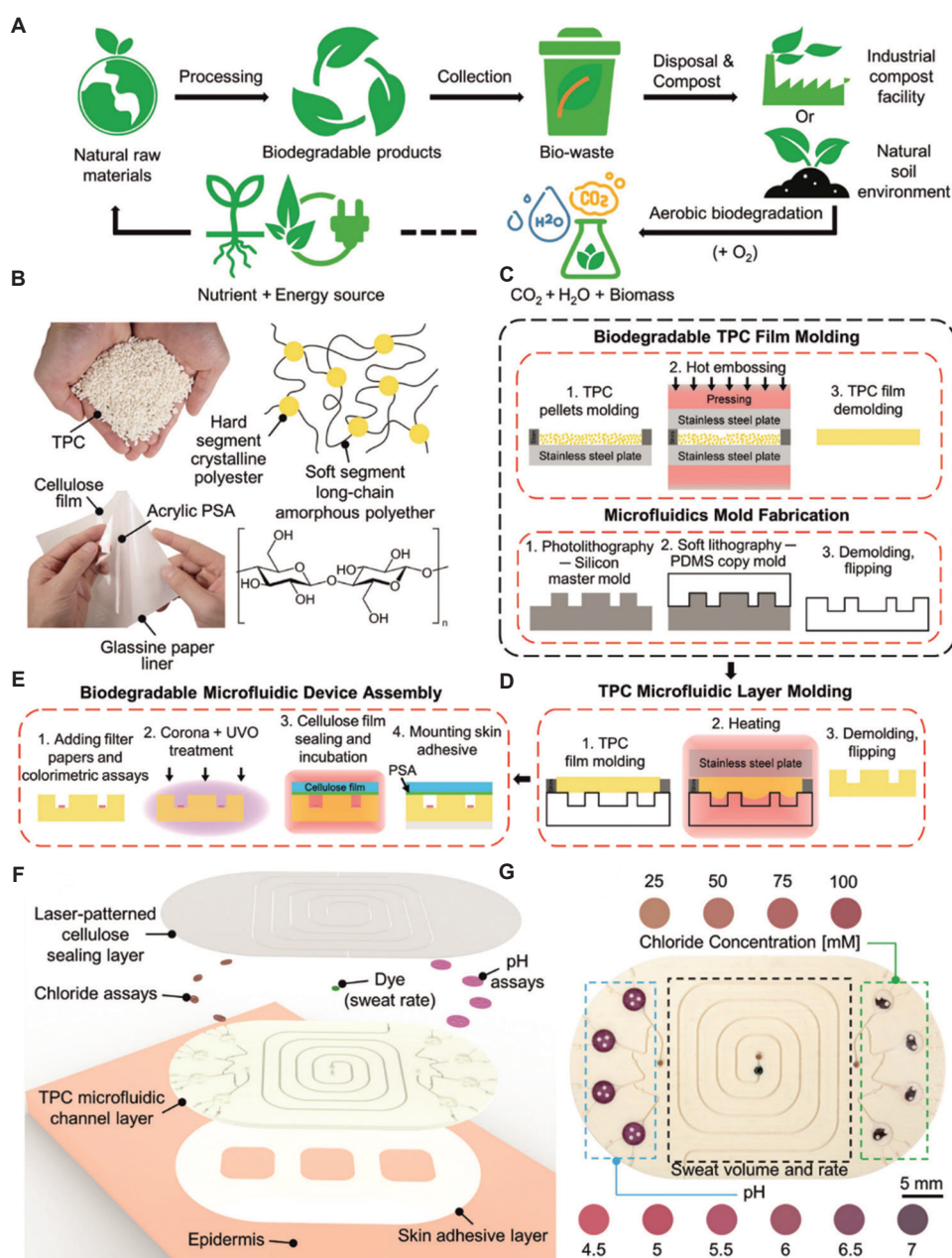


Figure 1. Demonstration of a transient electronics application as a biosensor. (A) Schematic illustrating the biodegradation process of biodegradable materials in natural soil environments. (B) Chemical structures of a biodegradable thermoplastic copolyester elastomer (TPC) as a microfluidic layer and a cellulose film with an acrylic pressure-sensitive adhesive for the sealing layer. (C-E) Step-by-step procedure of the device fabrication: (C) Fabrication of a silicon master mold, a polydimethylsiloxane 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 images 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

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 deionized water and biological solutions, while W and Mo display gradual but foreseeable rates of degradation. These behaviors offer diverse alternatives to fulfill the demand 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 disappear within a defined, limited time frame.⁴

3.2. 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. The categorization of biodegradable polymeric materials, both natural and synthetic is presented in [Figure 2](#).¹³

3.2.1. 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 renewability, which make it a desirable material for manufacturing biodegradable polymers for the application of flexible disposable organic electronics.¹⁴ Gelatin is another natural polymer extracted by thermal hydrolyzing of collagen, typically used in the food industry processes due to its good functional qualities.¹⁵

