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REVIEW

Green Extraction, Targeted Modification, and Multi-Domain Applications of Natural Polymers

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ABSTRACT: Natural polymers (NPs) are widely distributed in plants, animals, and microorganisms. They can be classified into three habitat-based groups, namely terrestrial polymers, marine polymers, and extreme natural polymers. This review summarizes their structural features, environmental adaptation mechanisms, and functional attributes. It also outlines the evolution of extraction technologies from traditional acid–alkali and mechanical methods to modern green solvent systems. The roles of physical modification and chemical derivatization in performance regulation and functional enhancement are examined. Artificial intelligence methods are introduced to support structure–property prediction, formulation design, and process optimization. Molecular dynamics and other computational approaches are also discussed to clarify the underlying mechanisms. Overall, as key materials supporting the green transition of industrial production, NPs are becoming a major focus in research on circular chemical resources. With continued advances in process optimization, artificial intelligence technologies and interdisciplinary integration, NPs are expected to replace conventional materials in a wider range of high-value applications scenarios and to achieve further breakthroughs in performance, thereby contributing to sustainable development.

KEYWORDS: Natural polymers; bio-based materials; extraction and modification technologies

1 Introduction

The increasing pressure of global environmental governance has intensified concerns about the depletion of petroleum resources, which remain a foundation of economic development [1]. Polymer materials are essential to modern industry and daily life, and synthetic polymers currently dominate the market. Synthetic polymers are typically derived from petrochemical feedstocks through addition or condensation polymerization, such as polyethylene (PE), polypropylene (PP), poly(ethylene terephthalate) (PET) and polyamide (PA). They offer strong advantages in molecular structure controllability, property uniformity, thermal and mechanical performance and large-scale production cost [2]. However, they rely heavily on fossil carbon sources, exhibit high environmental persistence and create significant burdens in recycling and degradation [3]. The chemical industry, as a major contributor to energy consumption and pollutant emissions, faces urgent demands for a green and low-carbon transition [4]. Against this background, sustainable materials represented by NPs have attracted increasing attention [5]. Their renewability, biodegradability, and low environmental footprint provide clear advantages in packaging, textiles, and biomedical applications [6–8].

NPs are complex organic macromolecules synthesized through multiple metabolic pathways in nature. They are essential components for sustaining biological functions and are widely distributed across living organisms, including proteins, cellulose, lignin, starch, rubber and chitin [9–13] (Fig. 1). A wide range of NPs has attracted increasing attention and has been extensively applied in conventional consumer-related sectors, including food, chemical products, cosmetics, electronic devices and automotive industries [13–17]. With continued advances in NPs research, their applications are no longer confined to traditional livelihood-related fields and have expanded into high-end areas with more stringent performance requirements, such as precision electronics, aerospace and medical applications [18–20].

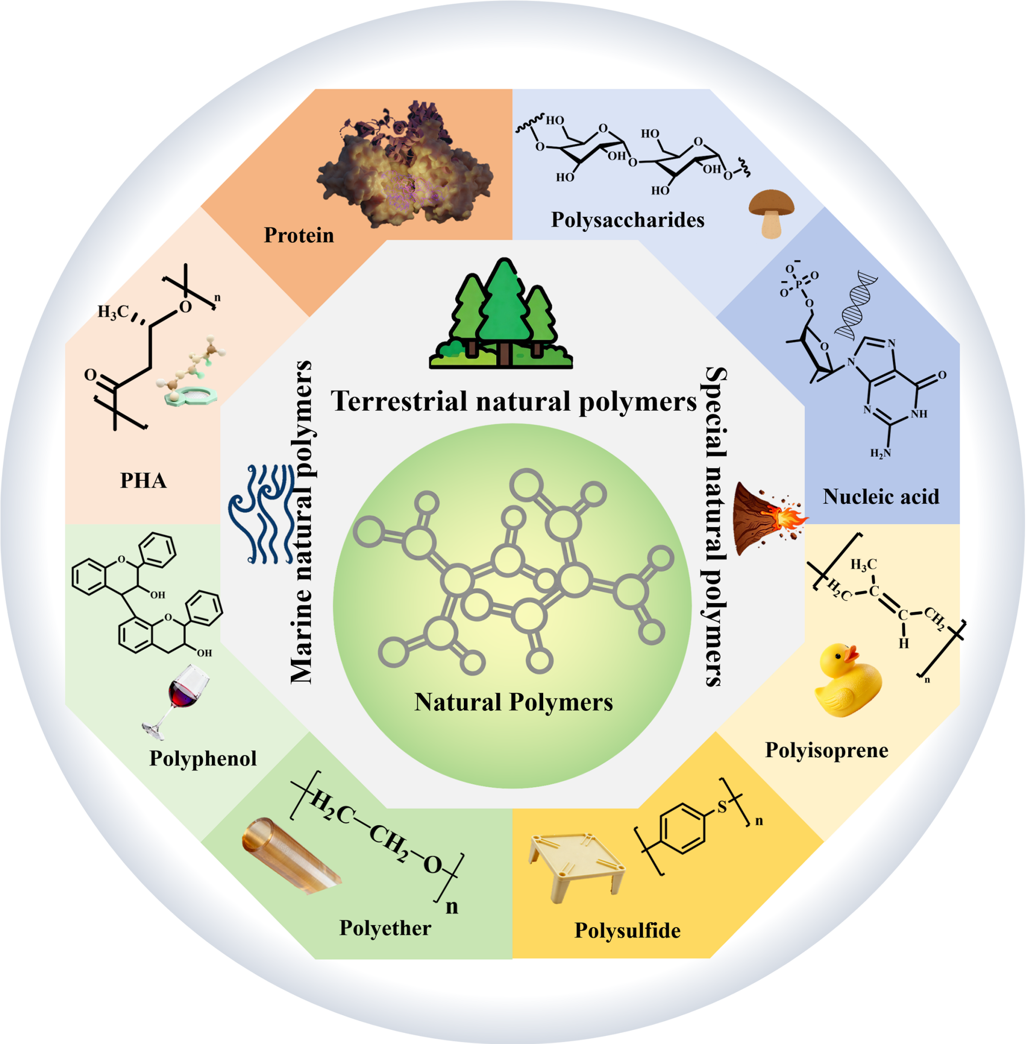

Figure 1: Classification and source framework diagram.

In light of the above background and application prospects, this review focuses on green functional material systems based on NPs. To clarify how this review differs from previous reviews, it is worth noting that many existing articles focus on one aspect—for example, alginate wound dressings in preclinical/clinical contexts or the use of deep eutectic solvents (DES) in chronic wound management—or they concentrate on a single process-intensification route such as ultrasound-driven polysaccharide modification [21]. In contrast, this review places NPs together with recent green extraction options and explains, with specific examples, how extraction media and conditions (e.g., DES/NADES and assisted extraction) can influence polymer quality and functional performance, thereby shaping subsequent modification choices and application feasibility. As a concrete translational example, hydrophobic DES (HDES) has been used to formulate printable emulgels for 3D-printed personalized wound dressings [22]. We also briefly note that data-driven modeling is increasingly being used to support NADES extraction optimization and prediction, complementing conventional experimental design [23]. This review systematically summarizes the sources, preparation approaches, and modification strategies of NPs, examines representative interdisciplinary application cases, and further discusses major development trends and future directions for sustainable applications.

NPs include several major categories, and their basic structural features largely determine how they are extracted, modified, and used in downstream applications. Polysaccharides such as cellulose, alginate, and chitin/chitosan contain abundant hydroxyl or ionic groups and often form hierarchical structures, which make them suitable for gelation, adsorption, and derivatization. Protein-based NPs show good bioactivity and biocompatibility, but their conformations can be sensitive to processing conditions. Nucleic acids have a charged phosphodiester backbone and specific recognition ability, yet stability and purity control remain important in practice. Microbial polyesters such as PHAs are biodegradable aliphatic polyesters whose thermal and mechanical behavior can be tuned by composition. In addition, polyphenols and polyisoprene represent functional natural-polymer families that provide antioxidant/UV-related functions and elastomeric behavior, respectively. Introducing these NPs types helps connect habitat-derived resources with appropriate green extraction routes, targeted modifications, and downstream applications.

2 Sources and Multidomain Applications of NPs

As bio-based functional materials derived from living organisms, NPs exhibit renewability, biocompatibility, and multifunctionality. They were widely used in the early stages of human civilization. Cellulose was applied in the textile and papermaking industries [24], starch served as a food binder and molding aid [25], and chitin was used in simple anticorrosive coatings [26]. However, limited research depth and technical conditions constrained early development. Modification strategies were largely restricted to physical approaches, which resulted in narrow performance ranges and limited functional diversity [27–29].

With the gradual establishment of systematic research on NPs, interdisciplinary integration has continued to deepen. Functional modification and advanced fabrication technologies have achieved key breakthroughs, leading to significant progress in polymer membranes, polymer fibers and biomedical polymer materials. Through chemical modification [30,31], self-assembly [32,33] and directed biosynthesis [34,35], precise molecular-level structural design and regulation of NPs have been realized. As a result, NPs have evolved from basic materials into specialized functional materials suitable for high-end application scenarios.

2.1 Sources of NPs

NPs are complex organic molecules synthesized by organisms through their intrinsic metabolic pathways. Based on chemical structure, they can be broadly classified into proteins, polysaccharides, nucleic acids, polyesters, polyphenols and polyisoprene [36]. Because organisms experience markedly different environmental pressures, their metabolic pathways are selectively regulated to produce functional NPs with specific environmental adaptability. Owing to their diverse functional attributes, these NPs have found broad applications in high-end technological fields [37–39].

2.1.1 Terrestrial Natural Polymers (TNPs)

Terrestrial natural polymers (TNPs) are primarily derived from terrestrial plants, animals and microorganisms, with typical examples including cellulose, hemicellulose, lignin, chitosan and collagen. Under the combined effects of diurnal and seasonal climatic fluctuations and biomechanical demands, most TNPs form stable three-dimensional network structures composed of cyclic monomeric units [40].

