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Review

Advances, Synergy, and Perspectives of Machine Learning and Biobased Polymers for Energy, Fuels, and Biochemicals for a Sustainable Future

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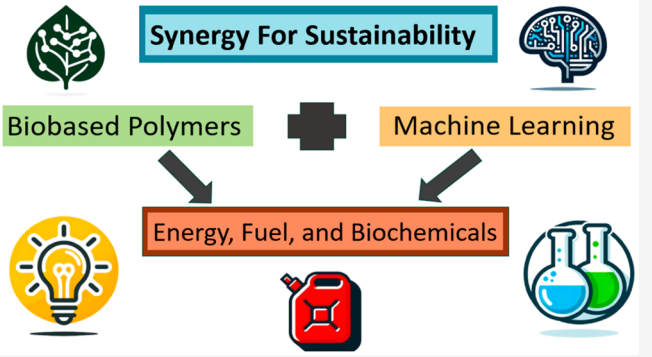
ABSTRACT: This review illuminates the pivotal synergy between machine learning (ML) and biopolymers, spotlighting their combined potential to reshape sustainable energy, fuels, and biochemicals. Biobased polymers, derived from renewable sources, have garnered attention for their roles in sustainable energy and fuel sectors. These polymers, when integrated with ML techniques, exhibit enhanced functionalities, optimizing renewable energy systems, storage, and conversion. Detailed case studies reveal the potential of biobased polymers in energy applications and the fuel industry, further showcasing how ML bolsters fuel efficiency and innovation. The intersection of biobased polymers and ML also marks advancements in biochemical production, emphasizing innovations in drug delivery and medical device development. This review underscores the imperative of harnessing the convergence of ML and biobased polymers for future global sustainability endeavors in energy, fuels, and biochemicals. The collective evidence presented asserts the immense promise this union holds for steering a sustainable and innovative trajectory.



1. INTRODUCTION

In the quest for a sustainable future, numerous challenges have been encountered.[1,2] Global reliance on nonrenewable energy sources has exacted a significant toll on the environment.[3−5] Traditional materials, primarily derived from finite resources, exacerbate the environmental burden, contributing to pollution and resource depletion.[6,7] The promise of biobased polymers, sourced from renewable biomass, is overshadowed by various obstacles, including their production, modification, and application in diverse fields.[8] ML, a subset of artificial intelligence, involves the development of algorithms and statistical models that enable computers to perform tasks without explicit instructions.[9−11] Instead, these systems learn from and make predictions or decisions based on data. This technology has become increasingly pivotal in various sectors, including energy, materials, and biotechnology.[12−17] The integration of ML offers a pioneering approach, potentially overcoming these barriers by optimizing biopolymer characteristics and their applications in energy, fuel, and biochemical domains.[18−20] However, a substantial research gap persists in the comprehensive understanding and effective deployment of this synergistic relationship.

In various sectors, initial strides toward integrating biobased polymers for sustainable energy, fuels, and biochemicals are being made.[21,22] Table 1 shows the Source and Overview of Biobased Polymers. The production and modification of these polymers are currently being refined, contributing to the gradual mitigation of the associated challenges. Despite these endeavors, optimizing biobased polymers for diverse applications remains a significant hurdle.[23,24] Parallel efforts are observed in the realm of ML where advanced algorithms and computational models are being developed to enhance the characteristics and applications of biobased polymers.[25−27] ML strategies for the improved production and application of biobased polymers are emerging. These efforts symbolize the budding synergy between ML and biobased polymers, showcasing the collective stride toward a sustainable future.

In this comprehensive review, an exhaustive and critical examination of the advancement and synergy of ML and biobased polymers is conducted. Insight into the inherent

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Table 1. Source and Overview of Biobased Polymers

source of biobased polymers	biopolymer types	potential application	reference
Corn starch	Polylactic acid (PLA)	Biodegradable packaging, agricultural products	28
Sugar cane	Biopolyethylene (bio-PE)	Food packaging, cosmetics, personal care, automotive parts, toys, agricultural and industrial purposes	29
Microalgae	Polyhydroxy alkanoates (PHA)	Medical devices, Biodegradable packaging	30
Cellulose	Cellulose acetate	Food packaging	31
Soybeans	Polyhydroxyerethane (PHU)	Adhesives and coatings	32
Potatoes	Starch-based biopolymers	Biodegradable packaging films	33
Castor oil	Polyamide 11 (PA11), Polyurethane (PU)	Footwear and automotive parts	34−36
Chitin from shrimps and crabs	Chitosan	Drug delivery and dressings	37
Whey	Whey protein-based films	Food packaging	38
Macroalgae	Alginate, agar, carrageenan	Edible films and lectins	39

attributes of biobased polymers and their cardinal role in bolstering sustainability in diverse applications is offered. The profound influences of ML on the enhancement of biobased polymers are elucidated. Discussions highlight the prominent role of biobased polymers in sustainable fuels and their production, alongside the substantial impact of ML on fuel efficiency and innovation. The notable contributions of both domains to the advancement of biochemical production are expounded. A conclusion is presented, summing the findings and providing a directional path for future research, solidifying the belief in the continuous collaborative growth of ML and biobased polymers for a sustainable global future.

This compelling review culminates in affirming the indispensable role played by the convergence of ML and biobased polymers in energy, fuels, and biochemicals. This review fills a gap in the current literature by providing a unique, integrated perspective on ML and biobased polymers, a combination scarcely addressed in existing studies, offering timely insights into emerging interdisciplinary solutions for sustainability. The path toward a more sustainable and innovative future is presented by thoroughly exploring the intersection of these two critical domains. The detailed analysis presented within these pages aims to inform and spur further research and development in these vital areas. The criticality of this synergy underscores a compelling opportunity for the global research community, highlighting the potential for enhanced exploration and investment in these areas, pivotal for driving sustainable advancements and innovations.

2. BIOBASED POLYMERS AND SUSTAINABILITY

A global shift toward sustainability is being witnessed.[40−42] An essential role in this transformative move is played by biobased polymers, which are derived from biological sources rather than petroleum bases.[43,44] Derived from biomass, these polymers are considered the more sustainable option, thereby increasing utilization across various industries.[45] In this significant transition, biobased polymers' properties, characteristics, and diverse applications are analyzed, highlighting their impactful role in advancing the sustainable agenda for the energy, fuel, and biochemical industries.[46] In their essence, biobased polymers carry properties that address many environmental concerns.[47] Being biodegradable, a significant reduction in waste pollution is associated with their use.[48,49] These polymers exhibit a commendable balance between lightness and strength and their flexibility, making them adaptable to a wide range of applications.[50] Their diverse properties open avenues for customizations suitable for specific needs, reinforcing their potential and adaptability across multiple sectors.

A swift surge in the application of biobased polymers in the energy sector is noted.[51,52] The efficiency and durability of renewable energy systems such as solar panels and wind turbines are being enhanced by integrating biobased polymers.[53,54] These polymers further facilitate the fostering of sustainable energy technologies, emphasizing their significant role in promoting renewable energy systems and contributing to the global sustainability movement. A marked influence of biobased polymers in the fuel industry is observed.[55] The enhancement in the production of biofuels is ascribed to the effective catalytic properties exhibited by these polymers. The efficient conversion of biomass to fuels is being facilitated, demonstrating their crucial contribution to bolstering sustainable fuel production.[55,56] This is an essential step in the global move toward more sustainable and cleaner energy solutions, further reinforcing the pivotal role played by biobased polymers.

The realm of biochemicals is not untouched by the extensive benefits of biobased polymers. Their use in developing biodegradable and ecofriendly packaging materials is reducing the environmental load considerably.[57,58] Moreover, a significant contribution to the production of sustainable chemicals and materials is made by these polymers, showcasing their extensive and versatile applications.[59] In the domain of

Table 2. ML's Capability in Property Prediction and Optimization Potential for Materials Science and Engineering

property or feature	ML's role in enhancement	potential impact	references
Material design	Guiding innovative design approaches	Enhanced material functionality	61, 84
Mechanical properties	Predicting and optimizing strength and durability	Improved product reliability and lifespan	85, 86
Thermal properties	Forecasting and enhancing heat resistance	Wider application range	87, 88
Environmental compatibility	Assessing and improving biodegradability	Increased sustainability	89, 90
Production efficiency	Enhancing process parameters for efficient production	Reduced production cost and time	91, 92
Performance characteristics	Ensuring robust and efficient material properties	Enhanced operational efficiency	79, 93
Application specific customization	Tailoring polymers for specific applications	Improved performance in diverse applications	94, 95
Cost-efficiency	Optimizing for low-cost production and material use	Economic and competitive advantages	96, 97
Integration in renewable energy systems	Customizing materials for energy systems	Augmented renewable energy efficiency	98, 99
Integration in energy storage	Developing advanced components for energy storage	Enhanced energy storage capacity and efficiency	73, 100

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energy storage and conversion, biobased polymers are making substantial contributions.[60] High-efficiency batteries and supercapacitors are being developed with these polymers, exhibiting advancements in energy storage solutions and contributing to the sustainable energy ecosystem.[19,51]

The encompassing role of biobased polymers in propelling global sustainability efforts is emphasized. From the energy sector to biochemicals, their diverse applications foster advancements in sustainable technologies and materials, leading the path toward a more environmentally conscious future. The ongoing research and exploration in biobased polymers signify the continuous enhancement and discovery of their potential, promising a sustainable and innovative future.

3. ML: REVOLUTIONIZING MATERIAL SCIENCE

In the evolving panorama of material science, the influence of ML stands out, predominantly steering the enhancement and development of sustainable materials and biobased polymers.[61−65] The prospect of designing advanced materials with precise properties for specific applications is heightened by employing ML algorithms for property prediction and optimization.[11,66,67] A comprehensive analysis of large data sets performed by ML efficiently discerns patterns and correlations that might remain unnoticed by conventional methods.[68] Through this, expedited and more informed decisions are made in the development of biobased polymers for diverse applications. Table 2 shows the ML capability in property prediction and optimization potential for materials science and engineering.

In the sector of renewable energy systems, a remarkable enhancement is noticed in the integration of biobased polymers, courtesy of ML interventions.[69,70] Renewable energy apparatuses like solar cells and wind turbines are experiencing a boost in operational efficiency by incorporating ML-optimized biobased polymers.[71,72] By understanding the intricate material properties and performance characteristics, ML aids in customizing biobased polymers to complement the unique requirements of different renewable energy systems.[27] This cooperation between ML and biobased polymers is proving to be instrumental in augmenting the sustainability and efficiency of renewable energy systems, contributing significantly to global sustainable energy goals.

Shifting the focus to energy storage, ML's impact in the refinement of biobased polymers for this purpose is substantial.[73] The ML algorithms, proficient in analyzing and predicting material behaviors, play a crucial role in the development of biobased polymer components for advanced batteries and energy storage systems.[27,74] The accurate prediction capabilities of ML aid in ensuring the robustness and efficiency of these storage solutions, further emphasizing ML's role in promoting the sustainability of energy storage technologies.[75,76] Real-time monitoring and predictive maintenance, facilitated by ML, enhance the lifespan and reliability of these energy storage systems, showcasing the comprehensive benefits of ML's integration.[77,78]

In energy conversion systems, the contribution of ML to the progress of biobased polymers is crucial.[79] The role of biobased polymers in fuel cells and other energy conversion devices is optimized by employing ML for the precise tailoring of material properties.[80,81] The potential of ML in guiding the development of high-performance, sustainable biobased polymer components for energy conversion is significant. It ensures the efficiency and sustainability of these systems, thus playing a crucial role in enhancing overall energy conversion processes and technologies.[79]

Further, integrating ML in the realm of biobased polymers fosters innovation in material design and performance. ML's capability in property prediction and optimization guides the development of biobased polymers with enhanced features for diverse energy applications.[82,83] The concurrent evolution of both these domains, facilitated by ML, ensures the timely advancement and integration of efficient and sustainable biobased polymers in the global energy landscape.

In summation, the integration of ML in material science, particularly in enhancing and developing biobased polymers, marks a significant leap toward comprehensive sustainability and efficiency in energy systems. Ensuring the continued collaboration and innovation in these intertwined domains is fundamental for the realization of global sustainable energy objectives, underscoring the essential role of ML in this endeavor.