3.2.2. Synthetic polymers

In addition to green polymers discussed above, synthetic polymeric materials have also been reported as promising candidates demonstrating non-toxicity and biodegradability properties for transitory electronics. 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), PLA, poly-lactic-co-glycolic acid (PLGA), polycaprolactone (PCL), and poly (vinyl alcohol) (PVA), which are shown in [Figure 2](#).¹⁶⁻¹⁸ PGA is one of the most promising biodegradable polymers available today. It has

a 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 a high degree of crystallinity. Besides, PGA is more susceptible to degradation than PLA due to its higher hydrophilicity. However, due to their high processing temperature, it is difficult to melt-mix them with other commercial biopolymers including PCL, polybutylene succinate, and polyhydroxybutyrate as well as biomass-based polymers such as cellulose and starch.¹⁹ The next well-studied polymer in transient electronics is PLGA, a hydrophilic polymer with a high degree of biocompatibility. It is composed of PLA and PGA that can be controllably degraded by tailoring the molecular weight and the ratio of its components.¹⁶ The next one is PCL, which is a synthetic linear polyester. This semi-crystalline polymer has a relatively lower degradation rate than either PGA or PLA. Yet another polymer is PVA, holding several benefits, such as non-toxicity, non-carcinogenic nature, and the ability to dissolve in various solvents.⁴ In comparison to PCL, PVA has a more rapid dissolution and degradation process.²⁰ The solubility of PVA in water is primarily determined by the degree of polymerization and the temperature of the solution. In addition, a noteworthy report demonstrated the tailoring of PVA dissolution rate by altering the composite structure.²¹

Generally, for both natural and synthetic biodegradable polymers, the degradation is influenced by the physicochemical characteristics of the polymer, such as its molecular weight, crystallinity, the presence of hydrolyzable bonds, and surface area. In addition, various environmental factors play crucial roles, including temperature, pH, humidity, oxygen availability, and ultraviolet light exposure. The process is further impacted by the presence and activity of specific microbial degraders that produce extracellular enzymes to catalyze the degradation of the polymer.²²

3.3. 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 endeavors to study the degradability of different electronic components in a material perspective including silicon-based semiconductors, metal oxides, organic semiconductors (OSs), and dielectrics.

3.3.1. Silicon-based semiconductors

The remarkable progress in silicon technology has spurred extensive research into degradability studies, with findings

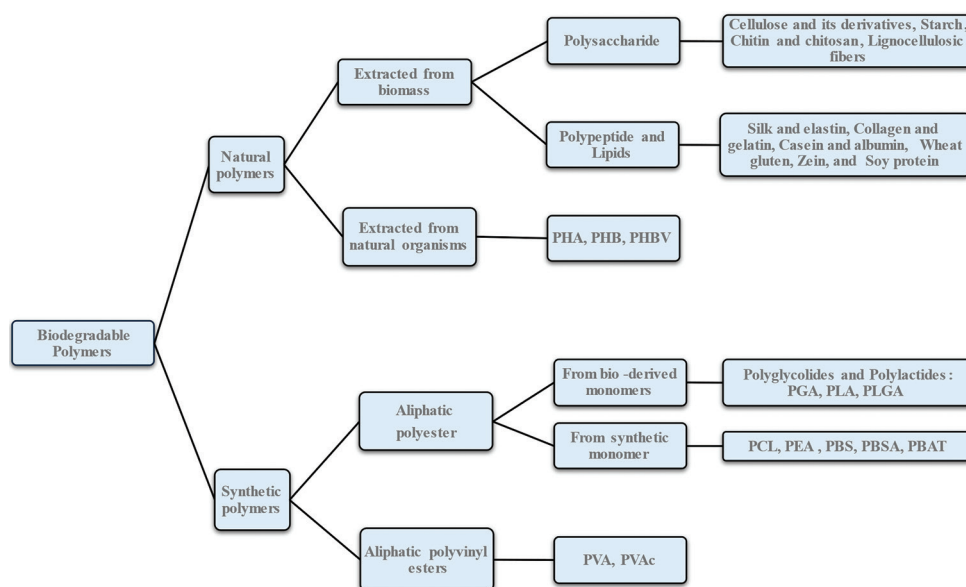


Figure 2. Categorization of biodegradable polymeric materials, both natural and synthetic¹³

highlighting the degradability of Si nanomembrane (30 – 300 nm), polycrystalline silicon (poly-Si), amorphous silicon (a-Si), and germanium (Ge), as well as the silicon germanium alloys (SiGe) in physiological aqueous solutions.²³⁻²⁶ Typically, the electronic components degradability studies have been conducted in deionized water or simulated bio-fluids such as phosphate-buffered saline, and phosphate-buffered solutions. Notably, the dissolution rate in Si nanomembrane and a-Si is controlled by several factors such as solution concentration,²⁷ temperature,²⁶ pH,²⁵ and the presence of the surrounding environment²⁸ in the solution. Elevated temperature and pH levels accelerate the dissolution rates of Si nanomembranes, whereas the high doping concentrations (10^{20} cm^{-3}) significantly decrease the dissolution rate.^{25,27} In fact, the different deposition techniques (electron-beam deposition, plasma-enhanced chemical vapor deposition, and low-pressure chemical vapor deposition) have been found to demonstrate different dissolution rates in SiO_2 films of 100 nm thickness. The mechanism behind the silicon dissolution behavior has been revealed using density functional theory and molecular dynamics 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

3.3.2. 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) and fluorine-doped indium oxide),^{29,30} only a few oxides have been found to demonstrate good biodegradability, including 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 ($\text{Zn}(\text{OH})_2$). Besides ZnO, the next attractive oxide that holds excellent biocompatibility is TiO_2 , which is 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 of composite. In addition, the high dispersion of these nanoparticles in a polymer is a key factor for enhancing the performance.³¹ Along the same line, TiO_2 nanoparticles have been added to different kinds of polymer matrices to improve their degradability. Instead of the parameters mentioned earlier, such as those associated with Si 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 a few tens of nanometers thickness slowly dissolves in deionized water, resulting in a byproduct of hydroxide and water.