Plants represent a major source of TNPs, including cellulose, lignin, hemicellulose, pectin, and starch. Among these, cellulose is a plant-specific TNPs composed of cyclic glucose units linked by β-(1,4) glycosidic bonds, forming a highly ordered linear long-chain structure [41] (Fig. 2a). This structure endows cellulose with excellent mechanical strength and chemical stability. Cellulose is abundant worldwide and is renewable and biodegradable. It is widely used in textiles, construction, packaging, and biomedical materials, including wound dressings, tissue engineering scaffolds, and drug delivery systems. Similar to cellulose, hemicellulose is also present in plant cell walls and is a highly branched polysaccharide composed of monosaccharides such as xylose, arabinose, and mannose [42] (Fig. 2b). Lignin is the second most abundant organic polymer in terrestrial ecosystems after cellulose. It is mainly formed by the random polymerization of phenylpropane units, including p-coumaryl alcohol, coniferyl alcohol and sinapyl alcohol, through ether and carbon–carbon bonds, resulting in a three-dimensional network structure [43] (Fig. 2c). Lignin is embedded within cellulose and hemicellulose networks via van der Waals interactions and hydrogen bonding, which enhances cell wall rigidity and mechanical support while imparting resistance to biodegradation and hydrophobic barrier properties. These functions are essential for maintaining plant structural stability and environmental adaptability [44].

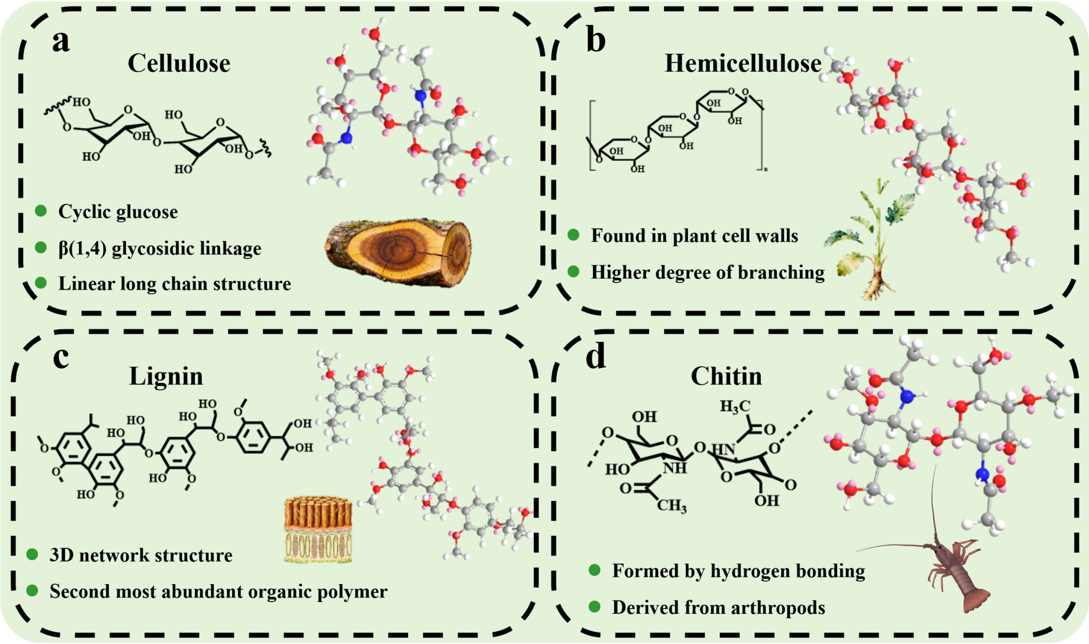

Figure 2: (**a**) Cellulose; (**b**) hemicellulose; (**c**) lignin; (**d**) chitin.

In animals, chitin is an essential TNP for terrestrial arthropods and is the second most abundant natural nitrogen-containing polymer. It is composed of N-acetyl-D-glucosamine units, and its limited exposure of hydrophilic groups reduces water loss under dry conditions [45,46] (Fig. 2d). Chitin molecules assemble through hydrogen bonding to form crystalline and amorphous regions, resulting in shell structures with high strength and flexibility [47]. This structural organization improves resistance to mechanical stress and reduces fracture caused by drying-induced shrinkage [48–50].

Polyhydroxyalkanoates (PHAs) are representative bio-based polyesters synthesized by microorganisms. They are produced under conditions of excess carbon and limited nutrients such as nitrogen and phosphorus. PHAs function as intracellular carbon and energy storage materials. Their polymer chains consist of repeating 3-hydroxy fatty acid units linked by ester bonds. The molecular weight and composition of PHAs can be tuned by adjusting carbon sources, oxygen levels, and nutrient supply during cultivation. Kumari and Venkata Mohan synthesized P-3HB, P-3HB-co-3HV, and P-3HB-co-3HD by controlling aerobic and anaerobic conditions and nutrient stress using levulinic acid and lignocellulosic derivatives as co-substrates. Among these materials, P-3HB-co-3HD exhibited high thermal stability [51] (Fig. 3). PHA biosynthesis also shows broad adaptability to different carbon sources. This feature enables the high-value utilization of organic waste. Ó Maoldúin et al. produced PHAs from residual sludge at a large wastewater treatment plant in Ireland, which markedly reduced production costs [52].

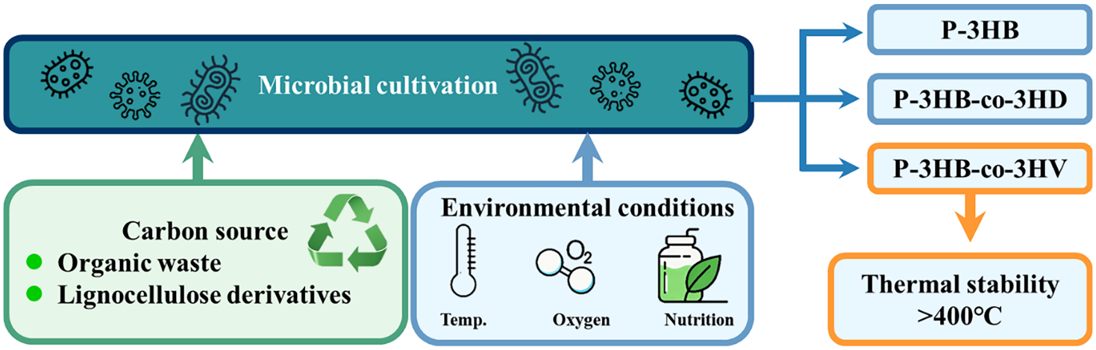

Figure 3: PHA production route diagram.

2.1.2 Marine Natural Polymers (MNPs)

Marine natural polymers (MNPs) are mainly derived from marine plants, animals and microorganisms, including algae, mollusks, crustaceans, fish and planktonic microbes. In practice, many widely used MNPs are predominantly composed of polysaccharides. MNPs typically exhibit low solubility and high molecular weight. Their backbones are mainly long-chain or macrocyclic structures, with ring sizes commonly ranging from 8- to 10-membered structures. In addition, MNPs are rich in nitrogen and halogens, particularly bromine, while their oxygen content is relatively low [40].

Algae are an important source of MNPs, with brown, red and green algae serving as major producers of plant-derived polysaccharides (Fig. 4(ai)). Alginate, agar and carrageenan are the most widely used and extensively studied polysaccharides. Alginate is a linear polysaccharide composed of β-D-mannuronic acid (M units) and α-L-guluronic acid (G units) arranged in different ratios and sequences (Fig. 4(aii)). The M/G ratio and sequence distribution strongly affect physicochemical properties. G-rich alginates form gels with higher hardness and mechanical strength through crosslinking with divalent cations such as Ca^{2+} [53]. By contrast, M-rich alginates exhibit improved elasticity, softness and water solubility [54]. This tunable mechanical behavior underpins the broad use of alginate in food, biomedical and pharmaceutical materials [55–57]. For example, Tan et al. prepared sodium alginate and carboxymethyl cellulose composite films loaded with functional nanoparticles, which enhanced water resistance and ultraviolet shielding and extended the refrigerated shelf life of pork [58] (Fig. 4(aiii)).

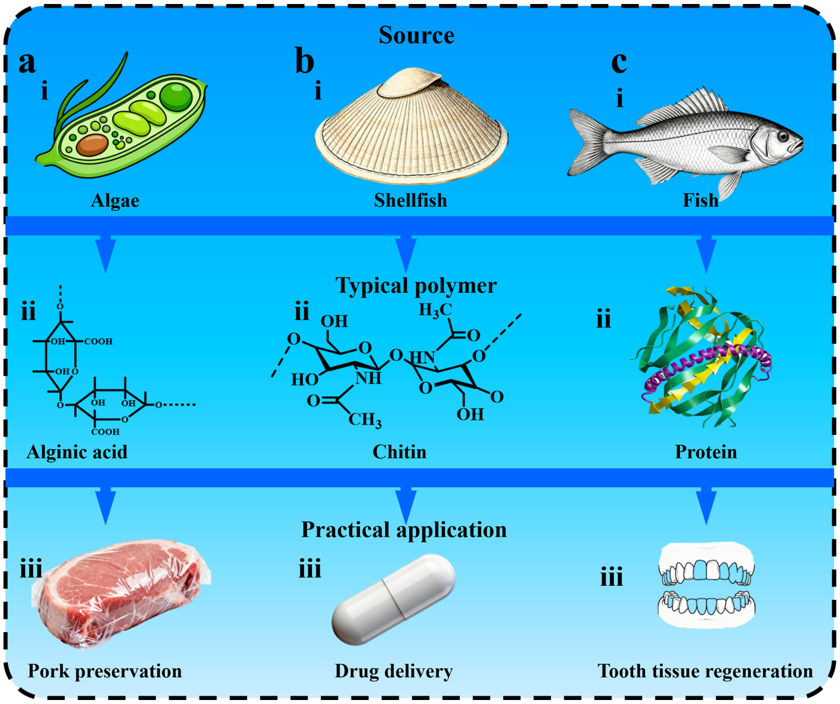

Figure 4: MNPs (**a**) algae, (**b**) mollusks, (**c**) fish.