4. ENERGY AND FUELS

4.1. Biobased Polymers for Sustainable Energy. The integration of biobased polymers such as chitosan, lignin, polypyrrole, PLA, PHA, and microalgae-derived biopolymers in the field of sustainable energy reveals significant promise for enhancing the performance and environmental compatibility of renewable energy systems, energy storage, and energy conversion.[101−104] Within the renewable energy sector, these polymers actively participate in constructing more efficient, environmentally friendly solar cells.[105] Their application is seen in organic photovoltaic cells, which serve as the active layer, enabling the absorption and conversion of solar energy to electricity.[106,107] For instance, in the fabrication of organic photovoltaic cells, chitosan is often employed due to its excellent film-forming properties and biocompatibility, enhancing the cell's ability to absorb and convert solar energy.[108,109] Additionally, PLA is another biobased polymer frequently used in these cells for its environmental sustainability and efficiency in aiding the conversion process from solar to electrical energy.[110,111]

In the realm of energy storage, biobased polymers show significant potential for the development of advanced, sustainable batteries.[112] Utilizing biobased polymers for making electrodes and electrolytes in batteries has witnessed notable advancements, contributing to the production of high-performance energy storage devices.[22,113] The introduction of these ecofriendly materials in batteries effectively supports the reduction of hazardous waste and the overall environmental footprint.[114] This application stands as a testament to the beneficial amalgamation of biobased polymers and energy storage systems. Additionally, the role of biobased polymers in energy conversion is crucial and is gradually gaining attention. These materials contribute to the enhancement of fuel cells and other energy conversion devices, ensuring higher efficiency and sustainability. Biobased polymers function as essential components in the membranes of fuel cells, promoting the efficient conversion of chemical energy to electrical energy.[101,115] By replacing conventional, petroleum-based materials with biobased alternatives in these applications, the industry makes substantial strides toward a more sustainable and ecofriendly future.

The infusion of ML with materials further catalyzes these advancements, providing an avenue for optimized material design and utilization.[116] Sophisticated algorithms and models

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facilitate the precise tailoring of biobased polymer properties to meet specific energy-related applications. ML assists in predicting and enhancing the performance, functionality, and environmental impact of these polymers within diverse energy systems.[117] Through this synergy, the potential for innovation and development in utilizing biobased polymers for sustainable energy is boundless.

In conclusion, the amalgamation of biobased polymers with sustainable energy applications bolstered by advancements in ML exemplifies a promising pathway for the future. These polymers' incorporation into renewable energy systems, energy storage, and energy conversion technologies demonstrates tangible benefits for these systems' efficiency, performance, and environmental sustainability. The continued exploration, research, and development in this domain are imperative to fully unlock and harness the potential of biobased polymers for a more sustainable and energy-efficient future. The commitment to this exploration and innovation will invariably lead to achieving global sustainability goals, ensuring a cleaner, greener, and more efficient energy landscape for future generations.

4.2. Case Studies of Advanced Biobased Polymers for Energy Applications. Exploring biobased polymers for energy-related applications holds significant promise in the journey toward sustainable energy solutions. Advanced biobased polymers, thoroughly investigated through various case studies, unveil opportunities for enhanced ionic conductivity, increased efficiency and longevity of energy devices, and improvement in other critical parameters, ultimately contributing to the evolution of green energy technologies.

The work by Rudhziah et al.[118] presented an innovative exploration into the realm of biopolymer electrolytes, specifically focusing on blends of carboxymethyl kappa-carrageenan and carboxymethyl cellulose. The blending was found to enhance material properties, particularly conductivity. The research reported a remarkable finding of the highest room temperature ionic conductivity, achieving 2.41×10^{-3} S cm^{-1} at 30 wt % of ammonium iodides. This result is indicative of the impactful role of salt concentration on ionic conductivity. A meticulous evaluation of the polymer-salt interaction revealed a significant interaction with NH_4I salt, which was instrumental in increasing the O−H band, indicating a noteworthy interaction with the biopolymer chain oxygen atoms. This aspect demonstrated the essential role of NH_4I in the enhanced conductivity of the blended biopolymer electrolyte. It was established that the system's conductivity heightened with the increase in temperature, reaffirming the Vogel−Tammann−Fulcher relation and uncovering an activation energy of a low 0.010 eV for the highest conducting sample. Future research could delve into the potential optimization of the biopolymer blend ratios and the concentration of NH_4I to enhance the electrolyte's conductivity and overall efficiency.

In the work by You et al.,[119] the utilization of a biopolymer heparin sodium (HS) interfacial layer to enhance the efficiency and longevity of methylammonium lead trihalide ($MAPbI_3$) perovskite solar cells is meticulously analyzed. The HS layer's application evidently mitigated the traps at the perovskite-TiO_2 cathode interface, resulting in a significant boost in power conversion efficiency from 17.2% to a commendable 20.1%. Remarkably, the HS interfacial layer's role in retarding device degradation is clear, with devices maintaining 85% efficiency after 70 days of exposure to ambient conditions. The intricate methods employed, including density functional theory calculations, affirmed HS's passivation of $MAPbI_3$ and TiO_2 surfaces, interacting with undersaturated ions and thereby enhancing the overall device performance. Furthermore, elucidating reduced hysteresis and enhancing device parameter consistency post-HS layer addition solidify the findings. The comprehensive assessment, including photoluminescence spectroscopy and time-resolved PL decay kinetics, reinforced HS's critical role in promoting charge transfer, reducing surface charge trapping, and improving film quality by diminishing void density. The evident increase in recombination resistance from 1345 Ω to 2138 Ω with HS, highlighted in the Nyquist plots, further supports the assertion of HS's impactful role in enhancing perovskite solar cell performance. In terms of stability, the HS interlayer proves crucial. A compelling 90% of initial performance is retained after 70 days in a nitrogen atmosphere, a notable improvement over the reference cell's 60% efficiency retention. These robust findings underscore the HS layer's crucial role in significantly enhancing perovskite solar cells' efficiency and durability.

In the work by Rasal et al.,[120] a novel and nature-inspired approach utilizing polydopamine (PDA)-based additives in polysulfide electrolytes was explored to enhance the efficiency and stability of quantum dot-sensitized solar cells (QDSSCs). The work reports a significant enhancement in the conversion efficiencies with P-PDA and Se-PDA electrolytes, yielding 7.83% and 8.59%, respectively, compared to a 7.62% efficiency from the reference electrolyte. This improvement is attributed to the suppression of electron−hole recombination at the TiO_2/QDs/electrolyte interface by the PDA-based additives. Moreover, the PDA-based additives greatly contributed to the performance stability of QDSSCs, with P-PDA and Se-PDA devices retaining 91% and 79% of their original performance after 60 h, contrasting sharply with the 11% retention of liquid electrolytes. The technical aspects were meticulously detailed in the work. The Se-PDA showed distinct sharp peaks at certain degrees, confirming successful Se doping on P-PDA nanoparticles. Additionally, XPS results suggested that PDA's strong chelating properties may be responsible for the interactions between Se ions and P-PDA, a finding crucial for understanding the mechanism underlying the observed performance improvements. The study also reported improved water dispersibility and homogeneity with PEG-NH_2 functionalization and Se doping, resolving the issue of partial water solubility of PDA nanoparticles, a critical factor for ensuring uniform application and consistent performance of the modified electrolytes in QDSSCs. For future work, it would be imperative to explore the environmental footprint of using PDA-based additives and Se doping in polysulfide electrolytes. Further research could also focus on the optimization of the PDA and Se concentrations to enhance both the efficiency and stability of QDSSCs even further.

The work by Yuan et al.[121] scrutinizes the development and assessment of advanced biobased polythiophenes (PTs) for enhancing organic solar cells (OSCs) efficiency. The work discusses the introduction of new PTs (P5TCN-Fx) with cyano-group substitutions and varying fluorination degrees for heightened efficiency in OSCs. The cyano-group awards PTs deep energy levels, and backbone fluorination elicits robust interchain interaction, leading to a marked polymer crystallinity improvement. Significantly, several PTs have registered over 16% efficiency in binary OSCs, with a noteworthy 17.2%

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power conversion efficiency (PCE) observed for P5TCN-F25 via a ternary blend design. This progress is underscored by a comparison of the synthetic complexity (SC) and the number-average molecular weights (M_n's) of the polymers. P5TCN-Fx shows a lower SC (49.2%) than other studied polymers and M_n's ranging between 70 and 96 kDa, indicating efficient and stable polymer structures. Despite the decline in solubility after fluorination, all PTs remain adequately soluble for solution processing from common organic solvents. The study reveals an increase in thermal stability (above 430 °C) and melting and crystallization temperatures, showcasing the polymers' suitability for long-term OSC operation. However, it is worth noting the decreased homologous orbital (HOMO) energy levels with increased fluorination and a discernible aggregation at room temperature, particularly for higher fluorinated versions (P5TCN-F35 and F50). These polymers require elevated temperatures (55 and 65 °C, respectively) for deaggregation. In terms of future research, exploring the nuanced interplay between fluorination degrees and the resultant polymer properties will be crucial. This includes a deeper investigation into the balance between solubility, thermal stability, and energy levels to further optimize PTs for enhanced OSC efficiency while maintaining cost-effectiveness and long-term operational stability.

In the work by Abdulwahid et al.[122] on advanced biobased polymers for energy, the use of potato and chitosan starch, doped with NH_4SCN as the host electrolyte, portrays an innovative approach to developing electrochemical energy storage devices. The researchers produced novel plasticized solid biopolymer electrolytes with nontoxic glycerol, which were used as mediators in electric double-layer capacitor (EDLC) applications. This methodology significantly reduced crystallinity, as confirmed by XRD patterns, enhancing the ion conductivity (1.62×10^{-3} S cm^{-1}) and large electrochemical potential stability (2.1 V), especially for the PSBE composition with 24 wt % Gly. However, ion movement restrictions were observed for Gly-loaded samples (32 and 40 wt %), impacting ion transport and conductivity negatively. The assembled EDLC device displayed a specific capacitance of 16.1 Cspc F/g at a 10 mV/s scan rate, exhibiting stable and high performance over 2500 cycles.

In the critical examination by Aziz et al.[123] on the MC:Dex polymer blend electrolyte system with NH_4I salt for EDLC applications, notable results and techniques unfold. The XRD and FTIR analyses unveiled the complexation of MC:Dex polymer blend and NH_4I salt, with a discernible decline in crystallinity upon increasing salt concentration. Remarkably, the electrolyte composition with 40 wt % NH_4I showcased an apex in ionic conductivity at 1.12×10^{-3} S/cm and a stability window of 1.27 V, presenting itself as predominantly ionic. These outcomes highlight its potential for high-performance EDLCs. The EDLC, equipped with activated carbon electrodes and utilizing the highest-conducting electrolyte system, exhibited an initial specific capacitance of 79 F/g, an energy density of 8.81 Wh/kg, and a power density of 1111.1 W/kg at a current density of 0.2 mA/cm^2. The electrochemical stability assessment of the MC:Dex:NH4I system under the LSV method underscored its stability up to 1.27 V, aligning it as apt for proton-based energy devices. Despite these advancements, the EDLC performance observed a diminishing trend in prolonged cyclic tests. For future research, the exploration into enhancing the cyclic durability of the EDLCs developed with this electrolyte system would be paramount. Diving deeper into understanding the ion dynamics and electrode/electrolyte interplay could unearth avenues to bolster the electrochemical stability and overall performance of such advanced biobased polymers for energy storage applications.

The work by Dannoun et al.[124] delves into the use of plasticized proton conducting polymer composite (PPC) for advancing supercapacitors, addressing the inefficiencies associated with polymer-based electrolytes. The exploration and analysis of a blended methylcellulose and dextran solution impregnated with ammonium thiocyanate and zinc metal complex have yielded notable results. The ionic conductivity of the resultant system was recorded at a notable 3.59×10^{-3} S/cm. The study's methodological approach, involving various analyses like transference number measurement and electrochemical impedance spectroscopy, has robustly supported these findings. Moreover, the glycerol plasticizer shown to enhance transport possesses an ionic mobility of 5.77×10^{-5} cm^2 V^{-1} s^{-1} and a diffusion coefficient of 1.48×10^{-6} cm^2 s, supporting an overall carrier density of 3.4×10^{20} cm^{-3}. Additionally, the linear sweep voltammetry results indicate stability up to 2.05 V, underscoring the material's suitability for energy devices. The absence of Faradaic peaks in the cyclic voltammetry plot and the low equivalence series resistance of 65 Ω reported in the galvanostatic charge−discharge experiment further reinforce the potential of PPC in the enhancement of energy devices, showing average energy density and specific capacitance of 15 Wh/kg and 128 F/g respectively. Future research could delve deeper into optimizing the ionic conductivity and enhancing the overall electrochemical stability beyond the reported 2.05 V.

The work by Monisha et al.[125] explored the development of a proton-conducting solid biopolymer electrolyte by employing a solution casting technique. They utilize cellulose acetate (CA) and ammonium thiocyanate (NH_4SCN) for the creation of the polymer electrolyte. Their comprehensive XRD analysis significantly highlights an increase in the amorphous nature of the CA complex with an escalation in NH_4SCN salt concentration, leading to higher ionic conductivity. Further, the work documents the testing of electrical conductivity using an AC impedance analyzer, showcasing an increase in ionic conductivity with heightened salt concentration up to 50CA:50NH_4SCN, which exhibits a maximum ionic conductivity value of 3.31×10^{-3} S cm^{-1}. The detailed electrochemical impedance spectroscopy analysis bolsters these results, emphasizing a decline in resistance from 924 to 8.6 Ω with increased NH_4SCN concentration. Such technical aspects underscore the potential application in developing fuel cells and primary proton batteries. Additionally, the authors provide an insightful observation regarding the 50CA:50NH_4SCN polymer electrolyte, which displays the highest ionic conductivity (3.31×10^{-3} S cm^{-1}) at room temperature, significantly outperforming pure CA (1.285×10^{-7} S cm^{-1}). This notable finding is attributed to the transition from a semicrystalline phase to an amorphous phase of the polymer complex, combined with an increase in charge carrier concentration.