3.3.3. OSs

Various OSs, such as polythiophenes, polypyrrole (PPy), polyaniline, 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.³² The conductivity in these OS materials is offered by the delocalization of electrons along the π -conjugated backbone. However, these polymers demonstrate less resistance 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, 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 such as PPy with PLA,³³ PPy with poly (L-lactide-co-glycolide) (PLGA),³⁴ and poly (3-thiophene methyl acetate) with biodegradable polyester,³⁵ poly(3,4-ethylenedioxythiophene)-poly(styrene sulfonate) with PLA composite,³⁶ poly(3-hexylthiophene) (P3HT) with PLGA,³⁷ P3HT blended with PCL,³⁸ *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.³⁹ Such reported strategies include polymerization of modified monomers, introducing hydrolyzable linkages into conjugated polymer backbone, and co-polymerization of conducting oligomers with biodegradable polymers.⁴⁰⁻⁴⁴ In general, the small OS molecules can be completely biodegradable since they can easily pass through the digestive system.⁴⁵ However, the degradation rate of the molecules in various environments depends on their chemical structure. As a rule of thumb, the resistance to biodegradation of a particular molecule increases when the solution contains strong electron-withdrawing substituents like chlorine.⁴⁶ Similarly, the presence of extensive branching has been found to reduce the susceptibility to biodegradation. Nevertheless, the solution condition and the environment of the molecule play 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. In general, the degradation process consists of three main mechanisms: (1) hydrolytic degradation where

the breakage of chemical bond happens by water; (2) enzymatic degradation through which bond breakage is induced by enzyme; and (3) oxidative degradation through which the oxygen molecules help in breaking the macromolecules by forming free radicals. The other factors affecting the biodegradation rates of the OS materials are molecular weight, temperature, pH of the medium, surface area of the material, and absence of crosslinks.⁴⁷

3.4. Dielectric materials

Dielectric materials are electrical insulators that exhibit polarization when subjected to an electric field. Upon application of an electric field, dipole moments alignment takes place, thereby resulting in an internal electric field that decreases the overall field contained in the dielectric material. Owing to this property, the applications of dielectric materials are widespread in field-effect transistors (FETs) and capacitive sensing devices, further leading to the realization of medical diagnostics and structural health monitoring devices. Typically, they are classified into organic and inorganic dielectrics.⁴⁸

3.4.1. Inorganic dielectric materials

Magnesium oxide (MgO), silicon dioxide (SiO₂), silicon nitride (Si₃N₄), and spin-on-glass are the available potential choices of inorganic dielectric materials capable of being utilized as gate or interlayer dielectrics, passivation coatings, and the encapsulation layers of biodegradable electronic devices.^{49,50} Among these, SiO₂ and Si₃N₄ are the two most widely used dielectric material in the fabrication of field effect transistors.⁵¹ Completely biodegradable electronic implants consisting of *n*-channel FETs have been developed on a silk substrate using SiO₂ and Si₃N₄ as a dielectric and an encapsulation layer, respectively. A complete degradation of the fabricated devices has been observed in deionized water in <5 min.⁴⁶ Notably, MgO has also been used as an inorganic dielectric material in numerous applications.⁵²

3.4.2. Organic dielectrics

The commonly available organic polymers such as PLA, PVA, polymethyl methacrylate (PMMA), polyvinylpyrrolidone, polypropylene carbonate (PPC), polydimethylsiloxane, and polyurethane (PU) have been extensively studied as a dielectric material in biodegradable organic electronic devices owing to their commercial availability and ease of processability.⁵³⁻⁵⁵ The alcohol or acid groups in these polymers can be polarized under an applied electric field, making them a potential candidate as dielectric materials.⁵⁶ Synthetic polymers

such as PPC⁵⁷ and PVA have demonstrated high dielectric constant and utilized in the organic field effect transistors and circuits; these polymers showed instant degradation via enzymatic degradation in the former and through hydrolysis process in the latter.⁵⁸⁻⁶⁰ 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.^{61,62} Besides, synthetic and elastomeric polymers, natural polymers such as cellulose,⁶³ silk fibroin,⁶⁴ keratin,⁶⁵ jute,⁶⁶ and bamboo⁶⁷ exhibit high k values and are used in organic thin film transistors. 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.^{68,69}

3.5. Summary of functional biodegradable materials

This review focuses on recent research concerning transient materials, covering metals, polymers, and semiconductor materials. In the realm of metals, researchers are exploring the potential of Mg, Zn, Fe, W, and Mo as soluble metals, each offering specific degradation characteristics suitable for various applications. In fact, Mg and Zn degrade quickly, whereas W and Mo degrade at slower but more predictable rates. In the domain of polymers, both natural and synthetic varieties are investigated for their biodegradability. Natural polymers such as cellulose and silk, polysaccharides such as starch and gelatin demonstrate excellent potential for transient electronics due to their biocompatibility and degrading capabilities, wherein synthetic polymers such as PGA, PLA, PLGA, PCL, and PVA offer tunable degradation rates, allowing for tailored transient behavior. PLGA, a blend of PLA and PGA, offers controlled degradation, while PCL and PVA are notable for their slower and faster degradation rates, respectively. In the field of semiconductors, the quality and characteristics of semiconducting materials are vital for electronic devices. Research in degradable electronics focuses on materials such as Si-based, metal oxides, and OSs. Both inorganic and organic dielectric materials are important components of electrical devices in the area of dielectrics. Inorganic dielectrics such as MgO, SiO₂, and Si₃N₄ are used in FETs and other applications, demonstrating complete degradation in deionized water. Organic polymers such as PLA, PVA, and PMMA are popular due to their commercial availability and biodegradability, with PPC and PVA showing high dielectric constants and facile processing.