Compared with alginate, agar consists of β-D-galactopyranose and 3,6-anhydro-α-L-galactopyranose units linked alternately by α-1,3 and β-1,4 glycosidic bonds to form a linear backbone. These chains assemble into three-dimensional networks through intermolecular hydrogen bonding, resulting in high gel strength [59]. Carrageenan is based on 3,6-anhydro-D-galactose as the fundamental structural unit. Its main chain consists of alternating α-1,3 and β-1,4 glycosidic linkages. Depending on the number and positions of sulfate ester groups along the chain, carrageenan is classified into three main types, namely κ, ι and λ [60]. κ-carrageenan can form thermoreversible elastic gels with high strength through interaction with K^+ ions, providing robust three-dimensional network frameworks for flexible electrochemical devices. Duan et al. constructed a fully physically crosslinked double-network gel polymer electrolyte based on κ-carrageenan and polyacrylamide. Polyaniline was polymerized *in situ* to fabricate integrated supercapacitors with high specific capacitance and good cycling stability. The κ-carrageenan-based hydrogel also maintains favorable electrochemical performance at low temperatures and exhibits self-healing capability and resistance to mechanical impact [61]. By comparison, ι-carrageenan preferentially forms soft gels through interaction with Ca^{2+} ions. Chan et al. combined ι-carrageenan with κ-carrageenan at different ratios in fermented sour cream. This approach significantly improved rheological and textural properties. The samples exhibited shear-thinning behavior while maintaining good microbiological stability [62]. In contrast, λ-carrageenan has a high degree of sulfation and strong electrostatic repulsion, which limits gel formation but provides pronounced thickening ability. The addition of small amounts of λ-carrageenan to gas and oil pipeline hydrate inhibition systems significantly prolongs hydrate induction time and reduces growth rates. Its kinetic inhibition performance surpasses that of conventional inhibitors [63].

Mollusks and crustaceans are species-rich marine groups with critical ecological roles [64] (Fig. 4(bi)). Their rigid shells are rich in chitin, which can be converted into chitosan through demineralization, deproteinization, decolorization, and deacetylation processes (Fig. 4(bii)) [65]. In animal feed, chitosan improves digestive function in young animals, promotes growth, reduces diarrhea and enhances reproductive performance and milk or egg quality in adults, and it is considered a potential alternative to antibiotics [66] (Fig. 4(biii)). In drug delivery, its biocompatibility, biodegradability, cationic nature and mucoadhesive properties enable the construction of nanocarriers, hydrogels, scaffolds and mucosal delivery systems [67]. In environmental applications, chitosan serves as an efficient adsorbent for the removal of heavy metal ions [68]. In addition, collagen extracted from fish scales and bones (Fig. 4(ci,cii)) is an important marine NP with good biocompatibility and mechanical performance. It has been widely used in tissue engineering, cosmetics, and medical materials and shows potential as a substitute in dental collagen-based applications [69] (Fig. 4(ciii)).

2.1.3 Extreme Natural Polymers (ENPs)

Extreme natural polymers (ENPs) are synthesized by extremophilic microorganisms in harsh ecological niches. Their habitats include deep-sea hydrothermal vents with high temperatures and pressures, hypersaline lakes, polar ice sheets, acidic mine drainage and highly alkaline salt lakes. To survive under extreme conditions and maintain physiological functions, ENPs have evolved unique and stable molecular structures. These structures resist thermal denaturation, pressure-induced collapse, salt-driven dehydration and degradation under extreme pH attack. As a result, ENPs exhibit high thermal stability, corrosion resistance and biocompatibility, which support their broad potential in industrial, biomedical, and environmental applications.

Exopolysaccharides (EPS) are heteropolysaccharides secreted by extremophilic microorganisms and represent key components supporting their adaptation to extreme environments [70]. For example, EPS produced by thermophilic microorganisms at deep-sea hydrothermal vents shows high thermal stability and resistance to denaturation. The strain *Bacillus licheniformis* B3-15, isolated from a shallow marine hydrothermal vent on Vulcano Island in Italy, secretes EPS to form a highly hydrated gel layer surrounding the cells. This layer buffers rapid temperature fluctuations and adsorbs heavy metal ions, thereby reducing toxicity. As a result, the microorganism can grow under extreme temperatures ranging from 45°C to 70°C [71]. In extremely low-temperature environments, psychrophilic microorganisms also rely on EPS for survival. These EPS typically exhibit high molecular weight (average ~16.2 MDa), and a high degree of branching (~56.7%). Such structural features create a viscous microenvironment that suppresses ordered water aggregation and ice crystal formation, thereby reducing freeze–thaw damage. EPS produced by the Antarctic strain SM20310 lowers the freezing point through its branched architecture and effectively protects cells during repeated freeze–thaw cycles [72]. In addition, the halophilic archaeon Haloferax mucosum (DSM 27191), isolated from Shark Bay in Australia, is capable of synthesizing the copolymer P(3HB-co-3HV). As salinity increases, the crystallinity of this copolymer rises, which slows the penetration of high extracellular NaCl concentrations into the cells and thereby markedly enhances stress tolerance [73].

NPs from extreme environments constitute an important reservoir of potential biological resources due to their unique molecular structures and adaptive functional mechanisms. They advance the understanding of biological adaptation under extreme conditions and provide new insights for expanding the application scope of functional materials.

2.2 Conventional Application Scenarios of NPs Materials

Materials based on NPs have consistently played an important role in societal development. Their application scale has expanded over time and has been continuously upgraded through technological progress. Owing to their wide availability, biodegradability and environmental compatibility, these materials are now widely used across agriculture, food and medical industries.

In agricultural production, NPs are mainly used in agricultural films, soil conditioners and plant growth regulators. Caputo et al. prepared a degradable sprayable coating by combining chitosan with galactomannan. The material showed strong inhibitory effects on weeds such as purslane, redroot pigweed, lamb's quarters and black nightshade, demonstrating significant potential for green and sustainable agricultural practices [74].

The film-forming ability and edibility of NPs enable their broad use in food processing and preservation. Isaiah et al. developed composite edible packaging films based on pork gelatin with glycerol, acetic acid and cellulose fibers. The films were characterized in terms of physicochemical properties, morphology, molecular structure and bioactivity. Compared with pure gelatin films, tensile strength and elongation at break were markedly improved to 61.84 MPa and 57.57%. In refrigerated pork packaging, the films maintained stable pH, inhibited microbial growth and lipid oxidation and thereby extended shelf life [75].

Pharmaceutical formulation and material development largely rely on the biocompatibility and controlled release behavior of NPs. Goswami et al. prepared linezolid-loaded calcium alginate lyophilized wafers for the treatment of diabetic foot ulcers. The wafers showed strong inhibitory activity against methicillin-resistant *Staphylococcus aureus*, with clinical cure and bacterial clearance rates comparable to vancomycin. The cumulative drug release reached 96.9 ± 0.1% within 24 h. The material absorbed wound exudate exceeding 3220% of its own weight and markedly improved the wound microenvironment. FTIR, DSC and XRD analyses confirmed good compatibility between the drug and excipients and high formulation stability. These results support the feasibility of NPs-based materials for local drug delivery in diabetic foot ulcer therapy [76].

The dependence of the textile industry on NPs is most evident in raw materials. NPs such as cotton fibers, wool and silk proteins have served as core textile materials for thousands of years. These materials provide goodwearing comfort and can be further functionalized through modern finishing technologies to impart wrinkle resistance, water repellency and antibacterial properties, thereby promoting the development of multifunctional textile products.

The development of biodegradable packaging materials is also a major research focus in the field of NPs. Akhtar et al. prepared high-performance biodegradable composite packaging films using carboxymethyl cellulose (CMC) as the film-forming matrix, mulberry leaf polysaccharides as additives and glycerol as a plasticizer. Optimized film thickness and moisture content significantly improved mechanical properties and degradability. The composite films exhibited notable antioxidant and antibacterial activity, with a maximum inhibition zone of 14.39 mm, and showed more than 50% weight loss after 21 days in soil. When applied to sunflower oil packaging, the films effectively delayed lipid oxidation, with a peroxide value of only 31.12 mA after 25 days, which was markedly lower than that of the control. These results further demonstrate the application potential of CMC-based composite films in biodegradable food packaging [77].

In papermaking, cellulose and hemicellulose have long been the primary raw materials for paper. The introduction of green chemistry and functional modification approaches enables the incorporation of NPs-based additives while preserving conventional mechanical strength and printability. These strategies improve water resistance, antibacterial performance and surface properties, thereby meeting the requirements of high-end functional paper products.

In construction and decorative materials, NPs are commonly used as matrices for coatings, adhesives and sealants to provide environmentally friendly protection for metal components under harsh conditions. A natural rosin-based hybrid sealant constructed from bio-based NPs and SiO_2–NH_2@GO nanocomposites significantly enhances the compactness and corrosion resistance of Fe-based amorphous coatings. The coating adhesion increases by 10.59%, porosity decreases from 6.2% to 1.1% and the decomposition temperature reaches 414.3°C. The three-dimensional NPs matrix works synergistically with GO sheets and SiO_2 nanoparticles to extend diffusion paths for corrosive species such as seawater, Cl^- and O_2 and to mitigate microcracks and pores induced by shrinkage, vibration or aging. Based on this mechanism, the rosin-based SiO_2–NH_2@GO hybrid sealant is suitable for marine service environments, including offshore oil and wind power platforms, pipeline exteriors, ship hull components near the waterline and steel housings of underwater ROVs and deep-sea sensors. After immersion in 3.5 wt% NaCl solution for 672 h, the corrosion current density is reduced by two orders of magnitude compared with unsealed coatings, demonstrating that NPs-based sealants can effectively extend coating service life [78].

NPs have established mature application foundations in agriculture, food, medicine, textiles, packaging, papermaking and construction. With the growing emphasis on green and low-carbon development and continued advances in modification and composite technologies, NPs retain substantial potential for functional expansion and performance enhancement. These advantages provide a solid basis for their extension into emerging application scenarios.