The research by Harikumar and Batabyal[126] portrayed a novel study into creating a flexible, transparent, and biodegradable supercapacitor electrode using a pectin biopolymer and a biocompatible electrolyte. The work comprehensively explored pectin biopolymer-based electrodes due to their stability and specific capacitance. Notably, the pectin electrode with 10% graphite retained an impressive 98.74%

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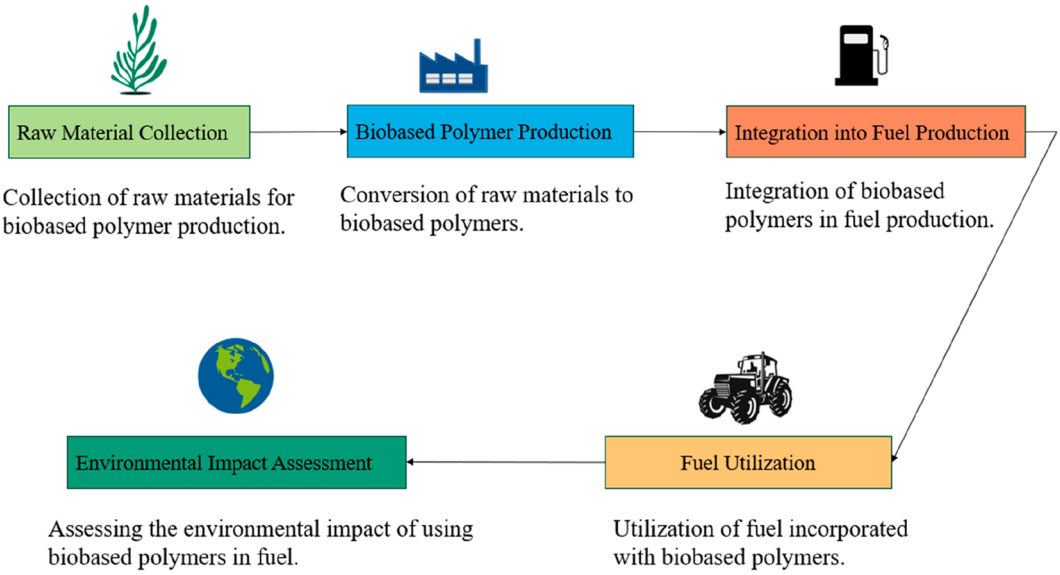

Figure 1. Biobased polymers process in the fuel industry.

capacitance after 2500 cycles at 11.48 mF/cm^2, showcasing its potential for enduring efficiency in energy storage. Moreover, the specific capacitances of supercapacitors, especially the PP supercapacitors, displayed encouraging results, showing 7.25 and 4.64 mF/cm^2 specific capacitance at 10 and 100 mV/s respectively with a notable capacitance retention of 86.8%. In terms of technical highlights, the methodological use of EDX and elemental mapping is crucial for showcasing a uniform distribution of various elements, aiding the establishment of the most effective supercapacitors. The work commendably indicates the enhanced ionic movement during charging and discharging to maintain the GCD shape after numerous cycles. For future research, the practical application of these advanced biobased polymer supercapacitors should be a primary focus. This includes testing under various environmental and operational conditions to ensure versatility and reliability. Furthermore, refining the graphite-to-pectin weight ratios and exploring alternative biocompatible materials can unearth more optimized solutions for sustainable and efficient energy storage systems, contributing to the advancement of ecofriendly technology in the energy sector.

In conclusion, the comprehensive investigation of energy-related advanced biobased polymer case studies elucidates the paramount importance of these materials in enhancing the performance and sustainability of energy devices. The revealed advancements pave the way for further research, aiming to optimize and expand the utilization of biobased polymers, fortifying their crucial role in the future of sustainable energy solutions.

4.3. Biobased Polymers in the Fuel Industry. A substantial contribution is being made by biobased polymers in developing sustainable fuels.[18,127,128] Figure 1 shows the biobased polymer process in the fuel industry. Extracted from biological sources, these polymers align with environmental sustenance.[129] The in-depth exploration of biobased polymers' roles in sustainable fuel production and enhancement is presented in this section, illuminating their fundamental contributions and future prospects. The biobased polymers, derived from renewable biological resources, are marking a crucial shift toward sustainable fuel production.[18,130,131] Their role in enhancing the production process of biofuels is prominent. The contribution of these polymers to the efficient conversion of biomass into fuel is being acknowledged, underscoring their critical role in promoting the production of environmentally friendly fuels. The promising potential of these polymers to improve and increase the output of biofuel production is being recognized, opening new avenues for sustainable fuel production and environmental protection. Among these biobased polymers, cellulose, PHA, and PLA are particularly notable for their roles in fuel industry applications, offering innovative pathways in producing sustainable fuels.

A growing usage of biobased polymers in biofuel production processes is being witnessed. The polymers are aiding in developing efficient and advanced biofuel production technologies. Their use in the production process enhances the overall efficiency, thereby contributing to the increased production of sustainable fuels. These advancements are vital in promoting ecofriendly fuels and addressing global energy demands without harming the environment. The practical applications of biobased polymers in fuel production processes showcase their substantial impact on the industry. Innovative biofuel production methods and technologies are being developed, credited to integrating these polymers. The advancements include enhanced production efficiency, increased output, and improved environmental sustainability. Promoting these advancements by biobased polymers is essential in establishing a solid foundation for sustainable fuel production, highlighting their crucial role in the industry.

Furthermore, the role of biobased polymers in fuel production is not limited to biofuels. These polymers significantly contribute to other sustainable fuel production processes, including creating hydrogen fuel and other alternative, sustainable fuel sources.[132,133] Specifically, biobased polymers like cellulose and lignin-derived materials are instrumental in the catalytic processes crucial for hydrogen production, enhancing hydrogen generation efficiency from biomass. Additionally, these polymers contribute to developing advanced bioelectrochemical systems, enabling more effective energy extraction from alternative sustainable fuels and thus broadening the scope of their application in the energy sector.

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The impact of biobased polymers on these alternative fuel production methods is being realized, supporting the continued growth and advancement of sustainable fuel technologies and promoting environmental sustainability. In summary, it has been demonstrated that biobased polymers play an indispensable role in the evolution of the fuel industry. Their contributions, extending beyond biofuel production to encompass alternative sustainable fuel sources, including hydrogen fuel, are pivotal in the transition toward a more ecoconscious energy sector. Incorporating these polymers not only enhances the efficiency and output of biofuel production but also signifies a leap forward in environmental stewardship.

4.4. Case Studies of Biobased Polymers in the Fuel Industry. In pursuing ecofriendly alternatives within the fuel industry, significant emphasis has been placed on developing and assessing biobased polymers. Various case studies in this section rigorously investigate the efficient conversion of biomass and biopolymers into sustainable fuels, showcasing innovative methods and catalysts that have the potential to revolutionize the fuel industry.

The work by Liu et al.[134] offers a comprehensive investigation into the production of high-density aviation fuel from cellulose, a bountiful, nonedible biomass. The process involves converting cellulose to 2,5-hexanedione with a yield of 71.4%, followed by obtaining a mixture of C12 and C18 branched polycycloalkanes with a carbon yield of 74.6% using the aldol method. The polycycloalkane mixture demonstrated low freezing points and high density, marking its potential as an advanced aviation fuel. The article underscores the utilization of HCl and Pd/C for cellulose hydrolysis and hydrogenation, attaining a carbon yield of 64.2% under specific conditions. The study further explores the effectiveness of the HCl + Pd/C catalyst in the hydrogenolysis of other carbohydrates, achieving carbon yields ranging from 40.4% to 74.0%. Further research could focus on exploring alternative catalysts and methods that may enhance the overall efficiency and sustainability of the fuel production process. In the context of producing high-density polycycloalkanes, the work presents the efficacy of both pure and metal-modified MgO as catalysts, achieving a conversion of 99.1% and a carbon yield of 98.3%. The bimetallic Cu-Ni/MgO-p catalysts showcased the highest total carbon yields, indicating their superior performance in producing C12 and C18 oxygenates. For future research, exploring more environmentally benign catalysts and further optimizing the fuel production process, focusing on maximizing yield while minimizing environmental footprint, remains paramount.

The work by Riaz et al.[18] posits a novel exploration into the potential of PHAs in biofuel production. These bacterial polymers exhibit versatility and compatibility for methyl esterification, making them suitable candidates for biofuel production, akin to biodiesel but with higher oxygen content and absent nitrogen or sulfur. The work delineates the production of hydroxyalkanoates methyl ester (HAME) and hydroxybutyrate methyl ester (HBME) from PHAs, showcasing a promising path for sustainable fuel generation. Notably, the work highlights a significant increase in combustion heat by 30% when HBME was blended with ethanol. The essential point is that the work asserts that these PHA-based biofuels do not necessitate significant purification, suggesting a possible cost-effective production pathway, utilizing wastewater as a source, thereby negating competition with food resources. Furthermore, the optimization of the production parameters is meticulously discussed. A notable highlight is the discernible increase in HBME yield, rising from 12.8 to 70.7% with a reaction time increase from 10 to 50 h. The document lays a foundation demonstrating the influence of diverse factors such as reaction time, temperature, and catalyst type on the yield of HAME-based biofuels. The presence of low cetane numbers and high heat of vaporization in oxygenated additives like HA esters may pose challenges in diesel engine fuelling.

The work by Akinwumi et al.[135] addresses the production and utilization of PHA-based biofuels, analyzing their pros, cons, and commercial viability. The PHA methyl esterification process, used to produce biofuels like 3HBME and 3HAME, is examined for its sustainable and petroleum-free approach. The work reveals that despite low octane and cetane numbers, which hinder performance, alternative PHAs with longer carbon lengths may provide improved biofuel qualities. This feature is critical for advancing biobased polymers in the fuel industry, indicating a need for more extensive research on various PHA types and their corresponding biofuel characteristics. The work uncovers crucial data, such as the significant increase in combustion heat when 3HBME and 3HAME are blended with ethanol, demonstrating the potential efficacy of these biofuels. However, it also highlights the issues of high production costs, estimated at $1,200/ton, which could limit the broad-scale application of this technology. The detailed analysis of HBME as a potential fuel additive is noteworthy, emphasizing its superior flashpoint, oxygen content, and temperature properties compared to ethanol. Despite these positive aspects, the low octane and cetane numbers and potential phase separation issues underscore the need for further development and optimization of PHA-based biofuels. In addressing the production process, the work reports on the effectiveness of both acid and alkali catalysts in PHA conversion to biofuels. The elucidation of the method involving chloroform solvent, methanol, and acid or base for esterification at 67 °C for 50−100 h is meticulously outlined. Explaining the subsequent processes, such as the separation and vacuum evaporation, adds depth to understanding the biofuel production methodology. Furthermore, the work sheds light on the comprehensive characterization of PHA-based biofuel, elaborating on its physicochemical properties, including dynamic viscosity, flashpoint, and oxygen content. The comparison with petrol, ethanol, and diesel strengthens the argument for the potential use of HBME as a fuel additive despite the highlighted challenges, such as its lower cetane number and research octane number, necessitating additives.

The work by Xu et al.[136] provides a comprehensive exploration into the solvent-free catalytic hydrogenolysis of PLA powder. Achieving a 100% conversion with a carbon utilization of 99%, the study presents an ecofriendly and efficient process. The fuel produced exhibited an HHV of 29.9 MJ/kg, and the carbon recovery for discarded PLA straws was reported to be 95%. One significant aspect is the meticulous scrutiny of reaction temperatures to optimize the hydrogenolysis process. The decomposition temperature of PLA, which was affected by the addition of Pd/C, lowered to 351 °C, underscoring the catalytic effect on the degradation of PLA powder. A careful selection of the reaction temperature range (170−300 °C) was employed, ensuring the complete conversion of PLA powder, yielding mainly light-yellow liquid products and CO-enriched gas. The extensive experiments indicated that hydrogen pressure was pivotal in enhancing the liquid product yield, from 69.6 ± 6.2 wt % to 93.9 ± 5.7 wt %

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upon increasing H_2 pressure. This indicates the potential scalability and reliability of this method. Furthermore, utilizing different catalysts besides Pd/C, such as Raney Co, Raney Ni, and Cu/Zn/Al, underlines the versatility of the hydrogenolysis process. The liquid products derived exhibit a considerable HHV of 29.9 MJ/kg, highlighting their practical utility in the fuel industry. Future research could delve deeper into enhancing the hydrogenolysis process by exploring novel catalysts that could optimize the reaction conditions and product yield.