4. ML modeling

The main steps in a traditional ML modeling process include data collection, characterization, model training, and model evaluation.⁷⁰ Data collection is a crucial stage in the ML workflow, essential for ensuring accurate predictions. High-quality and quantity datasets are vital, as they directly affect the potential performance of the ML models. The second step, also known as feature extraction, involves generating and selecting descriptors from the original data. This transformation is essential as it impacts the quality and interpretability of the resulting model. It is important to recognize that the attributes of the data determine the limit of maximum likelihood, with the algorithm only capable of approximating this upper limit.⁷¹ Algorithm design and model training, the third step, is pivotal in ML, where different algorithms may yield varying results on the same dataset. ML primarily comprises two types of learning: supervised and unsupervised. Supervised learning involves fitting a model to labeled data to predict outcomes, while unsupervised learning detects patterns in unlabeled data, employing techniques such as clustering and dimension reduction.⁷² The algorithm design and model training step can be challenging because different algorithms may perform variably on the same dataset, choosing and optimizing the right hyperparameters is crucial for achieving optimal prediction performance.⁷³ The last step involves utilizing various metrics to gauge their performance in regression and classification models. The efficacy of ML model is based on their capability to accurately forecast unknown data and effectively fit the available data points.⁷⁴

4.1. ML techniques in biodegradability

Determining the biodegradability of chemicals without relying on costly tests is both ecologically and economically advantageous. Quantitative structure–activity relationship (QSAR) models offer potential in this area. The QSAR prediction system is designed for classifying biodegradation datasets without the need for actual chemical experiments. QSARs are mathematical models that predict the physical, chemical, and biological properties of substances based on their molecular structures. These systems have gained attention as numerous countries have updated their environmental policies to reduce the use of environmentally harmful, non-biodegradable substances. For instance, European legislators incorporated chemical persistence in the registration, evaluation, and authorization of chemicals for chemical evaluation. These regulations utilize QSAR models for assessing chemical risks. The most recent, effective, and commonly used ML techniques in predicting biodegradability include classification and regression

trees (CARTs), support vector machine (SVM), K-nearest neighbor (kNN), regulated logistic regression (RLR) model, graph neural network (GNN), transformers, and Bayesian optimization (BO). Each of these techniques is briefly discussed below.⁷⁵

4.1.1. CART technique

CART is a robust and interpretable method for predicting the biodegradability of compounds using decision tree learning concepts; it constructs a binary tree by recursively splitting the dataset based on feature values to maximize the separation of biodegradable and non-biodegradable compounds (in case of biodegradability prediction).⁷⁶ Each node represents a decision based on a molecular descriptor (molecular weight, number of certain atoms, hydrophobicity, and other physicochemical properties), and the leaves represent the final prediction. This method is highly interpretable, allowing researchers to easily understand the decision-making process.⁷⁷ However, it can be prone to overfitting, which can be mitigated through pruning. CART's ability to handle non-linear relationships and its simplicity make it a valuable tool for assessing the environmental impact of chemicals.

4.1.2. SVMs

SVM is a powerful ML technique used to predict the biodegradability of compounds by finding the optimal hyperplane that separates biodegradable and non-biodegradable compounds in a high-dimensional feature space. By transforming molecular descriptors into this space, SVM maximizes the margin between the two classes, ensuring robust classification even with complex, non-linear relationships.⁷⁸ Kernel functions, such as radial basis functions, are often employed to handle non-linearity. SVM is highly effective for its accuracy and ability to manage high-dimensional data, making it a popular choice for biodegradability prediction in environmental science and chemical informatics.⁷⁹

4.1.3. kNN

kNN is another technique to determine the biodegradability of compounds by classifying a compound based on the majority class of its k closest neighbors in the feature space, in which the features are typically molecular descriptors. The choice of k (the number of neighbors) and the distance function are crucial hyperparameters that can be tuned to optimize the performance.⁸⁰ The distance metric, often Euclidean distance, determines the similarity between the compounds. kNN is intuitive and non-parametric without using any assumptions about the underlying data distribution. However, it

can be computationally intensive for large datasets and sensitive to the choice of k and feature scaling. Despite these challenges, kNN remains a valuable tool for biodegradability prediction due to its straightforward implementation and interpretability.⁸¹

4.1.4. RLR

RLR technique typically models the relationship between input variables and a binary outcome using a logistic function. An S-shaped curve is produced by a logistic function that maps the input to a probability value between 0 and 1 representing the predicted probability of a positive outcome. The model estimates the logistic function's parameters using maximum likelihood estimation. This technique prevents overfitting by utilizing regularization and improves generalization by adding a penalty term to the cost function. This penalty term reduces the magnitude of coefficients and prevents them from growing too large. The logistic regression model has two most popular regularization terms such as L1 (Lasso) or L2 (Ridge). The former adds the absolute values of coefficients to the cost function, causing some coefficients to become exactly zero and latter adding the squared values of coefficients to the cost function. Typically, the model estimates the probability that a compound is biodegradable based on its features, providing a clear probabilistic interpretation. Regularization helps in managing multicollinearity and ensures that the model generalizes well to new data, making it a reliable choice for biodegradability prediction in environmental science and chemical informatics.