2.3 *Emerging Application Scenarios of NPs Materials*

NPs materials offer clear advantages in emerging technological and industrial applications because of their sustainable sources, favorable interfacial compatibility, and ease of precise functional regulation.

In biomedical applications, NPs are widely used in drug delivery systems, tissue engineering scaffolds and medical dressings due to their biodegradability and tissue compatibility. As a representative example, Chunlin et al. constructed tissue-engineering scaffolds by integrating a natural plant-derived component (fresh lotus root) with methacrylated gelatin (GelMA), yielding a stable porous structure and skin-like mechanical properties; the scaffold showed good cytocompatibility with human umbilical vein endothelial cells, low hemolysis, minimal inflammatory response, and notable antioxidant activity. In a mouse full-thickness skin wound model, GelMA scaffold accelerated wound closure and promoted neovascularization, re-epithelialization, and collagen deposition, restoring a more skin-like tissue architecture (Fig. 5a) [79].

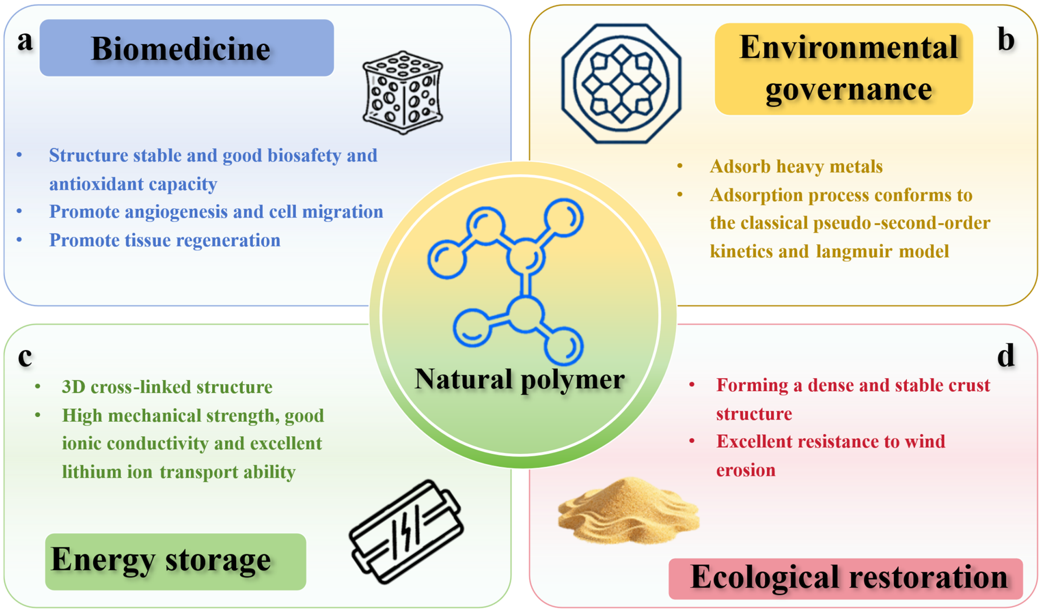

Figure 5: Application scenarios of NPs. (**a**) Biomedicine, (**b**) Environmental remediation, (**c**) Energy storage, (**d**) Ecological restoration.

In environmental remediation, NPs are widely used in wastewater treatment, soil remediation and air pollution control. This is due to their strong adsorption capacity and biodegradability. Youngeun systematically reviewed polysaccharide-based adsorbents for heavy metal removal. These materials were classified into homopolymers, blends, copolymers and composites. The study focused on chitin, chitosan, cellulose, starch and alginates. Functional modification has been shown to improve performance. The introduction of thiol and carboxyl groups by grafting or blending increases adsorption capacity and mechanical strength. Mechanistic analysis indicates that adsorption involves multiple interactions. These include π–π stacking, dipole–dipole interactions, hydrogen bonding and chelation. Adsorption kinetics and isotherms are well described by the pseudo-second-order models and the Langmuir isotherm (Fig. 5b). Repeated adsorption–desorption cycles demonstrate good regenerability and recovery efficiency. These results support a sustainable and cost-effective approach to heavy metal pollution control [80].

In the energy field, the application scope of NPs has further expanded. Dong et al. used chitosan and poly(ethylene glycol) diglycidyl ether (PEGGE) as precursors. A three-dimensional crosslinked chitosan–PEGGE gel polymer electrolyte (CP-GPE) was prepared by free-radical polymerization in an aqueous system. The material exhibits high mechanical strength, sufficient ionic conductivity at room temperature and good interfacial compatibility. These properties meet the requirements of solid polymer electrolytes for lithium-ion batteries. LiFePO4/CP-GPE cells show high initial discharge capacity and good cycling stability (Fig. 5c). Compared with conventional liquid electrolytes, commercial separators and PEO-based membranes, chitosan-based CP-GPE offers improved cycling stability and superior mechanical and thermal performance. The preparation process is also green and cost-effective, which enhances the overall safety of solid-state lithium battery systems [81].

Beyond energy and environmental applications, NPs also show broad potential in ecological management. Ankit Garg's group used sodium alginate, pectin and gum arabic to modify desert sand in India. The materials were applied by surface spraying, pouring or mixed compaction. The resulting biopolymer-modified sand exhibited enhanced mechanical strength. Experimental results showed a marked improvement in wind erosion resistance. Mass loss was negligible at wind speeds of 10–30 m s^{-1}. The average surface strength reached 313.81 kPa and a dense, stable crust was formed [82] (Fig. 5d). This strategy effectively improves sand stability and wind resistance and provides a practical approach to desertification control and soil improvement.

Owing to their structural diversity and tunable functionality, NPs have demonstrated distinct advantages in biomedicine, environmental remediation, energy storage and ecological restoration. They are increasingly emerging as key material systems supporting green manufacturing and sustainable development.

3 Extraction and Modification of NPs

NPs usually occur in nature as complex mixtures, and impurities are easily co-extracted from natural sources. These impurities can impair material performance or raise safety concerns. For example, cellulose extraction from plants requires effective removal of lignin and hemicellulose. Residual lignin causes darkening and reduces mechanical strength [83]. Chitosan production from shrimp and crab shells requires deproteinization and demineralization. Protein residues weaken antibacterial activity, while calcium carbonate residues reduce water solubility and biocompatibility [48]. In addition, the content of target polymers in natural feedstocks is often limited. Alginate typically accounts for only 12%–55% of seaweed biomass [84]. After water extraction followed by alcohol precipitation, alginate purity can exceed 90%. This approach markedly improves utilization efficiency [85].

In addition, many NPs exhibit insufficient mechanical strength and high brittleness. This limits their direct use as structural materials. Chitosan (CS) nanofibers are a representative example. Their intra- and intermolecular hydrogen bonds are easily disrupted, which leads to weak mechanical performance in standalone films. The incorporation of polyvinyl alcohol (PVA) as a flexible reinforcement improves toughness. Polyethylene glycol (PEG) can further regulate fiber morphology and hydrophilicity. These modifications markedly increase elongation at break and peel strength while maintaining high water absorption and air permeability. As a result, the performance of CS-based flexible films is significantly improved.

In terms of functional expansion, single-component NPs often fail to meet the multifunctional requirements of biomedical and smart materials. Native cellulose provides a typical case. Quaternary ammonium groups can be grafted onto cellulose, and silver nanoparticles can be introduced as functional fillers. Cellulose nanocrystals (CNCs) can also be oxidized to dialdehyde cellulose nanocrystals (DCNCs). Silver ions are then reduced *in situ* on the DCNCs to form DCNC–AgNP composites. These composites show both Pickering emulsion stability and antibacterial activity. When incorporated into chitosan films, they enhance mechanical strength and impart antibacterial activity. They also promote HaCaT cell migration and collagen synthesis. The resulting CS–PE–Qu composite films show no hemolytic effect and are promising for wound dressing applications [86].

Poor solubility and narrow processing windows are additional common challenges for many NPs. Chitosan is soluble in acidic aqueous solutions only when the degree of deacetylation exceeds 55%. Industrial applications usually require values above 70%. Chitosan is almost insoluble at pH values above 6.0. To address this issue, chitosan can be carboxymethylated with chloroacetic acid under alkaline conditions to obtain carboxymethyl chitosan (CMCS). Zwitterionic groups can be introduced along the polymer chain. This modification enables solubility in neutral water and maintains good solubility over a wider pH range. It substantially expands the application of chitosan in biomedical coatings and water-soluble wound dressings [87].

Extraction and modification of NPs transform natural materials into high-quality functional materials for specific applications. These processes are core enabling technologies that support the sustainable development of NPs-based materials in green manufacturing, biomedicine, and intelligent technologies.

3.1 Extraction Methods

NPs extraction methods are mainly classified into physical, chemical, and biological approaches. Conventional techniques are dominated by physical and chemical methods. These methods rely on different mechanisms for NPs separation and purification. Physical methods typically use heating, grinding, and filtration. A common example is starch extraction from plants by grinding followed by hot-water extraction. These methods are simple to operate and avoid chemical residues. However, they require high energy input and generate substantial waste streams (e.g., wastewater and solid residues). As a result, they are usually limited to laboratory or small-scale production and are less suitable for industrial applications.

Chemical methods use reagents to react with impurities or to alter the solubility of NPs for separation and extraction. Chitosan is typically obtained by acid demineralization of crustacean shells (e.g., using dilute hydrochloric acid), followed by precipitation and filtration [88]. Cellulose extraction commonly involves alkaline treatment to remove lignin and hemicellulose. Acid treatment is then used for further purification. These methods significantly improve extraction efficiency and broaden applicability [89]. However, they often rely on strong acids or bases. Such reagents cause equipment corrosion and secondary pollution. The toxicity of some chemicals also raises safety concerns. Reaction conditions therefore require strict control. Waste streams must be carefully treated.