Tseng et al.[137] examined the biological decomposability of PLA by thermophilic methane fermentation (TMF) and analyzed the microorganisms involved in PLA decomposition. The research utilized disposable cutlery and pure poly L-lactic acid (PLLA) pellets for both small and large-scale batch tests, observing a 70−77% decomposition of PLA by TMF based on weight changes, and CH_4 yield ranged from 321−343 mL CH_4/g PLA consumed, a significant figure underscoring the potential for methane production from PLA. The study identified a considerable role of microbial activity, specifically lactic acid-consuming bacteria, in enhancing PLA decomposition doubling the physicochemical degradation rate. The research unveiled that *Methanothermobacter*, a hydrogenotrophic methanogen, was the primary archaea in methane production from PLA degradation. The bacterial microflora involved in the depolymerization of PLA and/or degradation of LA were also analyzed, and bands such as B1, B7, B8, and B9 were identified as dominant in the PLA decomposition process by TMF. The bacterial genera involved included *Defluviitoga*, *Anaerosalibacter*, *Tepidimicrobium*, and *Jonquetella*. Interestingly, bands B2 and B3, associated with genera Streptococcus and *Tumebacillus*, were observed to become dominant during PLA degradation, although they had not been previously reported in PLA degradation, indicating potential new pathways for PLA decomposition. The exploration of carbon-13 isotope tracing in future studies is poised to elucidate the production of CH_4 and CO_2 from PLA decomposition, and the isolation and evaluation of *Tepidimicrobium*'s LA-consuming ability will fortify the findings of this study. The efficient PLA treatment by TMF is emphasized, and the critical role of microbial activity in this process is unambiguously highlighted, proposing a potential sustainable avenue for biofuel generation from biobased polymers. Further research into the precise microbial pathways and mechanisms, along with the optimization of TMF for PLA degradation, stands out as a crucial future direction to enhance the viability of this biotechnological approach for sustainable biofuel production.

The study by Saha et al.[138] stands out for exploring Lewis acidic metal chlorides in producing biofuel precursor, 5-hydroxymethylfurfural (HMF), from carbohydrates and biopolymers. The research reveals the superiority of $Zr(O)Cl_2$ as a catalyst, achieving 63% and 42% HMF yield from fructose and glucose, respectively, in a water-MIBK biphasic solvent system. This yield is impressively heightened to 84% and 66% in a [BMIM]Cl-MIBK biphasic solvent, showcasing the impactful role of solvents in catalytic efficiency. However, although thoroughly investigated, pH's impact on the catalytic process demonstrates some ambiguity. Despite the lower pH of $Zr(O)Cl_2$ leading to higher HMF yields, the trend does not consistently follow for all metal chloride catalysts. This suggests that other unaccounted factors could be influencing the catalytic effectiveness. The work emphasizes the superior HMF yield when using microwave-assisted heating compared to conventional oil-bath heating, and it elaborates on a detailed mechanism for the isomerization of glucose into fructofuranose, followed by the production of HMF, further solidifying the study's comprehensiveness. The recycling aspect of $Zr(O)Cl_2$ catalyst, which sustains activity across five cycles with only a 4% loss, is a promising finding for sustainable biofuel production. Yet, the formation of CMF and LA as side products indicates potential avenues for optimization to enhance the yield and purity of HMF. For future research, exploration into the anomalies in the catalytic effectiveness related to pH and different metal chloride catalysts is essential to optimize the process further. It would also be valuable to investigate the intricate impact of various solvents and heating methods on the HMF yield and potential ways to mitigate side reactions that result in CMF and LA, ensuring a more efficient and sustainable biofuel production using biobased polymers.

The study by Cheng et al.[139] on the synthesis of five Brønsted-Lewis acidic ionic liquids and their use in converting cellulose to levulinic acid (LA), a key intermediate in the fuel industry. The cellulose to LA conversion, in pure water without additives at 180 °C for 10 h, yielded over 49% more LA than utilizing Brønsted-Lewis IL $[HO_3S\text{-}(CH_2)_3\text{-py}]Cl\text{-}FeCl_3$, highlighting the efficiency and potential ecofriendliness of this method. Despite the formation of some solid residues, identified as benzene or amorphous fused benzene rings, the IL reusability and catalytic performance remained consistent after five reuses, an essential factor for sustainable and practical application in industry. The study's methodologies are thoroughly outlined, including the preparation of the Brønsted-Lewis acidic IL and the testing of its catalytic properties. The results show that the synthesized ILs had Lewis acidic centers, with $ZnCl_2$ being the strongest, followed by $FeCl_3$, CuCl, and $CrCl_3$. A cellulose conversion exceeding 70% and the highest LA yield of 57.6% were achieved, supporting the efficacy of the Brønsted-Lewis acidic ILs in cellulose to LA conversion. Furthermore, the IL $[HO_3S\text{-}(CH_2)_3\text{-py}]Cl\text{-}FeCl_3$ showed the best catalytic performance among all investigated, with cellulose conversion at 71.4% and LA and glucose yields at 49.1% and 10.2%, respectively. Future research in this area could focus on optimizing IL structures for maximized LA yield and cellulose conversion.

The work by Khan et al.[140] offers several valuable insights and findings in the realm of sustainable technology. The research focuses on utilizing cellulose for the production of levulinic acid (LA) through the use of dicationic ionic liquids as a catalyst. Notably, a significant catalytic activity for cellulose to LA conversion was achieved with $[C4(Mim)_2][(2HSO_4)\text{-}(H_2SO_4)_2]$, showcasing a 55% conversion rate at 100 °C within 3 h, without requiring an additional catalyst or solvent. This aspect underscores the potential efficacy and efficiency of the utilized ionic liquids, contributing positively to the sustainability and feasibility of the method. The research also provides a profound insight into the influence of factors such as IL type, amount, temperature, and reaction time on catalytic conversion, thereby ensuring a comprehensive exploration of the subject. The experiments performed at varying temperatures between 80 and 120 °C revealed an optimal yield at 100 °C, emphasizing the importance of temperature control in enhancing the LA yield.

In sum, the meticulously conducted case studies demonstrate significant advancements in biobased polymer conversion for fuel production. Despite the promising results,

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several research gaps and opportunities for optimization and enhancement are highlighted. Continual exploration in this realm is vital for realizing more sustainable and efficient fuel production processes using biobased polymers, contributing substantially to global environmental conservation efforts.

4.5. ML in Energy Systems. In recent years, a marked advancement in ML application in energy systems has been observed.[141,142] Significant enhancements in the efficiency and sustainability of these systems have been realized by harnessing the predictive and analytical capabilities of ML algorithms.[141,142] The optimization of renewable energy production, particularly from solar and wind sources, stands as a striking illustration of this trend.[143,144] Real-time data are analyzed to predict energy output, allowing for more efficient grid integration and energy distribution.[145] This analysis primarily utilizes data such as weather forecasts, historical energy usage patterns, and real-time sensor readings from energy generation equipment. Moreover, the capacity for accurate energy consumption forecasting by industries and households has been augmented. This improvement enables more effective demand-side management and aids in minimizing energy wastage, underscoring the crucial role played by ML in bolstering the efficiency and sustainability of energy systems.[146]

The domain of energy storage, too, has been positively impacted by the integration of ML.[75,76,78] Enhanced performance and lifespan of batteries are achieved through the real-time analysis and monitoring facilitated by ML, ensuring optimal functioning and reliability of energy storage systems. These improvements are largely attributed to predictive maintenance strategies, where ML algorithms anticipate maintenance needs and schedule interventions to prevent failures. Additionally, degradation modeling of battery components, enabled by ML, aids in understanding and mitigating wear and tear, further enhancing lifespan and performance. Strategies for effectively managing and maintaining these systems have been formulated, leading to substantial improvements in their overall efficiency and longevity. These advancements resonate with the global impetus toward bolstering the efficiency and sustainability of energy systems by leveraging cutting-edge technologies, exemplified by the integration of ML.

Moreover, in the field of energy conversion, ML has emerged as a transformative tool.[79,147,148] It aids in the refinement and optimization of energy conversion processes, ensuring maximized output and minimized waste. The fine-tuning of these processes, facilitated by ML, underscores its pivotal role in enhancing the efficiency and sustainability of energy conversion systems. Furthermore, its application in the assessment and optimization of novel energy conversion technologies expedites their development and integration into the existing energy infrastructure. This dynamic illustrates the substantial contribution of ML in advancing the efficiency and sustainability of energy conversion systems. In the realm of enhancing biobased polymers for energy applications, ML has displayed a substantial capacity for innovation. It has facilitated the rapid, efficient design and assessment of biobased polymers for diverse applications in renewable energy systems, energy storage, and energy conversion.[27,149] This accelerated development and optimization process ensures the timely integration of these ecofriendly and efficient materials into the energy landscape, further augmenting the sustainability and efficiency of energy systems globally.

In summary, from optimizing renewable energy production and consumption to ensuring the peak performance of energy storage systems and from refining energy conversion processes to advancing the development and integration of biobased polymers, ML has emerged as a critical ally in the global pursuit of a more efficient, sustainable, and ecofriendly energy future. The continued exploration and harnessing of its immense potential are paramount to realizing these global aspirations, reaffirming the indispensability of ML in the evolution of energy systems toward unparalleled efficiency and sustainability.

4.6. ML for Fuel Development. In the ever-evolving landscape of fuel development, the substantial influence of ML is being acknowledged.[14,150] A significant surge in efficiency, sustainability, and innovation in fuel development is being observed, owing to the integration of advanced ML algorithms.[67] An exploration into the multifaceted impact of ML on fuel development is explored in this section, underlining its pivotal role in reshaping and enhancing the industry.

The enhancement of fuel development processes is seen as a direct consequence of ML.[151,152] By processing vast data sets and deriving actionable insights, ML is aiding in the optimization of fuel production processes.[14] These advancements result in heightened efficiency, thereby reducing resource utilization and promoting environmental sustainability. Furthermore, the role of ML in the predictive maintenance of fuel production machinery is being realized, preventing unforeseen downtime and ensuring consistent and optimal production.[153,154] The technology is enabling the rapid development and testing of novel fuel formulations, contributing to the emergence of more efficient and environmentally friendly fuel alternatives. The ability of ML algorithms to analyze and model complex chemical reactions is being leveraged, resulting in the accelerated discovery and development of new fuels.[98,155] This innovative approach drives the industry forward, ensuring it stays abreast of the growing global energy demands while maintaining sustainability.

Moreover, the integration of ML in fuel development is promoting sustainability.[156] Through the optimized use of resources and enhanced production efficiency, ML is contributing to the reduction of the environmental impact of fuel production. It aids in the development of cleaner, more sustainable fuels by analyzing and predicting the environmental impact of various fuel types, thereby guiding the industry toward more ecofriendly alternatives.[157,158] This commitment to sustainability is crucial in addressing the urgent global environmental challenges faced today. In conclusion, the incorporation of ML within the realm of fuel development is bringing forth substantial advancements in efficiency, sustainability, and innovation. Its role in enhancing and optimizing fuel production processes, promoting the discovery of new fuels, and guiding the industry toward ecofriendly alternatives highlights its crucial significance in the ongoing and future developments within the fuel industry. The sustained exploration and integration of ML within the industry hold the promise of a more efficient, innovative, and sustainable future for fuel development.