4.1.5. GNNs

GNNs are increasingly utilized in predicting biodegradability due to their ability to model the complex, non-linear relationships inherent in chemical structures. By representing molecules as graphs, where atoms are nodes and bonds are edges, GNNs can effectively capture the intricate connectivity and properties of compounds. This allows for accurate predictions of biodegradability by learning from the structural features and patterns within large datasets of chemical compounds. Consequently, GNNs facilitate the design of environmentally friendly chemicals by enabling researchers to identify and optimize biodegradable properties early in the development process.⁸²

4.1.6. Transformers

By utilizing self-attention mechanisms, it effectively captures the relationships within molecular structures, analyzing how substructures influence biodegradability. This allows for a detailed analysis of how various substructures within a molecule influence its biodegradability. The transformer model processes the molecule as a sequence of tokens, where

each token represents an atom or a bond, and learns to predict biodegradability based on these sequential patterns. This approach has shown promising results in accurately predicting the biodegradability of chemical compounds, providing a powerful tool for environmental chemistry and drug design.

4.1.7. BO

The BO algorithm is widely used due to its efficiency in finding good solutions with few iterations. BO uses a surrogate function, typically a Gaussian process, to approximate the objective function, and an acquisition function, such as expected improvement (EI), to explore the solution space. BO achieves this optimization through a combination of surrogate models and acquisition functions as follows: (1) Sampling the objective function at random points to build an initial dataset and surrogate model; (2) using the acquisition function to find the next point that minimizes the surrogate model, and updating the dataset and surrogate model accordingly; and (3) repeating this process to iteratively improve the approximation of the objective function until the global minimum is found. In biodegradability prediction, BO helps in refining model parameters to enhance accuracy, enabling more precise assessments of how chemical compounds break down in the environment, which is crucial for designing environmentally friendly substances.⁸³

Besides classification techniques, regression techniques in ML are also increasingly being utilized in the field of biodegradability to predict how chemical compounds break down in the environment. This involves modeling the relationship between chemical structures and their biodegradation rates or degradation half-lives. Understanding and predicting biodegradability is crucial for assessing the environmental impact of chemicals, pharmaceuticals, and other substances. Typically, regression involves predicting a continuous numerical value for given input data using different regression models and evaluation metrics. To predict the rate at which a chemical compound degrades in the environment, different regression models are used including linear regression, polynomial regression, support vector regression (SVR), and more advanced techniques like random forests and neural networks. It uses further evaluation metrics such as mean absolute error, mean squared error (MSE), R-squared (RS), and root MSE techniques to predict the continuous numerical value. All these regression models are briefly explained as follows:^{84,85}

(1) *Linear regression (LR)*. This is a simple and effective model that can provide a baseline for predicting biodegradation rates. However, their simplicity might

limit accuracy when dealing with complex molecular interactions.

- (2) *Multiple linear regression*. It extends LR by considering multiple chemical descriptors. It is useful for capturing the combined effect of various molecular features on biodegradability.
- (3) *Polynomial regression*. It is suitable for modeling non-linear relationships between chemical properties and biodegradation rates. It allows for capturing more complex patterns other than those captured by LR.
- (4) *SVR*. Effective for handling non-linear relationships and high-dimensional data, SVR can provide more accurate predictions for complex biodegradation processes.
- (5) *Random forest regression*. It is an ensemble method that uses multiple decision trees to improve prediction accuracy and robustness. It is particularly useful for handling large datasets with many features.
- (6) *Neural networks*. These are deep learning models, including feedforward neural networks, that can capture intricate non-linear relationships between chemical structures and biodegradation. They require large amounts of data and computational resources but can provide highly accurate predictions.

Taken together, regression techniques in ML represent a powerful tool for predicting the biodegradability of chemical compounds, aiding in environmental protection and the development of sustainable products. The ongoing refinement of these models and integration with experimental data will further enhance their applicability and reliability. Here, we acknowledge the importance of regression methods for predicting continuous outcomes, such as degradation time. However, according to a recent investigation,⁸⁶ there is a notable scarcity of numerical data (<3200 records) necessary for regression analysis.⁸⁷ Specifically, the lack of available and standardized characterization of parameters, such as reaction setup, binary classification, and degradation time, represents a nearly insurmountable obstacle to the ML-aided design of transient materials, *i.e.*, experimental datasets containing properties such as degradation rate are limited. This scarcity hinders the ability to create robust regression models. For instance, degradation time is often not included in current databases, making it difficult to assemble a labeled dataset for training predictive models. Huang and Zhang⁸⁸ have attempted to address these issues by compiling a large dataset of 12,750 records, which encompass various biodegradation conditions, and developing robust regression and classification models. However, the regression model only achieved an R^2 of 0.54, while the best classification model reached an accuracy of 85.1%, which improved to 87.6% with chemical speciation considerations.⁸⁸ Furthermore,

the absence of standardized characterization parameters further complicates the integration of existing data into regression models. Variability in how data are collected and reported reduces the reliability and comparability of the data. Due to these challenges, the current focus of studies has been on classification techniques where sufficient data are available. We believe that enhancing data collection methods and standardizing parameter reporting will be crucial for future research. This will eventually enable the effective use of regression techniques in the ML-aided design of materials.