Conventional extraction methods for NPs often suffer from low efficiency, poor selectivity, insufficient product purity and complex processes. They are also highly sensitive to raw material sources, which increases process uncertainty. Collagen provides a representative example. The yield and purity of acid extraction and enzymatic methods strongly depend on the feedstock. Collagen yields from marine fish skin and scales can reach about 50% of dry weight. Collagen from bovine cortical bone and Achilles tendon can achieve purities up to 96.12% with extraction yields of about 75.34%. However, the products often contain non-collagen proteins, lipids and minerals. Multiple purification steps are therefore required, including defatting, demineralization, dialysis and precipitation [90]. Chitosan is traditionally produced by chemical methods. These involve strong acid demineralization and high-temperature alkaline deacetylation. The yield is usually limited to 4.41%–30%. Problems such as uneven deacetylation and polymer chain degradation are common. In contrast, enzymatic methods enable controlled extraction under mild conditions. When shrimp shells are used as the feedstock, chitosan yields can reach 19.04%. The degree of deacetylation remains stable at about 74.9%. Product quality consistency is significantly improved [91].

Process parameters such as temperature, pH and time are critical for the extraction efficiency and quality of NPs. Chitosan illustrates this effect well. Temperatures above 280°C cause thermal degradation, chain scission and reduced molecular weight, which weaken antibacterial activity and biocompatibility. Excessively low temperatures reduce chitin deacetylase activity or acid dissolution rates and limit mass transfer, leading to poor extraction efficiency. pH must be selected according to the acid–base stability of the target polymer. Different NPs show distinct pH tolerances and require tailored optimization. Studies indicate that extraction temperatures are generally optimal in the range of 50°C–80°C, with pH further adjusted based on material characteristics [92].

With growing demands for economic efficiency and environmental sustainability, industry is increasingly seeking more cost-effective and greener extraction processes.

Modern Green Extraction Technologies

Under green and sustainable development requirements, the extraction of NPs is shifting from conventional boiling and acid–base or organic solvent processes to intensified mass transfer coupled with green solvent systems. Common strategies include ultrasound-assisted extraction (UAE), microwave-assisted extraction (MAE), supercritical carbon dioxide extraction (SFE-CO_2) and enzymatic extraction (EAE). These approaches are often combined with natural deep eutectic solvents (NADES) and ionic liquids (ILs), as well as membrane separation and nanofiltration, molecular distillation and electromagnetic field assistance. These techniques operate under mild conditions and improve selectivity, yield and purity. They also reduce energy demand and environmental burden and better preserve polymer structure and bioactivity. Representative conventional and green extraction technologies for NPs are summarized in Table 1, and representative modification technologies are compared in Table 2.

Table 1: Conventional and green extraction technologies for NPs.

Route	Technology/Method	Mechanism	Conditions	Advantages	Examples
Conventional extraction technologies	Physical method (heating, grinding, filtration, hot-water extraction)	Physical separation and particle size reduction	Heating, grinding, filtration, etc.	Simple process; no chemical residues	Hot-water extraction of starch from plant materials; common issues include low efficiency, insufficient purity, and process complexity.
	Chemical method (acid, base, organic solvents)	React with impurities or change solubility to achieve separation	Strong acids/bases, solvents; acid/base cooking, precipitation, filtration	High extraction efficiency; broad applicability	Chitosan: demineralization with dilute HCl, followed by precipitation and filtration. Cellulose: alkali cooking to remove lignin and hemicellulose, followed by acid purification. Collagen: yields from fish skin and scales ≈50% of dry weight; bovine cortical bone purity up to 96.12%; bovine Achilles tendon extraction yield ≈75.34%, but requires multistep purification such as defatting, demineralization, and dialysis. Chitosan via chemical routes yields 4.41%–30%, with uneven deacetylation and chain degradation.
	Enzymatic extraction	Enzymatic hydrolysis to gently release target components	Appropriate temperature and pH; enzyme activity optimization	Mild; high selectivity; controllable product quality	Chitosan: enzyme activity 40.69 U/mL; shrimp shell yield 19.04%; degree of deacetylation 74.92%; crystallinity 21.16%.
Modern green extraction technologies	Ultrasound-assisted extraction (UAE)	Cavitation enhances solvent penetration and cell wall disruption, improving mass transfer	Power, frequency, time	Shorter time; higher yield or recovery	Bee pollen protein: reduced particle size; increased random coil content; increased surface hydrophobicity; extraction yield, solubility, emulsion stability, and digestibility significantly improved.
	Microwave-assisted extraction (MAE)	Directional heating of polar molecules accelerates diffusion and release	Low temperature, atmospheric pressure; short-time high-energy coupling	Fast; low energy consumption; minimal thermal damage	Sugarcane bagasse hemicellulose: practical yield 72.9% (theoretical 77.2%), about 35% higher than hot-water extraction.
	Supercritical CO_2 extraction (SFE-CO_2)	Tunable solvating power; low-temperature, residue-free; high selectivity	Adjustable processing window; optional modifiers	Suitable for heat-sensitive components; high selectivity and purity	Pomegranate peel phenolics: 4362 vs. 2554 mg GAE/100 g (+70.8%); antioxidant capacity enhanced.

(Continued)

Table 1 (continued)

Route	Technology/Method	Mechanism	Conditions	Advantages	Examples
	Enzymatic extraction (EAE)	Selective cleavage of chemical bonds while preserving activity	Aqueous phase; enzyme system optimization	Preserves activity; high purity; mild conditions	Protein purity about 55%, higher than several neutral or flavor protease schemes by 20%–25%.
	Natural deep eutectic solvents (NADES)	Biocompatible deep eutectic system for selective dissolution; can synergize with UAE	Designable composition (e.g., choline chloride:ethylene glycol = 1:3 + 25% water)	Renewable solvent; high selectivity; low energy demand	Abalone viscera polysaccharides (AVP): yield 16.84 ± 1.32%; sugar content increased from 39.47% to 58.76%; Mw reduced to 53.33 kDa; DPPH IC50 0.50 to 0.17 mg/mL.
	Ionic liquid aqueous two-phase system (IL-ATPS)	Imidazolium and other ionic liquids form ATPS for mild separation	High water content; tunable phase equilibrium; solvent and salts recyclable	Strong solvation or selectivity; low volatility; recyclable	Alginate/BSA separation: yields 90%/89%; purity 99%; solvent/salt recovery 99.9%.

Table 2: Comparison of modification technologies for NPs.

Route	Method	Mechanism/Object	Example	Key Performance Improvements	Limitations
Physical modification	Thermal treatment	Temperature-induced chain rearrangement, phase transition, and crystallinity control; no change to main-chain chemical bonds	PMMA/PVDF composite film, 120°C; PVDF:PMMA = 5.5:4.5	Breakdown strength 389 → 729.42 MV m^{-1}; energy density 7.47 → 21.12 J cm^{-3}; discharge efficiency 42.1% → 64.8%; dielectric loss essentially unchanged	Requires precise temperature and phase-behavior control to avoid phase instability
	Irradiation	Induces free-radical grafting and crosslinking; increases structural integrity and network density	Chitosan/acrylic acid; Gammacell 220; water radiolysis generates eaq^{-} and •OH	pH-responsive hydrogel; nanoparticles 30–200 nm; swelling ratio ≈ 750% at pH 5; yield increase in agricultural application	Scale-up challenges in dose and uniformity; control of residual radicals
	Mechanical processing	Screw extrusion changes segment orientation and rearrangement, and densifies morphology	Whole potato flour (WPF) extrusion pre-treatment	Crystallinity to 44.53%; pore size reduced to 73.21 μm; 3D printing accuracy 94.75%; storage modulus G' to 6583.67 Pa	Sensitive to feedstock moisture and temperature rise; scale-up requires steady-state control
	Ultrasound (ultrasound-assisted treatment, UAE)	Cavitation and shear disrupt aggregates; depolymerization–reassembly and interfacial strengthening	WPI–soy milk composite system, 400 W	Yield to 42.26%; tensile strength 1.62 MPa (+8%); elongation at break 58.87%	Requires optimization of acoustic field distribution and thermo–mechanical coupling
	Freeze-drying	Low-temperature vacuum sublimation removes solvent while preserving porous structure	m-CNF/SA-c; bidirectional freeze-drying + ionic crosslinking + MTMS	Porosity 97.85%; density 24.2 mg cm^{-3}; oil–water separation capacity 88.91 g g^{-1}; water contact angle (WCA) 144.5°; compressive stress 340 kPa at 90% strain; >60% stress retention after 50 cycles	High energy use and long cycle time; challenges in scale-up molds and crack control

(Continued)

Table 2 (continued)

Route	Method	Mechanism/Object	Example	Key Performance Improvements	Limitations
Chemical modification	Esterification/ transesterification	Introduces ester groups to increase hydrophobicity and thermal stability and improve processability	Cellulose + acetic anhydride to obtain cellulose acetate (CA); lipase-catalyzed transesterification with methyl myristate	WCA 20°–30° → 117 ± 9°; paper-based composites show markedly improved water and oil resistance	Cost and recovery of enzymatic catalysts
	Amidation	Introduces amide groups or amino-containing segments on side chains; tunes hydrophilicity and bioactivity	Chitosan hydrochloride (CSH) + 6-aminohexanoic acid (AA)	Solubility 11.39% → 32.34% (w/v); dissolution rate ×6.46; MIC (μg mL^{-1}) *E. coli* 125 → 75 and *S. aureus* 175 → 75; mouse hemostasis blood loss 0.062 ± 0.013 g; degradable within 30 d	Control of reaction selectivity and crosslinking side reactions
	Hydroxyalkylation (HE/HP)	Introduces $-CH_2CH_2OH$ and $-CH_2CH(OH)CH_3$ groups; increases chain mobility and solubility	Hydroxyethylated cellulose; hydroxypropylated chitosan; hydroxypropyl guar with DS ≈ 0.8	Cellulose solubility <1% → 15.6 ± 0.8%; 24 h viscosity drift 5.2%; HP-CS solubility at pH 7.4 is 28.3 ± 1.2% with cell viability >92.5%; HP-Guar consistency index K = 650 ± 20 Pa·s; applications include encapsulation 86.7%, adhesion 90%, water uptake 700%	Degree of substitution (DS) uniformity and solubility–strength trade-off
	Quaternization	Introduces quaternary ammonium cations; provides antibacterial activity and positive surface charge	ECNC template grafting with C8–C16 quaternary ammonium salts; PVA blended films	Antibacterial rate (*E. coli*, *S. aureus*) ≥ 99.9%–100%; extended freshness period (strawberries)	Cation migration and leaching; food-related regulations
	Sulfonation	Introduces $-SO_3H$ groups; increases hydrophilicity and enhances proton conduction and ion-exchange capacity	sCS/SiO_2 blended into PVDF; sPES composite with zwitterionic polymers	Ion-exchange capacity (IEC) 0.97 meq g^{-1}; proton conductivity σ (H^+) 1.06×10^{-2} S cm^{-1}; tensile strength 37.91 MPa; thermal stability below 500°C; WCA 59.2°; microbial fuel cell (MFC) power output increased and crossover permeation decreased	Balance between degree of sulfonation and mechanical or chemical resistance; methanol permeation resistance