4.7. Case Studies of ML Applied in Biopolymers for Fuel Development and Energy applications. *4.7.1. ML Applied to Biopolymers for Energy Applications.* In the exploration of biopolymers for fuel and energy applications, ML emerges as a paramount tool. Significant advancements are

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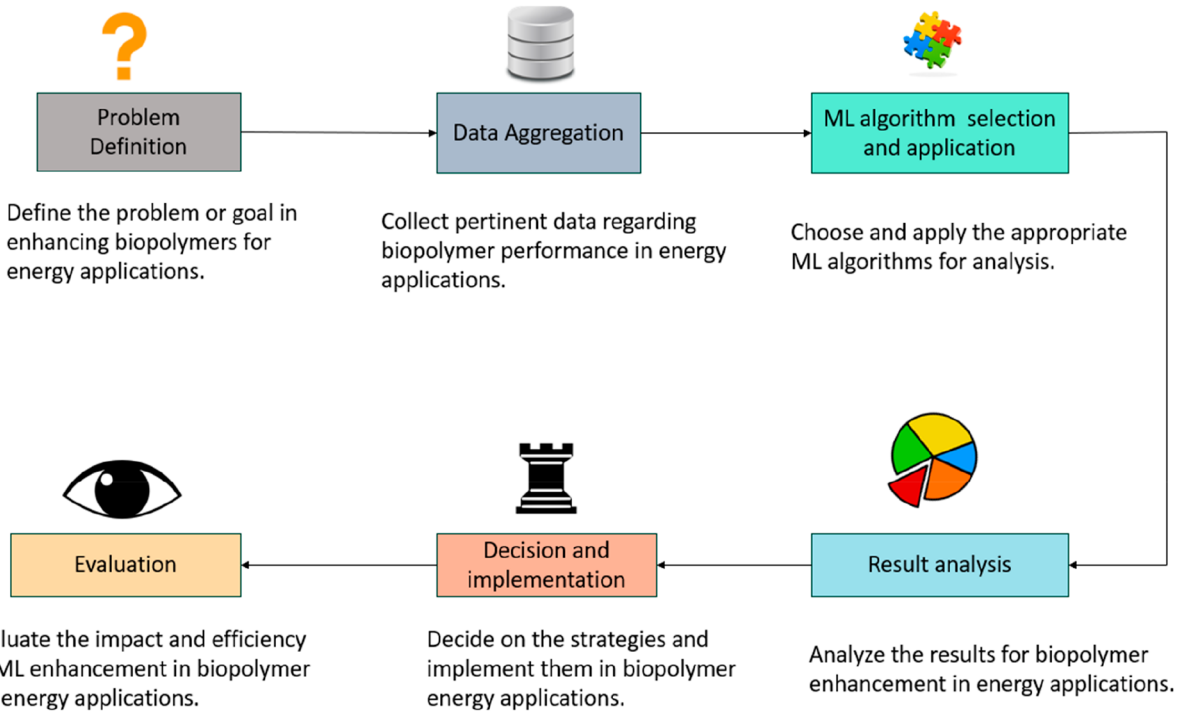

Figure 2. ML enhancement process of biopolymer in energy applications.

realized in fuel development, with ML optimizing biopolymer-based solid polymer electrolytes, enhancing fuel cell performance, and predicting ionic conductivity within biopolymer electrolytes for zinc-ion batteries. This section meticulously discusses various case studies to delineate the impact and potential of ML in biopolymer research for fuel and energy applications. Figure 2 shows the ML enhancement process of biopolymers in energy applications.

The study by Adam et al.[159] embarks on the optimization of cellulose and its derivatives-based solid polymer electrolytes (SPEs), leveraging ML. The research employs response surface methodology (RSM) and artificial neural networks (ANNs) for predicting and optimizing PC/MC-based SPE complexed with potassium phosphate (K_3PO_4) and glycerol. The study reveals significant influences of K_3PO_4 and glycerol on SPE's ionic conductivity and potential window, especially with higher potassium salt content. An optimal interaction of $\sim 3 \times 10^{-4}$ S cm^{-1}, 4.19 V is achieved at 60 wt % K_3PO_4 and 41.37 wt % glycerol, revealing effective numerical optimization. The research provides a detailed insight into the role of each variable, showing limited effects at low concentrations while pointing out the increasing ionic conductivity with a surge in salt concentration. This aspect is crucial as it highlights the interplay of these materials in enhancing ionic conductivity. The effectiveness of glycerol and K_3PO_4 in impacting the ionic conductivity and potential window is meticulously analyzed, giving readers a profound understanding of their roles and interactions. It is intriguing to note the linear correlation in the residuals of the two models, indicating a normal distribution of errors. In addressing ionic conductivity, the research demonstrates the minimal impact at low K_3PO_4 concentrations, a crucial observation for practical application. It portrays the intricate relationship between K_3PO_4 and glycerol, signifying their significant interaction in the PE. The detailed analysis using contour plots splendidly illustrates the interaction dynamics, helping to visualize the parameter synergy, a crucial aspect for material engineers. One significant highlight is the demonstrated accuracy of the ANN model in predicting ionic conductivity and potential window with high R^2 values of 0.999 and 0.998, respectively, showing a minuscule error margin. This accuracy is a compelling achievement in the realm of SPEs, as it provides a robust model for further experimental designs. Future research could be directed toward understanding the mechanical properties of these SPEs and their compatibility with other materials for diverse energy applications. This could pave the way for the development of more efficient and sustainable energy storage devices employing biopolymers. In essence, the work stands out for its in-depth analysis, the employment of ML tools, and clear, demonstrable results, setting a precedent for future research in the realm of biopolymer-based SPEs for energy applications.

The work by Tian et al.[160] presents a significant stride toward enhancing the efficacy of polymer electrolyte membrane (PEM) fuel cells. The work adeptly combines ANN and genetic algorithm (GA) to forecast and augment PEM fuel cell performance. Leveraging a robust 3D multiphysics model, the work meticulously trains the ANN, yielding a prediction error below 2.5% and 1.5% under varying current densities. The authors reveal a peak power of approximately 0.78 W/cm^2 at 368.8 K, achieved using the ANN-GA method, a pivotal insight for practical system design and expeditious control in fuel cell applications. The examination of diverse operational temperatures also provides essential perspectives on fuel cell performance. The work establishes a nonlinear relationship between temperature and maximum power, further underlining the temperature's critical influence on fuel cell output. Notably, a maximum power increase is identified until around 363−373 K, after which a subtle decline is observed. Such granular insights, notably the detailed analysis of relative humidity impacts on anode and cathode

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sides, offer substantial contributions to fuel cell operational understanding. The work demonstrates a thorough approach, utilizing the ANN-GA framework to confirm results with the 3D multiphysics model, showcasing robust alignment and underscoring the ANN-GA's prediction accuracy. In practice, the model enables swift adjustments to alterations in environmental temperature, a crucial capability for real-world fuel cell applications. For future work, it would be interesting to delve deeper into exploring the impacts of varying environmental factors and their intricate interplay on the fuel cell performance and how the ANN-GA model can be further optimized to adapt to these multifaceted conditions.

The work by Jha et al.[161] predicted the capacitance variation of lignin-based supercapacitors. The work has adroitly utilized four ML algorithms, including linear regression (LR), support vector machine (SVM), decision tree (DT), and ANN, ranking their accuracy as LR < SVM < DT < ANN. This is validated using the F-test, wherein ANN emerges as the most precise, reliable, and robust model, capable of anticipating specific capacitance variation even for material ratios not in the training set. In their methodology, the data set is divided into 80% for training and 20% for validation, which prevents model overfitting, ensuring higher prediction accuracy for optimal material weight percentage and specific capacitance (SPC) variation. The ANN model's superior performance is evident with the lowest root mean square error (RMSE) deviations of 0.234, 0.240, and 1.384 mF cm^{-2} for SC1, SC2, and SC3, despite training with reduced data. ANN's models for SC1 and SC2 displayed impressive R^2 values of 0.676 and 0.979 and RMSE values of 0.209 and 0.234, respectively. Furthermore, the ANN model predicts capacitance retention with significant accuracy, reflecting an understanding of nonlinear systems unattainable by parametric modeling. Further exploration of the ANN's robustness and accuracy with other biopolymer-based supercapacitors and varying compositions will enhance the understanding and applicability of ML in enhancing energy applications of biopolymers.

The work by Wei et al.[162] revealed a significant exploration into the potentialities of ML for predicting ionic conductivity within biopolymer electrolytes for zinc-ion batteries. Utilizing the gradient-boosting decision tree algorithm, the authors constructed models to predict the contribution of polymer functional groups to ionic conductivity, yielding promising and vital results. The synthesized and sulfonated series of cross-linked polymers denoted as SPTPT delivered noteworthy outcomes. The prepared membrane displayed a Zn^{2+} conductivity of 12 mS cm^{-1} and a proton (H^+) conductivity of 22 mS cm^{-1} in water at 30 °C, marking an encouraging achievement in the advancement of polymer electrolytes for zinc-ion batteries. The research demonstrated that the Zn/MnO_2 flow battery, utilizing the proposed membrane as the electrolyte, delivered a peak power density of 150 mW cm^{-2} and a significant specific capacity of 1.95 mAh cm^{-2}. This resulted in a robust cycling capacity retention rate of 71% after 1000 cycles at 30 mA cm^{-2}, signifying the potential for enhanced longevity and reliability in real-world applications. Notably, the tpt-SPTPT membrane exhibited exceptional ionic conductivity, offering 17 mS cm^{-1} to Zn^{2+} and 42 mS cm^{-1} to H^+ at 80 °C under 100% RH. Moreover, the tpt-SPTPT-based Zn/Zn flow battery showcased an admirable corrosion potential increase and reduced overpotential of nucleation, highlighting its operational efficiency and stability. These compelling results underscore the innovative integration of ML within the realm of materials engineering for energy applications. Future research could potentially delve deeper into enhancing the algorithm's predictive capabilities and exploring additional biopolymer candidates for diversified energy storage solutions.

The insightful case studies accentuate the indispensable role of ML in advancing biopolymer research for fuel and energy applications. These investigations not only highlight the optimization and prediction capabilities of ML models but also pave the path for future endeavors. Evidently, ML stands as a robust ally, promising enhanced efficiency and innovation in biopolymers for fuel development and diverse energy applications.

4.7.2. ML Applied to Biopolymer Fuel Applications. The surge in environmental concerns has necessitated innovations in sustainable energy, with particular emphasis on biopolymer fuels. The section illuminates the intersection of ML and biopolymer fuel applications. Herein, pioneering strides are expounded upon, providing a compelling narrative on the optimization of lignin depolymerization and hydrothermal liquefaction using sophisticated ML models.

The work by Liu et al.[163] is an exhaustive exploration into the optimization of lignin depolymerization, focusing on influencing factors for enhancing yields of bio-oil and high-value aromatic products through lignin hydrogenolysis. The study effectively utilizes ML models, namely xgboost, to simulate and predict optimal reaction parameters. The R^2 scores reflecting the reliability of these models are notably high, 0.92 for solid residue and 0.88 for aromatic yield, revealing a strong reliability in predictions. Crucially, the research highlights the paramount impact of the lignin-to-solvent ratio and average pore size on lignin hydrogenolysis results. It underscores that an optimal lignin-to-solvent ratio hovers around six, while the catalyst's pore size significantly influences the solid yield, positioning these factors as central in refining the hydrogenolysis process. Moreover, the ML models reveal that nickel and ruthenium exert higher effects on the models' output than other metals. However, the work indicates some limitations in its scope, particularly in the potential variation of lignin sources, which were not entirely considered in the models. The study's results are instrumental for advancing the field, providing clear insights into parameter significance, and offering direction for further optimization in industrial applications. Yet, it leaves room for expanding research into exploring diverse lignin sources and their distinct impacts on the hydrogenolysis process. Future research can delve into the comprehensive examination of various lignin types beyond alkaline and kraft lignin to ensure broader applicability and robustness in the ML models' predictive capabilities for lignin hydrogenolysis.

The work by Shafizadeh et al.[17] explores the use of ML in characterizing and quantifying hydrothermal liquefaction byproducts. The document provides an insightful analysis, demonstrating the application of ML models to optimize the biocrude oil yield, a significant aspect of fuel development. The work outlines that the Gaussian process regression (GPR) model showed the most promise, with a correlation coefficient above 0.926 and a mean absolute error below 0.031, showcasing robust predictive capabilities. The analysis of optimal biomass components for the highest biocrude oil yield, standing at 48.7−53.5%, presents clear, impactful statistics that reinforce the work's findings. It notes optimal conditions for biocrude oil production, specifically emphasizing biomass

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composition and operational conditions such as temperature (394−400 °C) and pressure (30.0−35.6 MPa). The article also elaborates on the process optimization and feature importance analysis, showing that biomass composition had a more significant impact on biocrude oil yield (58.18%) compared to operating conditions (41.82%). The article further provides practical data on how various factors, such as increasing biomass oxygen over 42%, could detrimentally affect biocrude oil yield. These specifics offer crucial insights for practical implementation, supporting the avoidance of nonoptimal conditions for biocrude production. Future research could focus on the development of universal ML models for nonwater hydrothermal liquefaction solvents, a potential area noted by the authors. The integration of ML in real-time monitoring and control of hydrothermal liquefaction reactors, as suggested in the article, could substantially enhance biofuel quality and quantity, presenting an exciting avenue for subsequent exploration and development.

In the work by Kartal et al.,[27] a novel application of artificial neural networks (ANNs) using the TensorFlow library is employed to model the thermal degradation of essential biomass biopolymers: hemicellulose (HC), cellulose (CL), and lignin. With an exceptional R^2 value above 0.998, the ANN model impressively demonstrates its robustness in predicting differential thermogravimetric (DTG) curves for HC, CL, and lignin, facilitating instantaneous calculation of biopolymer fractions in degraded biomass, a feat not previously achieved. A meticulous laboratory setup, including precise thermal conditioning and measurement using the NETZSCH STA 409 PC Luxx, underscores the reliability of the data used for ML training and evaluation. The neural network topology, incorporating layers with 5, 150, and 100 neurons, demonstrates a deft balance between complexity and computational efficiency, contributing to the model's exemplary predictive performance. In testing, R^2 values consistently above 0.998 highlights the model's excellent generalizability to unseen data, reinforcing its potential for broader application in biomass characterization and fuel development. Notably, the study reveals subtle variabilities in prediction accuracy among different biopolymers, with CL showing the most predictable DTG points and lignin the least. The findings suggest a more pronounced challenge in estimating lignin thermal degradation, underscoring an area warranting further research. The innovative application of ANN for the analysis of biopolymer thermal degradation signals a significant stride in enhancing the efficiency of biomass-based thermal processes, setting a firm foundation for the advancement of renewable fuel technologies while also elucidating clear pathways for future research, particularly in the nuanced prediction challenges presented by specific biopolymers such as lignin.