4.2. Challenges in ML for polymer degradation

Recent QSAR studies have primarily aimed for accuracy, often at the cost of transparency, employing models such as SVM, GNN, and kNN, which are mentioned above. Although it is established that integrating data and using ensemble analysis can enhance the reliability of QSAR models, they often encounter issues with uncertainty for several reasons. For instance, QSAR models may produce false correlations due to errors in the experimental process or may not fully capture the data characteristics because of the limited size of training datasets. In addition, these models inherently require the generation of suitable features for training, making feature selection a complex task. For example, certain structural features of molecules, such as halogens, chain branching, and nitro groups, have been shown to increase biodegradation time, whereas others, such as esters, amides, and hydroxyl groups, have the opposite effect. However, these structural features cannot be universally applied to represent both readily biodegradable and not readily biodegradable molecules.⁸⁹

Designing for multiple properties, particularly when considering degradation behavior, is becoming more imperative yet challenging, as optimizing one property often entails compromising others. Other significant hurdles in polymer informatics involve developing representations that account for stochasticity, acquiring larger datasets, and further exploring retrosynthetic design methodologies.⁹⁰ Moreover, the absence of standardized characterization for parameters such as degradation time and biocompatibility poses a significant challenge that is difficult to overcome in ML-assisted designs.⁸⁶ Even though only one or several interesting parameters of the original system are often focused, a more systematic treatment is required to understand the hierarchical relationships by appropriately integrating experimental chemistry, simulations, and data science. In the future, the establishment of additional pertinent databases is necessary to enable easy access to extensive datasets. Furthermore, the data currently employed

are primarily gathered manually from experiments or literature, but ML, particularly through widely used large language models, could aid in streamlining the data collection process. In addition, leveraging existing datasets for enhanced algorithmic refinement, including the application of data augmentation methods to increase dataset size, could contribute to greater efficiency. Collaborative sharing of domain expertise also offers a means to alleviate data scarcity, avoiding duplication in data collection efforts and thereby minimizing costs and resource utilization.⁷⁰

5. AI-driven material design

In the 21st century, the primary focus for material scientists is to strike a balance between performance and sustainability in materials. In general, the design of materials is influenced by their function and life cycles within specific environments. For example, when incorporating electronics into biological contexts, factors such as material biocompatibility, device implantation method, and overall design integration must be carefully considered.⁹¹ Molecular design serves as a method to achieve the desired functionality.

In the realm of polymer chemistry, key factors that influence their functionality include composition (such as monomer sequence, chain length, dispersity, end functionality, side chain type, and backbone) and topology (such as branching, regioregularity, and tacticity). The relationship between polymer composition and topology spans various chemical scales, from the molecular to the macromolecular level.⁹² Therefore, the molecular structure and polymer composition determine their mechanical, optical, and electrical characteristics. Even slight adjustments in the composition of polymers can directly affect the characteristics of macromolecules, especially their flexibility and water solubility. For example, after examining a collection of 51 low-band-gap polymers, Roth *et al.*⁹³ identified some major trends in the stiffness (tensile modulus) and ductility (crack-onset strain); wherein the presence of fused rings along the backbone tends to reduce ductility and increase the modulus. However, the opposite impact is experienced by branched side chains in the material. The side chains can act as solubilizing agents by introducing functional groups or interfering with crystallization.⁹³ In addition, 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. For instance, conjugated polymers are often insoluble in organic solvents, making them difficult to process into thin films. To enhance solubility in nonpolar liquids, branched alkyl chains, instead of linear ones, are

commonly used because their bulkiness could hinder interchain interactions. Simply, adding ionic side chains can also make them more soluble in water and polar organics.⁹⁴ Besides, structure-dependent characteristics can be fundamentally understood by examining polymer architecture, as it affects intra- and inter-molecular interactions in melts and solutions. Block copolymer structural characterization is an intriguing and developing field of study with great potential for advancement. Controlling the morphology at the nanoscale can be achieved by selecting the right blocks in terms of chemistry, composition, and architecture.⁹⁵ Sidky *et al.*⁹⁶ reported using data-driven ML/deep learning-based trajectory forecasting algorithms to reduce the computational load of simulating the complicated structures. ML techniques coupled with simulations hold useful potential for comprehending the underlying relationship between the complex architecture and the characteristics of grafted polymers.⁹⁶

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 the structural features of polymer networks at the molecular level. These techniques include programming topological information into network precursors or biasing of polymerization kinetics.⁹⁷ Notably, 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.⁹⁸ In a recent effort to enhance the understanding of the relationship between topology and elasticity, Zhong *et al.*¹⁰² conducted a study to evaluate 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.^{97,100,101} 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.¹⁰⁰ The effectiveness of this theory in predicting mechanical properties emphasizes the value of molecular

knowledge to comprehend the chemical basis of polymer network architecture.⁹⁰ Research in this subject area will continue to harness the topology of polymer networks as the study direction to a greater extent. By employing advanced characterization techniques and synthesis methods, researchers can achieve a better understanding of 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.⁹⁷

6. ML-guided biodegradation insights

A large range of biodegradable materials especially polymers are used in many products that require a limited lifespan. Every biodegradable polymer comprises hydrolyzable or oxidizable bonds. Owing 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 singularly 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.⁹⁹ Nonetheless, a key challenge here is to understand the mechanical behavior of biodegradable materials throughout their degradation. For example, a forecast model is utilized to read the mechanical properties in a composite of PCL and PLA. Here, a numerical method using ABAQUS® is provided, in which a user material subroutine 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.¹⁰² Yet a study by Jiang *et al.*¹⁰³ aimed to develop ML-based models to predict primary and ultimate biodegradation rates of organic chemicals, which are crucial for environmental risk assessment. The survey offers valuable tools for predicting biodegradation rates and insights into underlying mechanisms (Figure 3A).¹⁰³

Figure 3B shows the application of ML in the context of biomass-derived materials for water and agricultural systems. Analyzing and reviewing a collection of 53 papers published since 2008, Wang and Yao¹⁰⁴ categorized ML applications into material and process design, end-use performance prediction, and sustainability assessment.¹⁰⁴ The environmental fate of polymers, particularly biodegradable ones, has become a focal point across academic, industrial, and regulatory sectors. Albright and Chai examined test