UAE uses acoustic cavitation to enhance solvent penetration and disrupt cell walls, thereby promoting the release of macromolecules. Ultrasound can markedly damage plant cell wall structures. It also shortens extraction time and increases product yield. Li et al. applied an ultrasound-assisted enzymatic process to Camellia bee pollen. Cavitation reduced the particle size of the extracted proteins. It increased the proportion of random coils. It also increased surface hydrophobicity. These changes significantly improved protein yield, solubility, emulsion stability and digestibility [93].

MAE uses directional heating of polar molecules to accelerate diffusion and release. In hemicellulose extraction from sugarcane bagasse, MAE provides higher yields than hot water extraction or steam explosion. It also reduces high-temperature degradation. The practical yield reached 72.9%, which is about 35% higher than hot water extraction [94].

SFE-CO_2 offers tunable solvating power, low-temperature operation, no solvent residue and high selectivity. It is suitable for extracting heat-sensitive components. Phon et al. used carbon dioxide acidified water under supercritical conditions to recover collagen and gelatin from striped catfish skin and bones. The yields were about 36.9% and 8.1%, respectively. The process preserved the collagen triple-helix structure and thermal stability under mild conditions [95].

EAE uses water as the medium and provides high specificity. Enzyme systems can be optimized to balance purity and functional retention during protein extraction. In one study, alkaline protease produced proteins with a purity of about 55%. This value was higher than that obtained with several neutral or flavor protease systems [96].

NADES are green solvent systems built from natural components. They provide selective solubilization, biocompatibility, and renewability. Their formulations are also flexible and have a low environmental burden. Qu et al. used a choline chloride–ethylene glycol NADES at a molar ratio of 1:3 with 25% water. They combined it with ultrasound-assisted extraction to obtain polysaccharides, AVP (abalone viscera polysaccharides), from *Haliotis discus* hannai viscera. The yield reached 16.84 ± 1.32% and was about twice that of the boiling water bath method. The AVP content increased from 39.47% to 58.76%. The glucuronic acid proportion and antioxidant activity also increased. The DPPH scavenging IC_{50} decreased from 0.50 to 0.17 mg mL^{-1}. This strategy supports green and high-value utilization of marine by-products [97].

Dissolution using ILs is a green extraction approach with strong solvating power, high selectivity and recyclability. They are effective for separating complex biopolymer mixtures. Antunes et al. used an alginate and bovine serum albumin (BSA) model system to compare ILs. Water-insoluble phosphonium ILs such as trihexyl(tetradecyl)phosphonium bromide recovered about 86% of BSA by precipitation. Imidazolium ILs such as 1-butyl-3-methylimidazolium chloride, abbreviated as [BMIM][Cl], formed an ionic liquid aqueous two-phase system under high-water conditions. This system reduced protein denaturation and enabled efficient separation. The yields of alginate and BSA were about 90% and the purity reached 99% [98]. Extraction and separation using ILs have been increasingly reported as green approaches. Ionic liquid aqueous two-phase systems (IL-ATPS) show thermal stability, low volatility and strong tunability. They enable efficient and sustainable separation of NPs under mild conditions. This approach provides a practical route for green extraction.

Beyond the major methods, emerging external-field assisted techniques include electric field assisted extraction [99] and magnetically assisted extraction [100]. They introduce electrical or magnetic energy to enhance mass transfer and improve selectivity under mild conditions. With coordinated optimization of solvent systems and energy input, the extraction of NPs is moving toward greener and more efficient processes. This shift supports functional development and sustainable utilization. Cross-disciplinary integration in green chemistry, materials science and process engineering can facilitate scalable transfer from laboratory studies to industrial implementation.

3.2 Modification Methods

3.2.1 Physical Modification

Physical modification is an important approach for regulating the structure and properties of NPs, by altering the physical state, molecular orientation, and microstructure without breaking or forming main-chain chemical bonds. Common methods include thermal treatment, irradiation, mechanical processing, ultrasound treatment, and freeze-drying.

Thermal treatment controls temperature to induce chain rearrangement, crystal phase transitions, and changes in crystallinity. It is an effective way to regulate structural order and energy stability in NPs. In starch, thermal treatment adjusts the crystalline and amorphous fractions and thereby tunes gelatinization behavior and mechanical properties. Zhang et al. applied thermal treatment to PMMA/PVDF composite films to convert PVDF from the nonpolar α phase to the polar β phase and the weakly polar γ phase. At 120°C and a PVDF:PMMA ratio of 5.5:4.5, breakdown strength increased from 389 to 729.42 MV m^{-1}. Energy density increased from 7.47 to 21.12 J cm^{-3}. Discharge efficiency increased from 42.1% to 64.8%. Residual polarization decreased to 1.48 μC cm^{-2}. Dielectric loss remained nearly unchanged over a wide frequency range [101]. These results show that controlled orientation and phase regulation can improve the dielectric and energy-storage performance in NPs-based materials composites.

Radiation modification uses γ-rays, electron beams or X-rays to generate polymer radicals. These radicals drive grafting or crosslinking. This process tunes molecular structure and material properties. In a chitosan and acrylic acid system, a homogeneous solution was irradiated using Gammacell 220. Water radiolysis produced hydrated electrons (eaq^-) and hydroxyl radicals (•OH). These species initiated acrylic acid grafting onto chitosan at C-1 and C-4 sites. The CS–PAA network was formed. The electron-beam hydrogel showed pH responsiveness. Swelling depended on pH and irradiation dose. The resulting CS–PAA IPC nanoparticles were spherical and their size ranged from 30 to 200 nm. The maximum swelling reached 750% at pH 5. In sandy soil slow-release nitrogen fertilizer tests, maize height increased by 122 ± 21% compared with conventional fertilization. These results support radiation-induced grafting and crosslinking for agricultural functional materials [102].

Mechanical modification uses energy input to alter the physical structure of NPs. It drives segment orientation, chain rearrangement and morphology control. Wang et al. applied twin-screw extrusion to physically modify whole potato flour (WPF). The proportion of A chains decreased and the proportion of long B chains increased. Relative crystallinity increased to 44.53%. Free water decreased and bound water increased. The porous network became denser and the average pore size decreased to 73.21 μm. After modification, the 3D printing accuracy reached 94.75%. The storage modulus (G') increased to 6583.67 Pa. The material showed improved rheological suitability and structural stability. These results confirm the utility of mechanical processing for NPs functionalization [103].

Ultrasound modification uses cavitation to generate local high temperature, high pressure and strong shear. These effects disrupt aggregates, promote molecular depolymerization and recombination and strengthen interfacial interactions. In a WPI–soy milk composite system, Chen et al. found that ultrasound induced protein dissociation and reassembly. More hydrophobic groups and free thiols became exposed and β-sheet content increased. A denser and more stable protein network was formed. At 400 W, the yield increased to 42.26%. The tensile strength reached 1.62 MPa, about 8% higher than that of the untreated group.

The elongation at break remained at 58.87%. These results show that ultrasound can significantly improve structural stability and processing performance in bio-based composites [104].

Freeze-drying removes water by solvent sublimation under low temperature and vacuum. It preserves the microstructure without changing the chemical composition and yields highly porous, low-density materials. Liu et al. used bidirectional freeze-drying combined with ionic crosslinking and methyltrimethoxysilane (MTMS) hydrophobic modification to prepare cellulose nanofiber and sodium alginate composite aerogels (m-CNF/SA-c). The aerogels showed a porosity of 97.85%, a density of 24.2 mg cm^{-3}, a maximum adsorption capacity of 88.91 g g^{-1}, and a water contact angle of 144.5°, indicating excellent oil–water separation performance. The compressive stress reached 340 kPa at 90% strain, and more than 60% of the stress was retained after 50 compression cycles. These results show that freeze-drying is effective for constructing structurally stable functional porous NPs-based composites [105].

Physical modification can optimize properties by regulating physical states. It does not enable the precise introduction of specific functional groups. It also cannot construct complex molecular architectures. These limitations hinder its use in high-end functional materials. Such materials require tailored functional groups and strengthened interfacial interactions. Chemical modification is therefore needed for molecular-level precision control. It is a key step for expanding the functional scope of NPs.

3.2.2 Chemical Modification

Chemical modification is a core strategy for precise optimization of the physical, chemical, and biological properties of NPs. It works by introducing, transforming, or regulating functional groups within NPs. Common reactions include esterification, amidation, hydroxyalkylation, quaternization, and sulfonation. These reactions can tune key properties. They can improve thermal stability and mechanical strength. They can also regulate hydrophilicity, hydrophobicity and antibacterial performance. As a result, chemical modification enables functional expansion of NPs-based materials.

Esterification is widely used to increase the hydrophobicity and thermal stability of NPs. Esterification of cellulose with acetic anhydride yields cellulose acetate (CA). CA shows good transparency and processability. It is widely used in films and packaging materials. Sharma et al. performed lipase-catalyzed transesterification between cellulose and methyl myristate. They obtained cellulose fatty acyl derivatives with markedly improved hydrophobicity. The water contact angle increased from 20°–30° to 117° ± 9°. When applied in paper based composites, water and oil resistance improved substantially. The spreading areas of water and oil droplets decreased by about 50% compared with unmodified paper. This material can serve as a functional component for green paper packaging [106].