The work by Vinitha et al.[164] utilizes an ML-based optimized decision-making system (OD-MS) to enhance the yield of glucose and ethanol from biomass. With a substantial data set of 250 experimental results, the study claims a remarkable 95% accuracy in predicting the optimal conditions for enzymatic hydrolysis saccharification and fermentation, achieving an R^2 value of 0.97623. The intricate model considers various parameters, such as cellulose content, temperature, and pH levels, and their influence on yield. For instance, an increase in cellulose (>73%) and specific temperature (55−60 °C) and pH (7−9) conditions for saccharification markedly enhanced the yield. However, a critical examination of the study reveals areas where the application and interpretation of ML could potentially be refined. The work states that a reduction in hemicellulose and lignin to below 10% will result in enhanced yields, confirming this with glucose yields exceeding 50 g/L and ethanol yields over 40 g/L under these conditions. While these numbers are compelling, the work could provide more insight into the robustness of the model against varying biomass types and conditions. The real-world biomass samples might not always align with the ideal conditions prescribed, thereby affecting the practical applicability of the model's predictions. A notable strength of the work is the comprehensive 3-D surface analysis, lending a visual and quantitative dimension to the relation between various factors like cellulose content, temperature, and yield. This kind of multidimensional analysis is pivotal for the holistic understanding and optimization of biopolymer processing for fuel development. In future research, a more diverse range of biomass types and real-world conditions should be incorporated to enhance the model's robustness. Additionally, the model could be expanded to predict other essential metrics of the biofuel production process.

The work by Castro Garcia et al.[165] elaborates on the underutilized potential of lignin, a significant component of plant matter, in depolymerization for renewable aromatic chemicals and biofuel production. The research emphasizes using ML to develop predictive models for bio-oil and solid residue yields using limited reaction variables. These models, exhibiting an R^2 score of 0.83 and 0.76 for bio-oil and solid residue, respectively, were validated through experimental comparisons. The study emphasizes temperature and reaction time as critical predictive variables for experimental outcomes. The models displayed good performance in predicting bio-oil yields, with an R^2 of 0.836 and RMSE of 10.522, notably at lower to middle bio-oil yields (20−60 wt %). Key variables include reactor volume to H_2O volume ratio, ratios of lignin to H_2O, lignin to catalyst, temperature, and reaction time. However, the research revealed the complexity and variability in the role of these variables, reflecting on the diverse nature of lignin and its solubility, highlighting the challenges in comparing one variable to another within a limited experimental space. The study recommends the establishment of concrete guidelines for reporting in lignin depolymerization, underscoring the critical importance of specific variables like the reactor-H_2O volume ratio and reaction time and their intricate interplay in influencing bio-oil and solid residue yields. Nevertheless, while the ML models provided significant insights and predictions, deviations in experimental results from model predictions, particularly in bio-oil yield, call for careful consideration and further refinement in modeling approaches. For future research, the emphasis should be laid on the advancement of ML models to enhance the precision of predictions, alongside a more detailed exploration of the key variables and their interactions. The work hints at the need for a more comprehensive and clearer understanding of lignin's diverse characteristics and behavior in depolymerization reactions, as well as the crucial role of reaction variables in optimizing bio-oil and solid residue yields for sustainable fuel development.

In conclusion, the exploration of ML in enhancing biopolymer fuel applications heralds a promising horizon. While significant advancements have been observed, especially in optimizing reaction parameters and understanding biomass composition, the need for continual refinement in ML models is paramount. The unfolding journey bears potential for a

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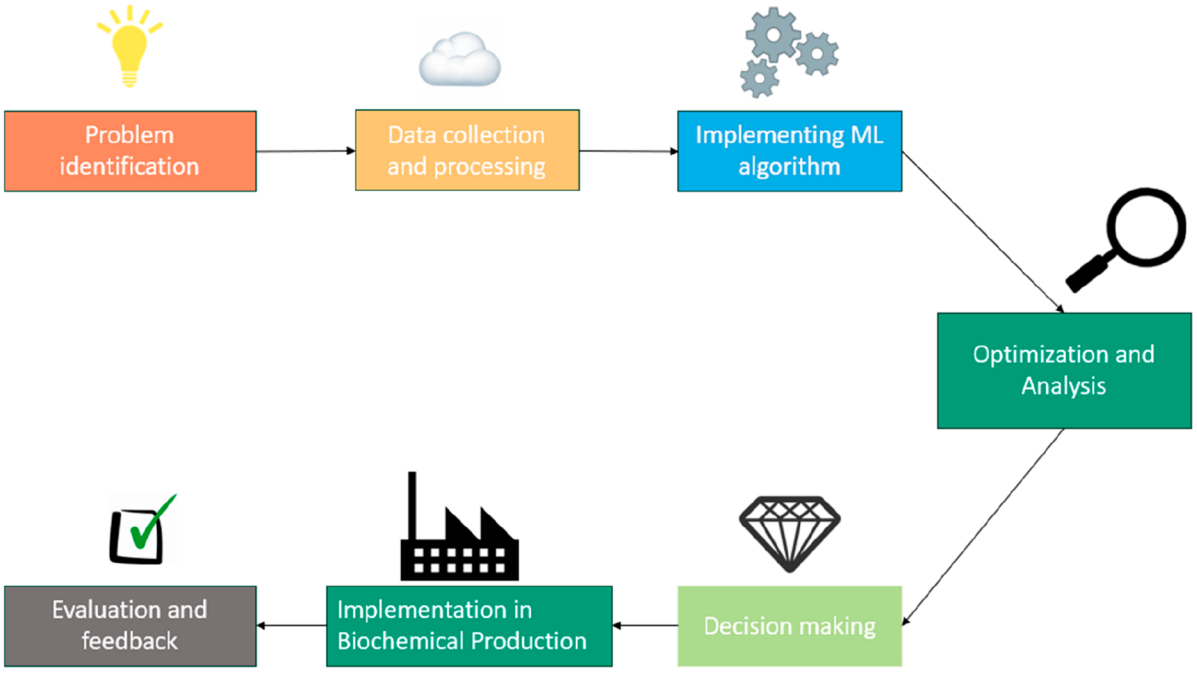

Figure 3. ML process in biobased polymer for biochemical production.

cleaner and more sustainable energy frontier, driven by a deeper grasp of biopolymer properties and innovative computational approaches.

In summarizing the potential of ML in enhancing biopolymer fuel applications, it is crucial to acknowledge inherent challenges and propose clear future research directions. Implementing ML in this field often encounters obstacles such as the variability of biomass materials, the complexity of biological processes, and the need for extensive data to train accurate models. These challenges necessitate a more nuanced approach to data collection and model training, ensuring that models are both robust and adaptable to diverse conditions. Looking ahead, research should focus on developing universal ML models that can adapt to various biomass types and conditions, enhancing the predictive accuracy for different biopolymers. Additionally, expanding the scope to include real-time monitoring and control in biopolymer processing using ML can significantly improve both the quality and efficiency of biofuel production. This approach not only addresses current limitations but also sets a solid foundation for advancing sustainable fuel technologies, contributing to a cleaner energy future.

5. BIOCHEMICALS

5.1. Biobased Polymers and Biochemical Production. Insights into utilizing biobased polymers permeate various sectors, particularly emphasizing their crucial role in biochemical production. This critical evaluation elucidates their multifaceted applications, chiefly in drug delivery and medical devices. The production of biobased polymers, predominantly derived from biological resources, significantly curtails the reliance on fossil fuels.[166] Their biodegradability and compatibility with the environment strengthen their position as sustainable alternatives to conventional polymers.[167] The prominence of biobased polymers is further heightened by the incorporation of ML, enhancing their development and application.[168]

A diverse array of biobased polymers, such as PLA and PHAs, offer unique characteristics that have been extensively exploited in the biomedical field.[169,170] In the arena of drug delivery, the employment of these polymers facilitates the controlled and targeted release of pharmaceutical agents.[171] This capability ensures not only enhanced therapeutic efficacy but also minimizes adverse effects. The biocompatibility and biodegradability of biobased polymers remain paramount for their utilization in medical devices.[172] These materials underpin the creation of prosthetics, sutures, and various other medical implements, underscoring their indispensability in healthcare.[173]

In conclusion, the critical role of biobased polymers in biochemical production and beyond remains unequivocal. Their beneficial attributes, such as biodegradability and biocompatibility, coincide with the global impetus toward sustainability. The intersection of ML technologies further emboldens the advancements in biobased polymers, propelling research and development in drug delivery, medical devices, and energy solutions. The continual exploration and enhancement of biobased polymers, augmented by ML, signal a promising trajectory for realizing a sustainable future.

5.2. Case Studies of Advanced Biobased Polymers for Biochemical Production. In recent years, advances in biobased polymer biochemical production have been examined meticulously. A focus has been laid on optimizing biodegradable food packaging materials such as polylactic acid (PLA), its reactions with food simulants, and enhancing its properties. Additionally, exploring novel materials like Pennisetum purpureum/Napier cellulose nanowhiskers (NWCs) PHA for diverse applications, including ecofriendly packaging and personalized implants, is gaining momentum. Figure 3 shows the ML process in biobased polymers for biochemical production.

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The work by Aznar et al.[174] explored the utilization and analysis of polylactic acid (PLA) for food packaging, an emerging field due to its environmental benefits. The methodological approach employed included the optimization of a dissolution/precipitation sample treatment using dichloromethane/ethanol as solvent/antisolvent, with recovery rates reported between 100.9−114.0%. The study is methodologically sound, identifying the main nonvolatile components of PLA by UPLC-MS(QTOF) analysis. The investigation's unique aspect is the in-depth analysis of PLA-polyester blend pellets and films. The outcomes detailed significant findings, wherein the four most intensive compounds in pellet samples were cyclic oligomers from the polyester blend, comprising adipic acid (AA), phthalic acid (PA), and butanediol. The research reported new compounds in migration solutions resulting from PLA components reacting with food simulants. In terms of migration experiments using different ethanol percentages as food simulants, the results indicate the emergence of new compounds, contributing to the study's comprehensive insights. Such compounds, specifically 14 new ones, were potentially formed by reactions with the packaging material components. A notable statistic is the similarity in composition between pellets and films, with a Pearson correlation factor of 0. 996. The work concludes effectively by outlining the high intensities of cyclic oligomers from the polyester part in PLA blend samples and migration studies, offering essential data for further research and practical applications. For future research, a profound exploration into the reactions between PLA components and various food simulants will be beneficial. Additionally, a detailed quantitative assessment of detected compounds is essential for a comprehensive material risk assessment, aiding in the further enhancement and safe application of biobased polymers in food packaging.

The work by Muller et al.[175] fundamentally investigates the potential of poly(lactic) acid (PLA) and starch as ecofriendly replacements for conventional nondegradable petrochemical polymers used in food packaging. The research analyzes the barrier and mechanical properties of PLA and starch films, utilizing strategies like blending or creating multilayer films, which show promising results in enhancing polymer compatibility and performance. Highlighting some notable results, a smoother microstructure and a higher tensile strength (68 MPa) were observed in the PLA-starch blend (55:45) with 0.5 wt % MDI, signifying improved compatibility and mechanical properties. Yet, the use of MDI, classified as a harmful substance, underscores a significant limitation for food packaging applications, emphasizing the need for safer alternatives. Another method explored was the use of maleic anhydride for enhancing polymer phase interfacial adhesion, resulting in a stable and homogeneous interface and enhancing water resistance and tensile properties. However, despite these advancements, the work reveals persistent challenges with phase separation in the PLA-starch blends, necessitating further research into innovative compatibilizers or treatment methods to optimize the blends for practical application. Moreover, the work demonstrates the improvement in functional properties of multilayer assemblies due to the complementary barrier capacity of each polymer, offering high resistance to both polar and nonpolar molecules and thus emerging as an effective packaging material. Furthermore, the study illustrates the advancements with PLA-starch bilayer films, showcasing improved tensile and water vapor barrier properties, with a noteworthy increase in tensile strength and a significant reduction in water vapor permeability in a 50−50 PLA-starch ratio. In terms of future research, exploring safer, more effective compatibilizers is essential to overcome the existing limitations of PLA-starch blends and multilayer films for food packaging.