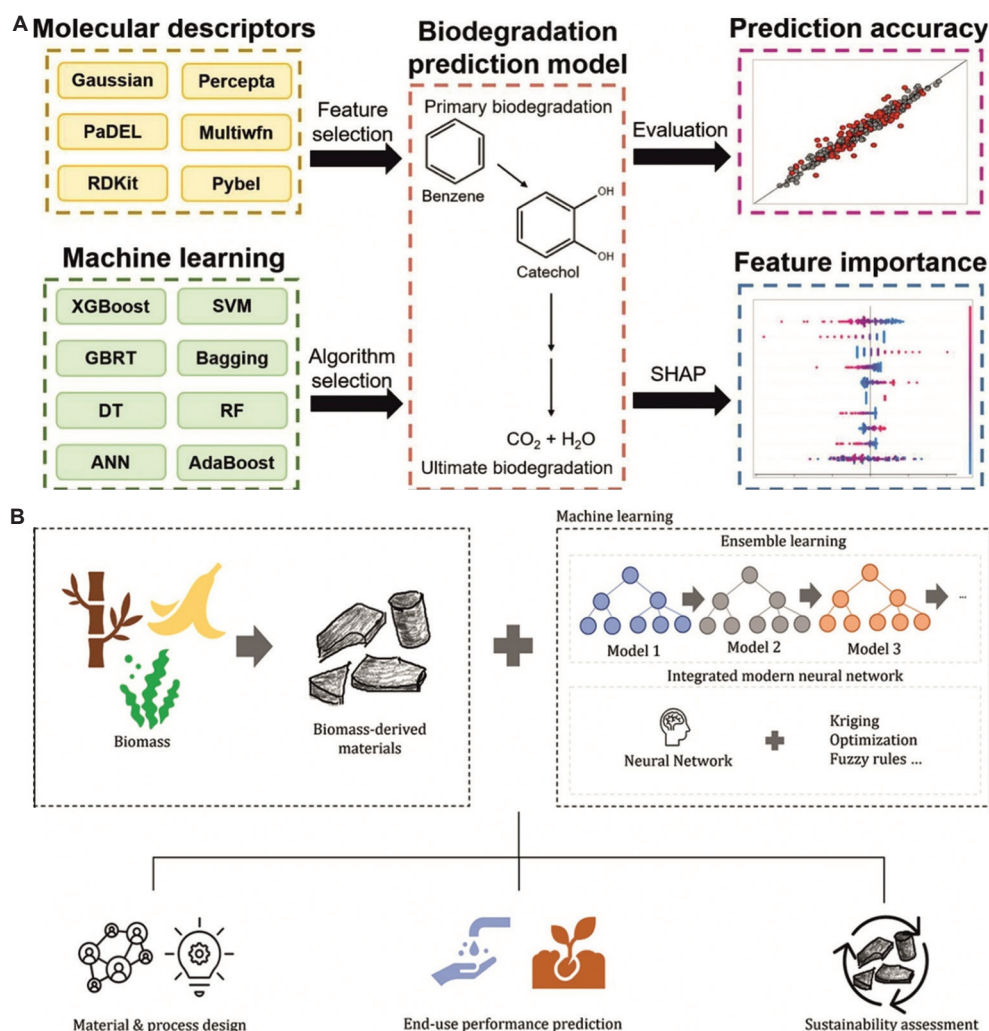


Figure 3. Prediction of biodegradation rate through machine language (ML) models/techniques. (A) Schematic showing the utilization of different ML-based models to predict and understand the biodegradation rate by giving the input of molecular descriptors. Reproduced with permission.¹⁰⁴ (B) The symbiosis 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.¹⁰⁵

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, and the advantages and limitations of analytical methods (Figure 4A). The authors identify crucial knowledge gaps and propose four recommendations for advancing polymer biodegradation studies: (1) Establishing standardized guidelines for various environmental matrices; (2) devising accelerated biodegradation and predictive methods for polymers; (3) adopting an integrated analytical approach using simple and effective methods; and (4) developing new

frameworks for assessing overall polymer persistence accepted by the scientific community.¹⁰⁵

As shown in Figure 4B, the 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 GNN, which aids in reducing the design space of renewable feedstocks, streamlining the discovery process of high-performance, bio-based 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 bio-based polymer practitioners