Amidation introduces amide bonds and amino-containing segments on NPs side chains. It can tune hydrophilicity and bioactivity. Chen et al. reacted chitosan hydrochloride (CSH) with 6-aminohexanoic acid (AA). Amide and ester linkages were introduced on hydroxyl and amino groups. The amino group of AA increased surface positive charge and weakened intermolecular hydrogen bonding. Water solubility improved markedly. Solubility at 25°C increased from 11.39 ± 0.98% to 32.34 ± 1.23% (w/v). The dissolution rate increased by 6.46-fold. Antibacterial activity also improved. The MIC against *E. coli* and *S. aureus* decreased to 75 μg mL^{-1}. In a mouse liver bleeding model, blood loss was 0.062 ± 0.013 g. The material showed antibacterial and hemostatic functions. It also showed good biocompatibility and degradability. It degraded almost completely within 30 days. It is suitable for wound repair applications [107].

Hydroxyalkylation introduces hydroxyethyl or hydroxypropyl groups onto NP chains. It increases segment mobility and solubility and also improves solution stability and processability. Hydroxyethylated cellulose shows much higher water solubility. Solubility increases from less than 1% (w/v) to 15.6 ± 0.8%

(w/v). Viscosity drift over 24 h is about 5.2% and the solution shows shear-thinning behavior. Hydroxypropyl chitosan reaches a solubility of 28.3 ± 1.2% (w/v) at pH 7.4. Cell viability remains above 92.5%. Hydroxypropyl guar shows suitable rheology at a degree of substitution of 0.8. The consistency index K is about 650 ± 20 Pa·s. Hydroxyalkylated NPs have been used in drug delivery, tissue engineering and wound dressings. Encapsulation efficiency can reach 86.7%. Cell adhesion can reach about 90%. Water uptake can reach 700% [108].

Quaternization introduces positively charged quaternary ammonium groups onto NPs surfaces or side chains. It can markedly enhance antibacterial activity. Using esterified cellulose nanocrystals (ECNC) as a template, Meng et al. grafted tertiary-amine-derived quaternary ammonium salts with different alkyl chain lengths from C8 to C16 to obtain ECNC-Qn. The antibacterial mechanism involves electrostatic interactions between quaternary ammonium cations and negatively charged bacterial membranes. It also involves hydrophobic insertion and disruption of the membrane by the alkyl chains. ECNC-Qn achieved inhibition rates of at least 99.9% against *E. coli* and *S. aureus*. PVA-blended PVA/ECNC-Qn films retained high antibacterial performance. They also suppressed microbial proliferation during strawberry storage and delayed quality deterioration. These results support practical applications in food preservation and packaging systems [109].

Sulfonation introduces–SO_3H groups onto NPs chains. It markedly increases hydrophilicity and ion exchange capacity. Sulfonated chitosan (sCS) provides a representative example. Blending sCS with functionalized SiO_2 and incorporating the mixture into PVDF enables the fabrication of proton exchange membranes (PEMs). These membranes maintain high proton conductivity and show improved mechanical strength. Proton-conducting membranes can also be prepared by radical copolymerization of zwitterionic polymers with sulfonated polyethersulfone. These membranes exhibit good tensile strength, thermal stability and surface hydrophilicity. Higher degrees of sulfonation further enhance anti-biofouling performance. Such materials perform well in microbial fuel cells, direct methanol fuel cells, alkaline fuel cells and electrochemical energy conversion systems coupled with wastewater treatment [110].

Chemical modification introduces new functional groups and reconstructs covalent structures in the main chain or side chains. It changes the chemical composition and interfacial energy state of NPs at the molecular level. This enables targeted property control and functional expansion. Stable covalent bonds can improve thermal stability, mechanical strength and chemical durability. Chemical routes often require harsh conditions, solvent dependence and by-product management. Physical modification uses external fields such as heat treatment, plasma, irradiation and mechanical stress. It regulates microstructure and molecular orientation. The process is simpler, more environmentally compatible and leaves no chemical residues. Its effects are often less deep and may show limited long-term stability.

Material design should select and combine both strategies based on application needs. Physical modification supports rapid surface and morphology control. Chemical modification enables structural reconstruction and durable performance. Their combination can support more sustainable NPs material systems for biomedicine, energy devices and functional packaging (Fig. 6).

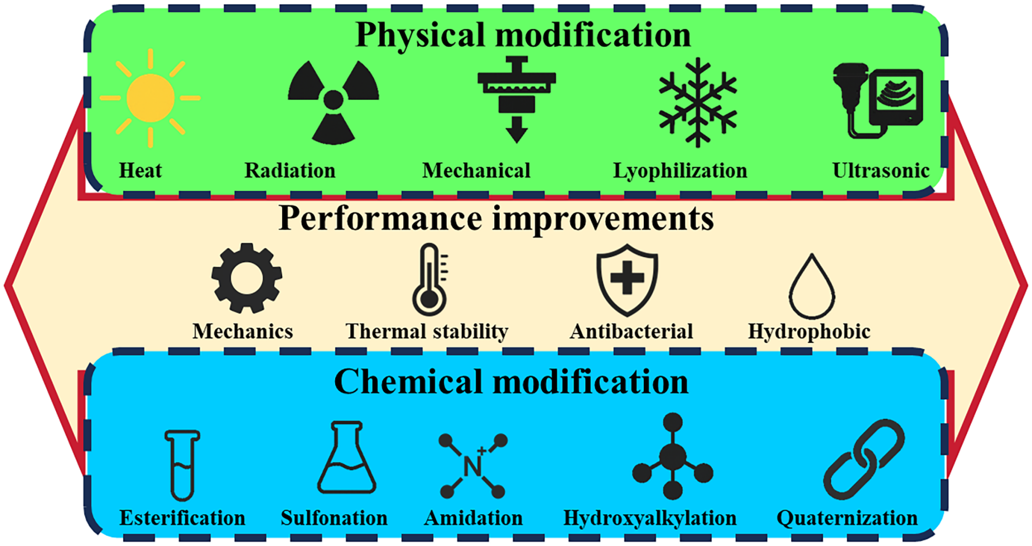

Figure 6: NPs modification pathways and performance enhancement.

4 AI-Enabled Structural Analysis and Modification Optimization of NPs

4.1 Artificial Intelligence for NPs Optimization

In recent years, artificial intelligence (AI) has introduced new paradigms for the structural design, property prediction and process optimization of NPs. Conventional studies rely heavily on repetitive experiments and empirical screening. This approach is time-consuming and costly. It also rarely reveals the relationships between structure and properties in a systematic manner. Machine learning, deep learning and data mining enable model development from multi-source datasets. These models link structure, processing conditions and performance. They quantify macroscopic properties such as mechanical, thermal and dielectric behavior. They also quantify structural descriptors such as crystallinity, pore architecture and phase morphology. These models support property prediction. They also enable formulation optimization and process parameter optimization. Inverse design and experiment planning can be implemented as well.

AI has shown strong capability in modeling polymer structure and properties for performance prediction. Malashin et al. built a database covering 18,311 polymers and 66,981 records of thermal, mechanical, electrical and optical properties. They used RDKit to convert SMILES (simplified molecular input line entry system) into 1024-bit fingerprints. They evaluated multiple regression algorithms using R^2, MSE, MAE and RMSE. Random forest achieved the best overall performance. It obtained R^2 values of 0.88 for glass transition temperature, 0.73 for thermal decomposition temperature and 0.71 for melting point. To address missing labels, they proposed predictive imputation. The model filled missing parameters and used variance to estimate confidence. This approach formed a scalable data-driven framework and provided methodological guidance for NPs databases and model selection [111]. A similar framework can be applied to NPs. Structural descriptors can be extended from SMILES and fingerprints to sequence features and supramolecular parameters of polysaccharides and proteins. This extension can support thermal and mechanical property prediction for NPs.

Beyond property prediction, AI also supports the design and optimization of NPs-based drug carriers. Models can learn noncovalent interactions between carriers and drugs and predict binding capability. These predictions guide the selection of anchoring sites, surface functional groups, and backbone structures. Generative adversarial networks (GAN) can generate candidates such as modified cellulose carriers with good water dispersibility and biocompatibility. Machine learning models have also been applied to drug-delivery studies. Random Forest (RF), Support Vector Machines (SVM), and LightGBM have been used to classify solid dispersion stability, identify drug interactions and fit release behavior of long acting injectables. Long short-term memory networks (LSTM), graph neural networks (GNN), and artificial neural networks (ANN) are used to generate pharmacokinetic concentration time profiles, predict binding affinity and optimize 3D-printed tablet processes. Bayesian models improve the use of low concentration data [112]. For chitosan, alginate and gelatin carriers, these models can screen optimal degrees of substitution, crosslinking and formulation ratios and reduce experimental workload.

Overall, data-driven modeling and intelligent optimization are moving NPs research toward more systematic and predictable workflows. They link structure, processing conditions and performance using multi-source experimental data and complex structural descriptors. This linkage enables accurate property prediction and controllable structural optimization. Progress in data integration, model interpretability and adaptive algorithms is strengthening these approaches. Data-enabled modification is becoming a key support for structure design, synthesis route planning and functional regulation. It offers efficient, cost effective and sustainable solutions for biomedicine, functional packaging and green energy applications.

4.2 Artificial Intelligence for Modification Process Optimization

AI-driven computational methods are increasingly applied to chemical, physical and biological modification of NPs. In chemical modification, deep learning and pattern recognition can jointly model variables such as temperature, time and catalyst type and concentration. These models predict reaction outcomes and optimize conditions using large experimental datasets. Park et al. combined the chemical markdown language (CMDL), the IBM Materials Notebook extension and a regression Transformer model. The model was pretrained on ChEMBL and USPTO data and then fine-tuned. CMDL polymer graphs were used to encode structures and continuous flow conditions. They generated about 2.5 million monomer and catalyst combinations. The model predicted ring-opening polymerization conversion and dispersity with correlation coefficients above 0.8. Experiments showed that selected catalyst systems achieved near complete monomer conversion within four minutes and produced polymers with dispersity of ~1.15. This approach can substantially shorten process exploration for chemical modification and polymerization [113].