The study by Sucinda et al.[176] introduces an inventive approach for producing ecofriendly packaging material reinforced with Pennisetum purpureum/Napier cellulose nanowhiskers (NWCs) in a polylactic acid (PLA) matrix. The bionanocomposite films exhibited promising thermal stability ranging between 343−359 °C. Distinctive observations were made regarding the dispersion of NWC in the PLA matrix. Optimal dispersion was noticed at 0.5−1.5 wt % NWC, leading to a smoother and denser surface structure as opposed to the 3.0 wt % NWC films, which had a rough surface due to the aggregation of NWCs. The tensile strength peaked at 21.22 MPa with a modulus of 11.35 MPa for the PLA/1.0% NWC film, demonstrating superior mechanical properties. Water absorption was recorded highest at 1.94%, providing insights into the hydrophilic behavior of the bionanocomposite films. However, a decline in transparency to 16.16% at λ800 and UVA and UVB transmittance to 7.49% and 4.02%, respectively, was noted for PLA/3.0% NWC film. This aspect, although beneficial for UV protection, may have limitations in specific packaging applications demanding higher transparency. A comprehensive evaluation, including FESEM analysis, revealed a more uniform and compact surface structure with lower NWC content. The study presents a critical analysis of the integration of NWC in PLA to enhance its properties. Yet, the agglomeration at higher wt % NWC indicates a crucial need for research to optimize the NWC content for balanced mechanical and physical properties. Further research might explore the practical implications of these findings, particularly the scalability of this technology for industrial applications and assessing the long-term performance and biodegradability of these bionanocomposite films in real-world conditions. The critical exploration of other biobased nanofillers and their comparative performance with NWC can be another potential avenue for advancing this field of research. Additionally, the environmental impact assessment over the life cycle of these bionanocomposite films could provide a more holistic understanding of their sustainability profile.

In the work by Zhang et al.,[177] the spotlight is cast on PHA, a category of biopolyesters known for their mechanical, biodegradable, and tissue-compatible properties. A distinct innovation seen within the work is the utilization of PHA, particularly polyhydroxybutyrate (PHB) composites, for the 3D printing of personalized implants. This offers a remarkable step forward by maintaining stable local pH during degradation, thus ensuring cellular and immune system tolerance. This innovation is further evident in the 3D-printed custom tricalcium phosphate-PHB scaffolds, achieving successful osteogenic differentiation. PHB's application does not halt here. It shows potential as an osteoplastic material, notably in the construction of porous 3D implants that promote attachment, proliferation, and directed differentiation. Beyond 3D printing, the work details other PHA production methods, such as lithography and nanofiber creation. Lithography, particularly soft lithographic methods, is harnessed to produce PHBHHx microstructures. This technique demonstrates the potential of PHA polymers to mimic the cellular microenvironment, enhancing our understanding of microstructure-

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cell function relationships. Similarly, the work highlights the use of PHA in nanofiber matrices. These matrices, emulating the extracellular matrix, present a promising frontier for tissue engineering due to their supportive role in cell growth and their nontoxicity to NIH 3T3 mouse fibroblast cells. For injectable implants, the use of PHBHHx dissolved in nontoxic organic solvents forms a nontoxic film around the animal's injection site, preventing surgical tissue adhesion. In bone tissue engineering, the combination of PHA with other materials, such as hydroxyapatite, showcases enhanced cell growth and alkaline phosphatase activity, reinforcing its potential in the field of bone tissue engineering. Future studies could explore the possibilities of combining PHA with other biodegradable polymers to enhance its properties, potentially leading to developing more advanced and effective biobased polymers for biochemical production.

The work by Siracusa and Blanco[29] presents a comprehensive examination of the progress of biobased polymers. It is reported that biobased materials' production is substantially less, being under 2% of the total plastic production, despite an astonishing ability to process large amounts of biomass. The global production of polymers from natural resources like starch and cellulose is about 20 million tons per year, a mere 7% of the total plastics production. The study highlights significant advancements in processing technologies for refining biomass feedstocks to obtain biobased monomers, especially focusing on Bio-PE, Bio-PP, and Bio-PET. The geographic analysis reveals the United States and Europe as predominant in biobased plastic production, trailed by the Asia Pacific region and South America. The work delineates technological challenges, noting the variance in development stages for diverse biobased polymers, from research and development to large and commercial stages. The production of Bio-PP is emphasized as especially difficult due to limited knowledge and technological barriers. Furthermore, the work discusses the impact of competition with food, feed, and biofuels for raw materials, recognizing the potential of lignocellulosic feedstocks as future starting chemicals. This aspect highlights the technological complexities in transforming cellulose into sugar monomers. The work also provides a critical evaluation of environmental performance, comparing various routes to obtain bio-PTA for the synthesis of bio-PET, emphasizing the greenest route to be that using orange peels. The study concludes by presenting an optimistic scenario for the future of biobased plastics, projecting a rise in worldwide capacity and emphasizing the importance of biobased PE and PHA alongside PLA and starch plastics. It underscores the interest in biobased durable plastics to curtail waste, taking advantage of biomass from food and agricultural waste. Despite the promising outlook, the work underscores the challenges of reducing production and processing costs and minimizing environmental impacts, crucial for commercial applications of biobased polymers. For future research, focusing on enhancing the technological efficiency of biomass processing, exploring more sustainable and less competitive feedstock alternatives, and comprehensive environmental impact assessment of various biobased polymer production routes will be crucial in advancing the sector and overcoming delineated challenges.

The research by Tyagi et al.[178] delves into the creation of functionalized tissue paper by hydrophobic spray-coating of chitosan (Ch) and cellulose nanocrystals (CNCs). A noteworthy finding in the study is the impressive inhibition of microbial growth by 98% with the ChCNC-coated tissue paper. This statistic emphasizes the robust antimicrobial activity of the developed material. The method of enhancing the antimicrobial properties by plasma treatment showcases innovation, enhancing the coating's antimicrobial activity. However, the variation in water absorption—with CNC increasing it and Ch decreasing it—reveals a critical balance that needs to be maintained for optimal performance. The ChCNC-coated glass slide's contact angle was found to be 41°, a crucial statistic that indicates a balance between hydrophilicity and hydrophobicity. Using various sophisticated techniques such as SEM, ToF-SIMS, and Auger electron microscopy reinforces the comprehensive assessment and verification of the ChCNC-treated substrate's morphology and chemical characterization. Despite the commendable antimicrobial activity, the study shows that only the ChCNC-coated tissue paper inhibited the human hand-collected microbial sample, which highlights a possible limitation in its broad-spectrum antimicrobial activity. This could be a vital area for future research—expanding the antimicrobial spectrum of the ChCNC coating.

In the study by Aristri et al.,[179] an emphasis on tannin-based biopolyurethanes (bio-PUs) and their potential for environmentally friendly applications is highlighted. The research highlights the successful synthesis of tannin-based bio-PUs, confirmed through various analytical techniques like FTIR, DSC, TGA, MALDI-TOF mass spectrometry, and GPC. Notably, a key finding is that as the tannin content increased, the transition glass (T_g) temperature decreased from 32.91 to 11.91 °C, indicative of an increase in backbone stiffness and chain interactions. This phenomenon emphasizes tannin content's role in enhancing bio-PU's thermal properties. The thermal analysis showed three degradation stages of PU resins, with the initial one occurring at 220 °C, attributed to urethane bond degradation. Significantly, no weight loss was observed, in line with the low isocyanate concentration used in the PU formation, highlighting the potential for a more stable and sustainable product. The thermogravimetric analysis showcased the degradation of ester and carbonyl groups from tannins at 290−300 °C, providing essential insights into the thermal stability and potential applications of these bio-PUs in various industrial sectors. Moreover, the research leveraged MALDI-TOF to determine the condensed tannin oligomer's distribution and derivatives. The MALDI-TOF results reveal a clear differentiation in the molecular weight ranges between the tannin-based bio-PUs produced at room temperatures and a reference mix, further accentuating the unique properties attained through tannin incorporation. In view of future research, a comprehensive investigation into the long-term stability and performance of tannin-based bio-PUs in practical, real-world applications is imperative. Additionally, exploration into the optimization of tannin content for enhanced material properties, alongside a detailed cost-benefit analysis, would significantly contribute to the field, offering a more holistic understanding and paving the way for the extensive industrial adoption of tannin-based bio-PUs.

The work by Alinejad et al.[180] gives an extensive and detailed review of the substitution of lignin for polyol in producing polyurethane products. Using lignin, an underutilized renewable aromatic polymer, is a unique approach to producing polymeric materials. The work outlines the procedure of making rigid polyurethane foams with lignin, emphasizing the significance of thermal conductivity in this

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process. Despite the environmental concerns surrounding using certain blowing agents, the work indicates a transition to more environmentally friendly options such as pentane and water, ensuring sustainable production. The production process explained in the document, beginning with water and isocyanate, elucidates how the exothermic reactions involved led to the creation of amine and CO_2 and, subsequently, the polyurethane. The work discloses the issues with unmodified lignin—leading to brittle foams with low compression strength, especially with incorporation over 30 wt %. To counter this, chain extenders like castor oil, polypropylene glycol triol, and butanediol have been employed. The work's extensive exploration of using various lignins in rigid polyurethane foams shows a comprehensive effort to ascertain optimal materials and procedures. Despite detailed investigation, the study suggests the ambiguity in the relationship between lignin properties and foam performance, pointing to an area that needs more detailed research to enhance understanding and refine processes. In the domain of flexible polyurethane foams, the document offers an analysis of lignin's potential as a filler and cross-linker. Even though some success was reported with modified lignins in enhancing thermal stability and mechanical properties, complete replacement with certain types of lignin resulted in inferior products. The detailed comparison with control foams is appreciable for its depth, providing clear insights into the practical advantages and limitations of lignin use. As for the production of polyurethane-lignin elastomers, the work reveals the constraints imposed by lignin's high glass transition temperature and low flexibility. Nevertheless, the findings that lignin fillers enhance mechanical properties and tensile modulus signify its potential use in polyurethane elastomer synthesis, contingent on selecting appropriate types of lignin. Future research could focus on improving the reactivity of lignin, exploring more environmentally friendly modification methods, and detailed investigations into the influence of lignin types and modification methods on the properties of the resulting polyurethane products.

In conclusion, significant progress is observed in the field of advanced biobased polymer biochemical production, from enhancement of PLA properties to exploration of new, innovative materials and methodologies. Despite the advancements, several challenges and areas for future research and optimization are unveiled, emphasizing the continual need for innovation and scrutiny in this critical field to ensure safety, efficiency, and environmental sustainability.

5.3. ML in Biochemicals. The impact of ML on the biochemical sphere has become increasingly profound. Its role in boosting and fine-tuning biochemical production is pivotal.[181] An expansive collection of data inherent in biochemical processes is effectively managed and analyzed through ML algorithms. This data management allows for the identification of patterns and trends that would be otherwise obscure, granting an enhanced understanding of diverse biochemical processes. Optimal conditions for biochemical production are effectively identified through ML, facilitating increased yields and process efficiency.[69,70,182] Enhanced efficiency conserves resources and substantially reduces production time and costs. ML's influence transcends traditional boundaries, imbuing the biochemical realm with unprecedented precision and control.

In the biochemical industry, the production of enzymes, amino acids, and other biobased materials is central.[183,184] The use of ML facilitates the prediction and optimization of production parameters for these crucial biochemical entities.[185] Accurate predictions ensure that the biochemical production processes are not only streamlined but also made more environmentally friendly and sustainable. Through ML, the biochemical industry is rendered more adaptable to the burgeoning demands for sustainability and efficiency.[186] This adaptation embodies a significant stride toward a more sustainable and ecofriendly future in biochemical production.

Additionally, ML plays a fundamental role in the optimization of fermentation processes, a core aspect of biochemical production.[155,187,188] The optimal conditions for fermentation are crucial for maximizing yield and product quality. ML algorithms help in determining these optimal conditions, leading to enhanced production efficiency. The precision afforded by ML ensures that the resources are used judiciously, and waste is minimized, aligning biochemical production with sustainability goals. The enhanced control over fermentation processes is a noteworthy advancement in biochemical production, offering a promising avenue for further research and development.

ML further finds its application in biocatalysis, a significant aspect of biochemical production.[189−191] Through ML algorithms, the most suitable catalysts for specific biochemical reactions are efficiently identified, ensuring that the reactions proceed optimally. This efficiency leads to enhanced productivity and sustainability in biochemical production. The integration of ML in this domain exemplifies the seamless amalgamation of technology and biochemistry, heralding a new era of enhanced and optimized biochemical production.

In essence, the infusion of ML into the biochemical sector signifies a monumental leap toward optimized and sustainable production. ML's capability to analyze vast data sets, identify patterns, and make accurate predictions is invaluable in enhancing and fine-tuning biochemical production. Its role in optimizing production parameters, fermentation processes, and biocatalysis is instrumental in ensuring increased efficiency, reduced waste, and alignment with sustainability goals. This synergy between ML and biochemical production stands as a beacon of progress, illuminating the path toward a more sustainable and efficient future in biochemical production.

5.4. Case Studies of ML Applied to Biopolymer for Biochemical Purposes. This section presents a critical examination of various case studies addressing ML applications to biopolymers for biochemical purposes. The focus remains on understanding the effective utilization of different ML models in enhancing and optimizing biopolymer properties and processes. The breakthroughs, limitations, and future perspectives are extensively analyzed, providing a well-rounded view of the impact and potential of ML in the sphere of biopolymer research and application.