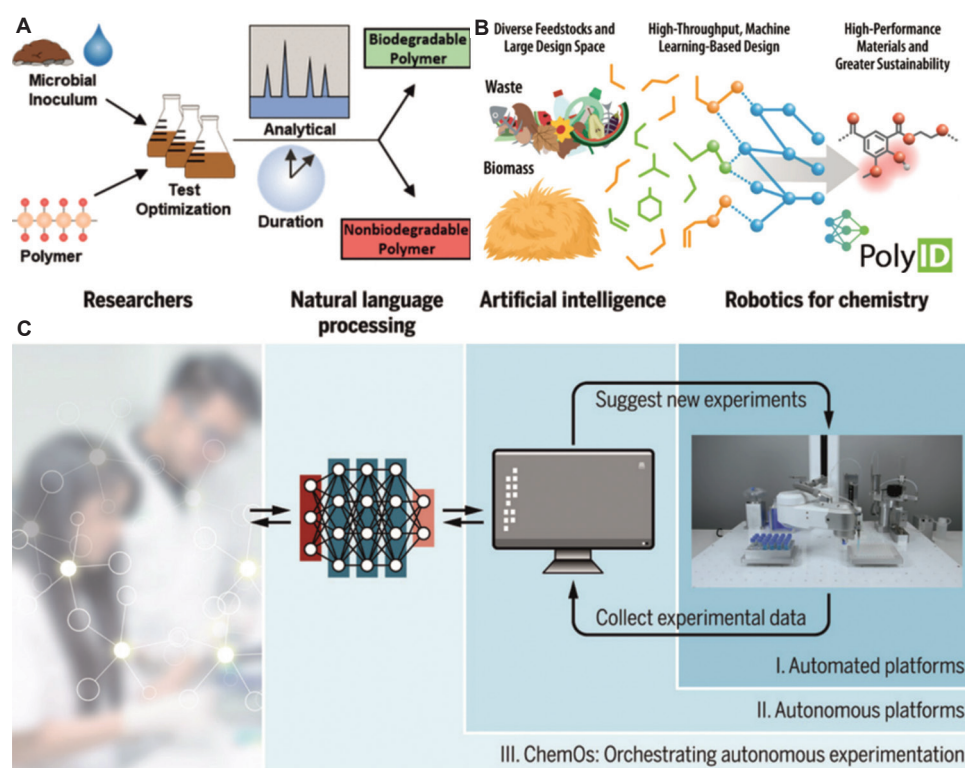


Figure 4. Machine learning (ML)/artificial intelligence (AI) techniques for automating experimental procedures in polymer research. (A) Example of an ML technique demonstrating the identification of crucial knowledge gaps and proposal of methods to determine polymer degradability and non-degradability. Reproduced with permission.¹⁰⁶ (B) Schematic illustrating ML-based PolyID tool describing the usage to reduce the design space of renewable feedstocks to enable efficient discovery of performance-advantaged, bio-based polymers. Reproduced with permission.¹⁰⁷ (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.¹⁰⁸

in discovering sustainable materials with enhanced performance.¹⁰⁶ In addition, AI algorithms are used with automated robotics platforms to create autonomous laboratories to conduct experiments independently. AI designs and recommends experiments, validated by robotics platforms, and analyzes results to enhance experimental strategies and propose better hypotheses for subsequent experiments (Figure 4C).¹⁰⁷

7. AI-assisted materials discovery

AI possesses the capacity to become a revolutionary force, catalyzing progress across diverse scientific and technical domains, including chemistry, materials science, and engineering.¹⁰⁸ The ability of AI to extract insights from complex systems has been shown to boost productivity, lower capital costs, and improve product quality and user satisfaction. However, AI's actual worth is grounded in its ability to advance scientific discoveries and provide answers to difficult worldwide issues related to the global environment, economy, and society.¹⁰⁹ Bringing together specialists

in the green and sustainable domains, the AI experts expedite the development of the 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, reducing the need for experimental and computing resources. AI-assisted materials discovery represents a paradigm shift in scientific exploration, leveraging advanced algorithms and data analytics to expedite the identification and development of novel materials with tailored properties. By harnessing the power of ML and computational modeling, researchers can efficiently navigate vast chemical spaces, accelerating the pace of innovation and opening new avenues for breakthroughs in various industries such as healthcare, energy, and electronics. This interdisciplinary approach not only enhances our understanding of materials at the atomic level but also promises to revolutionize the way we design and engineer materials for diverse applications, ultimately leading to the creation of next-generation

technologies with unprecedented performance and functionality.

The primary difficulty in new material discovery lies in analyzing the materials data with numerous dimensions. To address this challenge, ML techniques are utilized, adjusted, and enhanced. There are several ML methods that can be used based on the task of the experiments. These methods are classification, regression, clustering, dense neural network, sequential learning, dimension reduction, variational autoencoders, convolutional neural network, and BO. The AI algorithms analyze the validation of results to enhance experimental strategies, thereby enabling more precise predictions for subsequent experiments. Unlike in automated laboratories, where researchers preset experimental procedures, this closed-loop approach is adopted. Consequently, autonomous laboratories could refine traditional trial-and-error methods, accelerating the discovery of chemicals and materials. Moreover, they might mitigate the trade-off between the cost of human-driven testing, which may have reached its peak in terms of efficiency gains, and the expected time to discovery. Besides, AI-driven quantum mechanics and computing resources have the capability to revolutionize predictive toxicology, an underlying aspect of sustainability analysis.¹¹⁰

Through advanced algorithms and ML 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 multistage task, mainly involving 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 surpass human processing capabilities. Thus, AI can assist by automating and enhancing the characterization process, reducing manual labor, 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.^{111,112} 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.¹⁰⁹ Thus, 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.

8. Summary and perspectives

This paper contains a concise review of the recent advancements in transient technology, specifically in the context of transient electronics, with a focus on analyzing the materials, designs, and performances of these devices. A major part of this review focuses on transient materials, encompassing metals, polymers, and semiconductor materials. Further research should target 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 a suitable balance. The development of AI and robotics-based molecular design tools for autonomous high-throughput experimentation is accelerating. These technologies hasten the process of generating and optimizing commercially viable materials and equip chemists with tools for predicting molecular properties.¹¹³ This versatile and data-driven approach is required to address the time-consuming and expensive 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 translate to bulk properties.¹¹⁴ 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 repurposing of existing molecules for novel applications.¹¹⁵ 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 is necessary to compile comprehensive data related to the planned behavior 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.¹¹⁶ 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 applied to the field of chemical research because of the growing multidisciplinary nature of research. Although using AI has grown commonplace in some sectors, this technology has not yet had a significant influence on certain fields of burgeoning research, such as sustainable technology. Hence, more interdisciplinary research and advancements in self-training of AI data will help these fields move forward efficiently.

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Conflict of interest

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