In physical modification, AI is often combined with molecular dynamics and multiscale simulation. The goal is to link microstructural evolution under external fields to macroscopic mechanical behavior. Chen and Xu developed a framework for SiC fiber-reinforced SiC composites (SiCf/SiC). The framework integrated high-throughput molecular dynamics, a generative adversarial network and a genetic algorithm. Shear stress and strain data were generated under varied interfacial morphologies, PyC layer numbers and defect densities. These data were used to train the model. The generative model learned the nonlinear relationship between interface structure and shear performance. Prediction errors were about 1.6%–4.0%. A genetic algorithm then performed inverse search at 900 K to identify interface parameters that meet target shear properties. This strategy enabled rapid bidirectional mapping between interfacial microstructure and mechanical response [114]. Similar approaches can be extended to ultrasound and microwave-assisted modification. They can model and optimize frequency, power and treatment time. This enables finer control of NPs structure and properties.

In biological modification, AI is mainly used to screen and engineer enzymes and microbial systems. The goal is to improve the efficiency of NPs degradation or functionalization. Zhongbiao Tan et al. summarized this area into process optimization and molecular engineering. In process optimization, machine learning integrates variables such as fermentation temperature, pH, agitation, aeration, medium composition and immobilization parameters. This approach can increase lipase yield and stability and maintain reproducibility during scale-up. In molecular engineering, models link amino acid sequences and three-dimensional structures to catalytic performance. Hybrid quantum mechanics and molecular mechanics calculations and convolutional neural networks help identify key active residues. These tools guide mutation design and improve activity, enantioselectivity and thermal stability. Feedforward neural networks and support vector machines have also been used to optimize immobilization and mutation parameters. In some cases, lipase thermostability increased by an order of magnitude [115].

Overall, AI can integrate structural information, process conditions and performance metrics within a unified framework. It supports condition screening, interface and backbone design and biocatalytic system optimization. These capabilities are shifting NPs modification from empirical trial and error toward data-driven and model-guided rational design.

4.3 AI Based Mechanistic Analysis of NPs Functions

AI technologies also show strong potential for elucidating the functional mechanisms of NPs functions. Machine learning, deep learning and data mining can systematically analyze structural features, functional responses and interactions with the environment. These approaches can reveal latent patterns and governing factors. Recent advances at the interface of computational chemistry, bioinformatics and materials science have further accelerated progress in this area.

Data-driven methods are becoming important tools for quantifying relationships between structure and performance in molecular structure analysis and property prediction. Tashiro et al. investigated systems with different vinyl acetate contents. They processed spectroscopic and diffraction data using baseline correction, peak separation and integrated absorbance to distinguish hydrogen bond types. Lambert–Beer quantification was then used to obtain the critical continuous sequence length for vinyl acetate crystallization. This approach improved the accuracy of X-ray diffraction peak extraction and complex identification. It also supported process parameter setting for polarizing films [116]. Mulla et al. described multiscale features of natural fiber polymer (NFP) and poly(lactic acid) (PLA) composites using DScribe descriptors, Coulomb matrices and many-body tensor representation. They trained convolutional neural networks, deep multilayer perceptrons and random forest models to predict performance. Random forest achieved an R^2 close to 0.99 for glass transition temperature prediction. A k-nearest neighbors model (KNN) further quantified the relationship between three-dimensional printing parameters and porosity [117]. Combining detailed structural descriptors with machine learning models can strengthen quantitative structure–performance analysis in NPs systems.

In mechanistic analysis and application optimization, Chen et al. built a dataset that covered hydrogel composition, functional parameters and wound microenvironment indicators. They used machine learning to quantify the matching between materials and the microenvironment. They also differentiated the requirements of inflammation mitigation and tissue repair across healing stages. They then aligned drug release kinetics with the wound healing trajectory. This strategy yielded a predictable formulation system for diabetic wound therapy [118]. In degradation mechanism studies, multivariate models were built by integrating biochemical oxygen demand (BOD), molecular dynamics outputs, atomic volume, electrotopological indices and functional group descriptors. The models quantified the relationship between structural features and degradation rate. They indicated a strong negative association between chlorinated cyclic structures and degradation rate. The correlation coefficient was about 0.68 in magnitude and negative in sign. Cumulative local effect analysis and Williams plot diagnostics supported model robustness. The results highlight key roles of topology, functional group identity and electron localization in the design of degradable polymers [119].

Integration and modeling of multidimensional experimental data are advancing mechanistic studies of NPs toward higher precision and stronger system-level understanding. This approach improves analysis efficiency and predictive capability. It also provides quantitative decision support for structural optimization, functional regulation and application expansion. An overview of the AI-enabled research framework for NPs is shown in Fig. 7.

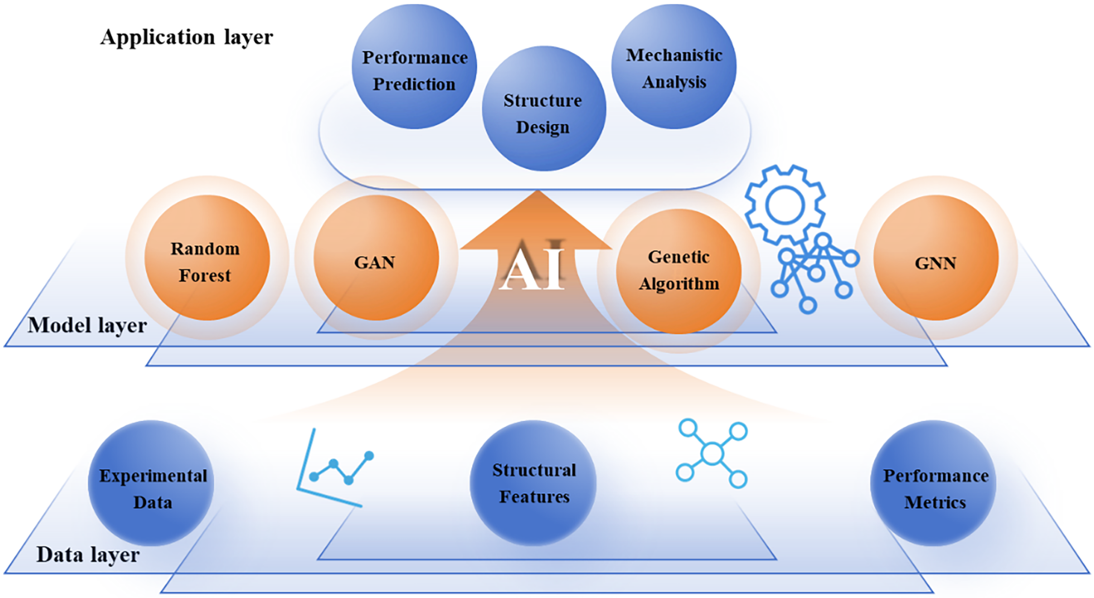

Figure 7: AI enabled research framework for NPs.

4.4 Current Bottlenecks and Future Research Directions

Despite the rapid progress of NPs in extraction, modification, and functional applications, several bottlenecks still limit their broader translation. A central challenge lies in the inherent variability of natural feedstocks and the resulting fluctuations in composition, purity, and performance, which reduce reproducibility and complicate the establishment of unified standards for pretreatment, processing, and quality evaluation [120–122]. Another major bottleneck concerns the industrial implementation of green solvent and process systems. Although DES/NADES-based strategies and assisted extraction technologies have demonstrated clear advantages at the laboratory scale, their robustness across different feedstocks, solvent recyclability, water-content sensitivity, scale-up feasibility, and cost-effectiveness still require more systematic validation under practical manufacturing conditions [123,124]. Mechanistic understanding also remains limited in many NPs systems, especially those involving multicomponent assemblies, hierarchical architectures, and dynamic intermolecular interactions, which restricts the transition from empirical screening to rational design [125,126]. At the application level, current studies often emphasize enhancement of a single target property, while the trade-offs among mechanical strength, thermal stability, moisture resistance, degradability, and long-term service stability are not yet sufficiently addressed [121,122,127]. For translation into biomedical and other high-value applications, more rigorous evaluation is still needed regarding degradation behavior, biocompatibility, and real-use performance, so that material safety and functional reliability can be assessed in a more application-relevant manner [128,129]. Future progress will depend not only on improved material and process design, but also on the development of standardized datasets, reliable polymer representations, and AI-assisted modeling frameworks that can better support structure–property prediction, reverse design, and reproducible optimization [125,130–132].

5 Conclusions

NPs are sustainable materials that have advanced rapidly through multidimensional innovation. Their diverse sources, including cellulose, lignin and alginate, enable broad functional adaptability. Green extraction and modification technologies, including ultrasound-assisted processing and ionic-liquid-based systems, have improved material performance. AI approaches, including machine-learning-based prediction and generative-adversarial-network-driven structural optimization, have further enabled precise and efficient design. Despite these advances, large-scale implementation remains constrained. Green processes can incur high costs. Precise regulation of complex structures is still challenging. Long-term stability in high-end applications remains insufficient. Future work should be guided by life-cycle-based principles. Recyclable solvent systems should be developed and integrated with process intensification and continuous manufacturing. Feedstock standardization and pretreatment specifications should be established. Online process analytics and closed-loop control should be deployed. Multifunctional integration should be strengthened. Unit production costs should be reduced, and scale-up cycles should be shortened. Looking ahead, several challenges still need more attention. These include improving reproducibility and standardization, making scale-up more practical, enhancing solvent and process robustness, and developing a clearer understanding of structure and performance relationships. Better ways are also needed to balance different properties without sacrificing long-term stability. At the same time, stronger evidence for safety and practical translation, along with more quantitative sustainability assessment and standardized datasets, will be important for supporting reliable data-driven optimization and wider real-world application.

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