The work by Löfgren et al.[192] demonstrates an innovative application of Bayesian optimization in enhancing the process of lignin biorefinery for efficient biochemical applications. The study focuses on optimizing AquaSolv omni biorefinery for lignin, an abundant biopolymer, using a ML framework. This approach enables linking various biorefinery conditions to the experimental outputs effectively. The research reported the use of Bayesian optimization for training two surrogate models for lignin yield and β-O-4 content. The authors efficiently visualized these models using 2D contour plots, revealing substantial improvements in lignin yield and β-O-4 content as new data were acquired using the CA strategy. The work's

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most crucial highlight is the revelation of optimal processing conditions for lignin yield and β-O-4 linkages for depolymerization into platform chemicals, showing the profound impact of ML in accelerating sustainable chemical processing methods. Further insights from the work discuss the comparison between two acquisition strategies, CA and PA, providing a deeper understanding of their effectiveness in the biorefinery process. The study illustrates that CA generates a more accurate and developed surrogate model than PA, proving to be a better acquisition strategy for BO-driven experiments. This comparative analysis strengthens the work's contribution by demonstrating the relative efficacy of different strategies in lignin biorefinery. However, despite these commendable findings, the work could offer more extensive insights into the potential impact of the optimized biorefinery process on broader sustainable development and biochemical applications. The study's results significantly contribute to enhancing lignin biorefinery, yet the discussion on its far-reaching implications appears limited. In terms of future research, the work sets a solid foundation for further exploration of ML applications in optimizing other biopolymer refineries. It opens avenues for investigating the effectiveness of other ML algorithms in improving biopolymer refinery processes and their subsequent impact on the production of high-value byproducts. In summary, the study presents a commendable integration of ML in optimizing biopolymer biorefinery, providing valuable insights for enhancing lignin yield and β-O-4 content effectively. The comparative analysis of acquisition strategies further enriches the work's contribution to the field while highlighting opportunities for expansive future research in this domain.

The work by Patnode et al.[193] focused on soy and zein for the development of sustainable bioplastic films is not only innovative but timely. The employment of ML to forecast and enhance the properties of proteopposite films shows a commendable intersection of materials science and computational technology. An R^2 value of 0.85 underpins the model's accuracy, reinforcing the credibility of the ML predictions and their practical application. The study eloquently blends experimental and computational research to assess the synergistic impact of zein, soy, and POBM-latexes in proteopposite films. The work observed a significant enhancement in the flexibility and moisture resistance of the soy-zein films with the integration of POBM-latexes. Considering the films' targeted application in food packaging, this aspect is pivotal, where these properties are paramount. Specifically, the elongation at the break of the films surged by over 400%, a staggering improvement that holds practical and industrial relevance. Yet, the exploration did not end here; the study delved deeper, examining the influence of POBM-latex particle size, unveiling that smaller particle sizes afford greater uniformity and enhanced interaction in the proteopposite film structure. Despite the advancements and the high prediction accuracy, there lies a necessity for further validation and testing in real-world applications. This is crucial for assessing Bioplastic films' true efficacy and feasibility in replacing traditional petrochemical food packaging. Moreover, while the study delivers insights into the mechanical and barrier properties of the modified soy-zein proteopposites, a comprehensive assessment of their antimicrobial properties and surface morphology remains uncharted, presenting a clear pathway for future research endeavors. The comprehensive ML-based QSAR model successfully predicted the mechanical attributes of the films, showcasing a robust R^2 value of 0.84, emphasizing the model's reliability in navigating the complexities of bioplastic film properties.

In the work by Bejagam et al.,[26] ML models were employed to predict the melting temperature (T_m) of various PHAs, utilizing a data set of experimentally measured T_m values, molecular weights, and polydispersity indices for many PHA homo- and copolymer chemistries. The model showcased robust predictions with an average RMSE in T_m predictions of 8.47 °C for training and 10.69 °C for the test set, demonstrating the model's efficacy and lack of overfitting. The work underlines the critical feature importance of first-order topology (Chi1) and second-order shape/connectivity indices (Kappa2) in the prediction models, emphasizing their role in understanding the atomic spatial density in a fragment. Furthermore, applying an evolutionary algorithm-based search strategy optimizes polymer design by identifying candidates that best meet the target chemical space criteria, underscoring the model's practical utility in real-world applications. In future research, enhancing the model's robustness through integration with other ML algorithms or expanding the data set for a more comprehensive analysis would be a constructive step forward. Moreover, assessing the model's performance across various biopolymer types and exploring its potential in predicting other crucial properties beyond T_m could offer more extensive insights and applications in the realm of sustainable Bioplastic formulations and biochemical applications.

The work by Pilania et al.[82] offers insight into the application of ML to polyhydroxyalkanoate-based biopolymers, emphasizing the prediction of glass transition temperature (T_g). The work collected experimental T_g values, molecular weights, and polydispersity indices for PHA-based polymers, developing a fingerprinting scheme based on topology, shape, and charge/polarity to represent polymers numerically. The constructed model demonstrated the ability to efficiently predict new PHA polymer properties with notable accuracy, citing a Pearson correlation coefficient of 94.67%, RMSE of 4.80 K, and mean absolute error (MAE) of 18.99 K. The uniqueness of this study lies in its methodical approach, using a large feature space recursively to enumerate analytical functions describing T_g, producing 283, 86.7×10^3, and 12.5×10^9 elements for various feature sets. The surrogate model, combined with an evolutionary algorithm-based search strategy, was able to find multicomponent polymer compositions with a specified T_g efficiently. The model's robustness is confirmed by its consistent performance on 20 randomly selected training/test splits, producing an average RMSE of 4.76 K and a variance of 1.19 K^2. The research adequately addresses the significance of T_g prediction for various biopolymers, successfully utilizing ML models to forecast T_g values and explore the chemical space of PHAs. Nevertheless, a critical evaluation reveals that the model's applicability may be limited to the data and features utilized in the study. The discussion emphasizes the model's resistance to overfitting and highlights the established parameters for the RF model, including a maximum tree depth of 6 and the number of estimators set to 35. However, these fixed parameters might pose restrictions for other biopolymers not considered in this study. In terms of future research, the exploration of other ML algorithms for predicting different properties of biopolymers beyond T_g and the enhancement of the current model for broader chemical spaces could be undertaken.

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The work by Jiang et al.[194] endeavored to predict the performance properties of PHAs using a deep neural network (DNN) model is remarkable. The methodological approach is comprehensive, utilizing variables such as molecular weight and monomer percentages to estimate PHA glass transition temperatures (T_g). The study achieved a substantial R^2 value of 0.869, MAE 4.010, and RMSE 5.339 K, demonstrating the model's high level of accuracy and reliability in prediction. This approach outperformed other ML models, further solidifying its credibility. However, the issue of model symmetry and sensitivity to missing data require attention. The initial DNN model did not capture symmetry, making it sensitive to monomer order and highlighting a significant limitation. Nevertheless, the researchers astutely addressed this by retraining the model, achieving improved results with R^2 increasing to 0.897. Although the DNN model's performance is laudable, the study illuminates the crucial aspect of symmetry in ML models for biopolymer prediction. Moreover, the investigation into the DNN model's robustness with missing or inaccurate data is praiseworthy, offering insights into the potential practical challenges of employing ML in predicting biopolymer properties. Despite the decrease in R^2 to 0.5 with omitted variables, the research insightfully demonstrates the critical role of fractional composition in the DNN model, underscoring its importance in maintaining prediction accuracy. Moving forward, potential research could delve deeper into enhancing the DNN model's robustness against missing data. Furthermore, exploration of additional ML frameworks might yield more streamlined or effective approaches, potentially further improving the prediction accuracy and reliability for biopolymer applications and expanding the study's implications for sustainable technology and engineering.

In conclusion, examining case studies reveals the pivotal role ML holds in augmenting biopolymer research for biochemical applications. Despite some limitations, the diverse machine-learning approaches discussed significantly enhance the prediction and optimization of biopolymer properties and processes. The explored studies underscore the burgeoning potential and avenues for further research in this innovative intersection of ML and biopolymer, driving advancements in sustainable and efficient biochemical applications.

6. FUTURE WORK

The intersection of ML and biobased polymers represents a significant and rapidly evolving field for research. This convergence unlocks unprecedented opportunities for developing sustainable energy, fuels, and biochemical solutions.[12,195] As we delve into this dynamic domain, the potential for innovative breakthroughs that can drive us toward a more sustainable future is immense.

A significant avenue for future research lies in enhancing the efficiency of biopolymers. ML has shown promise in optimizing various properties of biopolymers, but there is still room for improvement. Future studies could focus on refining ML algorithms for more precise predictions and optimizations of biopolymer properties, such as thermal stability, mechanical strength, and degradation rates. For instance, research could explore deep learning models to predict the interplay of biopolymer molecular structures with environmental factors, thereby enhancing their performance in specific applications.[196,197]

The development of robust ML models relies heavily on the availability and quality of data.[198,199] One of the challenges in this field is the limited access to comprehensive data sets that capture the complexity of biopolymer systems. Future research should prioritize the creation of extensive, high-quality data sets. This could involve collaborations between academic and industrial sectors to pool resources and data. Also, there is a need for standardizing data collection and reporting methods to ensure the consistency and reliability of the data used in ML models.

Another critical research direction is the application of ML in biopolymer recycling and waste reduction.[12,200,201] As the world grapples with plastic pollution, biopolymers offer a sustainable alternative. ML can be leveraged to improve recycling processes, optimize waste management systems, and develop new biodegradable materials. Future research could explore ML models that predict the recyclability of biopolymers based on their chemical compositions and environmental conditions.

The integration of ML in producing and processing biopolymers is a promising research area. ML can be used to optimize production parameters, reduce energy consumption, and enhance the overall efficiency of biopolymer manufacturing processes. Future studies could investigate the use of ML in real-time monitoring and control of biopolymer production, focusing on maximizing output while minimizing environmental impact.

Biopolymers such as alginate, cellulose, PLA, chitosan, and lignin have great potential in energy storage systems, such as batteries and supercapacitors. ML can play a pivotal role in enhancing the performance of these systems. Research should be directed toward developing ML models that can accurately predict and optimize the ionic conductivity, charge−discharge cycles, and overall efficiency of biopolymer-based energy storage systems.

Designing and developing novel biopolymers using ML algorithms is an exciting future prospect. Using ML, researchers can predict and create new biopolymer structures with desired properties for specific applications. This approach could revolutionize the field, developing innovative materials for various industries, from healthcare to aerospace. Furthermore, understanding the interactions between biopolymers and other materials is crucial for broadening their application scope. Future research could use ML to model and predict the behavior of biopolymer composites, blends, and hybrids.[85,202,203] This would enable the development of materials with tailored properties for specific uses, such as biocompatible medical devices or high-performance construction materials.

While biopolymers are inherently more sustainable than traditional polymers, there is a need to further enhance their environmental friendliness. Future research could explore how ML can be used to analyze and optimize the life cycle of biopolymers, from production to degradation. This would involve developing models to assess the environmental impact of biopolymers and finding ways to reduce their carbon footprint.

The use of biopolymers in drug delivery systems offers a promising research avenue.[204,205] ML can assist in designing biopolymer-based carriers that optimize drug release profiles and target specific tissues or cells. Future studies could develop ML models that simulate the interactions between biopolymers and various pharmaceutical compounds, aiding in creating

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more effective and safer drug delivery systems. Furthermore, the exploration of ML applications in biocatalysis within biochemical production is deemed promising, likely leading to enhanced productivity and sustainability in biochemical production.[189,191,206]

Finally, the future of ML and biopolymers research lies in collaborative and cross-disciplinary efforts. Combining the expertise of chemists, material scientists, computer scientists, and engineers will be key to advancing this field. Collaborative projects can lead to breakthroughs in understanding and leveraging the capabilities of ML in biopolymer research, leading to innovations that can significantly impact various sectors and contribute to a sustainable future. In conclusion, the path forward in converging ML and biopolymers has exciting opportunities and challenges. By addressing these key areas, the scientific community can unlock the full potential of this synergy, paving the way for groundbreaking advancements in sustainable materials and energy solutions.

7. CONCLUSION

The nexus between ML and biobased polymers heralds a transformative phase in energy, fuels, and biochemicals. Biobased polymers, with their sustainable origins, are progressively influencing the energy and fuel domains. Their integration with ML amplifies their inherent potential and optimizes renewable energy processes, storage solutions, and conversion mechanisms. Through diverse case studies, the efficacy of these polymers in energy applications is accentuated, while ML's potential to enhance fuel efficiency stands elucidated. The cusp of this synergy also brings to light groundbreaking strides in biochemical production, notably in drug delivery and medical instrumentation. It is evident that the symbiotic relationship between ML and biobased polymers offers a beacon for global sustainability in the energy and biochemical realms. Embracing this amalgamation is paramount to ushering in an era of innovation and steadfast commitment to a sustainable future.

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