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Review article

Recent advances in the applications of nanocellulose for sustainable development

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Abstract. The environmental and ecological concerns drive researchers to synthesize functional materials using components from natural resources. Nanocellulose (NC), derived from plants, marine animals, or microorganisms, is a green material attracting attention due to its abundance, biocompatibility, and biodegradability. NC's interstice properties enable the synthesis of functional nanocomposites in forms like aerogels, foams, paper, sheets, or hollow filaments. This review briefly describes NC classification and production while comprehensively presenting its mechanical, rheological, optical, and electrical properties, offering foundational knowledge for future research. Additionally, it highlights recent developments in NC-based products across fields such as papermaking, water treatment, civil engineering, electronics, cosmetics, food, and medicine. For the first time, this paper explores recent advances in NC molecular simulation, providing insights into structure, arrangement, and interactions through molecular dynamic simulation. Finally, future prospects for NC-based applications are discussed to encourage studies addressing current challenges.

Keywords: *nanocellulose, functional composite, molecular simulations, biobased polymer, biodegradability*

1. Introduction

Cellulose is the most important non-petroleum-based polymer and is naturally derived from biomass, which includes plants, selected marine organisms, and microorganisms [1–3] (Figure 1). The nanocellulose market was valued at $291.53 million in 2019 and is projected to reach $1053.9 million by 2027, reflecting a significant compound annual growth rate (CAGR) of 19.9% over the forecast period. Additionally, several companies have already initiated the industrial-scale production of cellulose nanofibers (CNF) and cellulose nanocrystals (CNC), with some achieving annual production capacities exceeding 200 t [4]. similarly, the expected revenue growth from 2021 to 2026 is expected to increase from $346 million to $963 million [2].

As Figure 1 indicates, in addition to botanical sources, nanocellulose can be obtained from other routes, including microorganisms (such as algae and bacteria) and marine organisms (Figure 1). Nanocellulose can be obtained from plant cell walls or agricultural residues through various deconstruction processes, which are outlined in Figure 2. Further details for each procedure can be found in other published materials [1, 2, 5–15]. Marine sources such as tunicates are limited and difficult to access thus making them less commonly exploited. Producing nanocellulose using microorganisms has attracted more attention as a sustainable and green method. This type of nanocellulose exhibits some exceptional properties compared to those derived from plant sources. These outstanding properties include higher purity, crystallinity, degree of polymerization, water absorption capacity, transparency and mechanical stability [12, 13]. However, this method faces different challenges that need to be resolved. The most important ones

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are finding suitable culture media with reasonable prices and productive microorganisms. Designing a bioreactor that provides an appropriate environment for cellulose formation is another issue that researchers are working on.

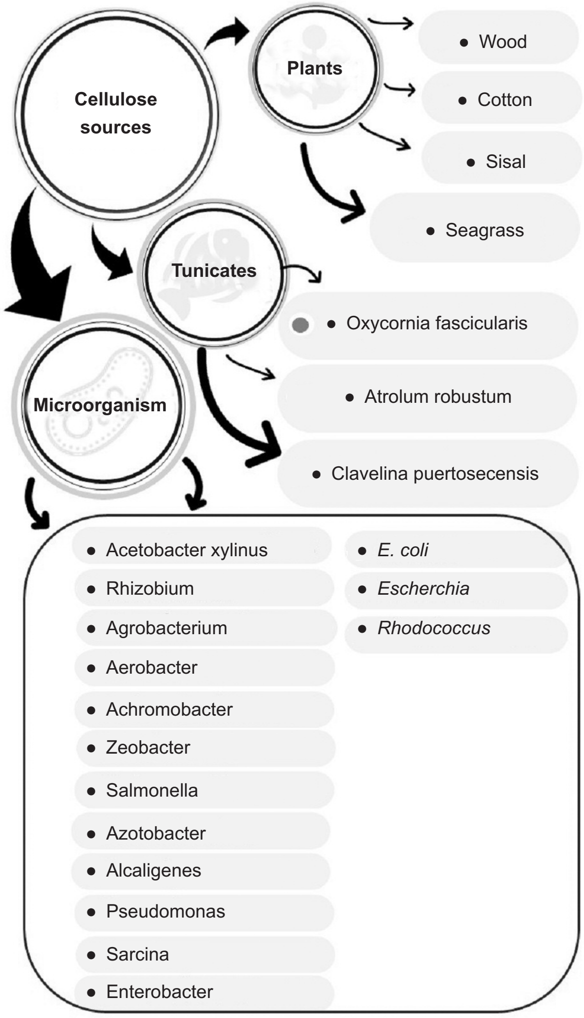

Figure 1. Different sources of cellulose.

Habibi *et al*. [16] proposed a relatively different procedure for the fabrication of NC-based products through a three-dimensional self-assembly method. This technique involves forming a 3D pattern of CNCs through sol-gel processing, followed by the infiltration of this structured network with a chosen polymer. Yang *et al*. [17] also demonstrated that cellulose-based materials can effectively form various three-dimensional structures through self-assembly. The phenomenon of self-assembly was examined by studying the chiral nematic phases where CNCs with end-attached ligands were used [18]. Self-assembly in these nanocrystals is highlighted as a crucial process for achieving these phases more rapidly compared to non-attached CNCs. The recent advancements in the self-assembly of CNCs can be found in [19], which describes the basics of liquid crystals and self-assembly as well as the main approaches used in order to form CNC-based composite films. Detailed knowledge of the structure and properties of nanocellulose is essential for its diverse applications in various industries. In recent years, molecular dynamics (MD) simulation has emerged as a cornerstone tool in polymer science and engineering for this purpose [20]. MD provides engineers and scientists with a means to unravel the intricate relationship between the macromolecular structure of polymers and their functionalities while reducing research costs. It plays a central role in the development and design of products as diverse as adhesives, membranes, drug carriers, and emulsions.

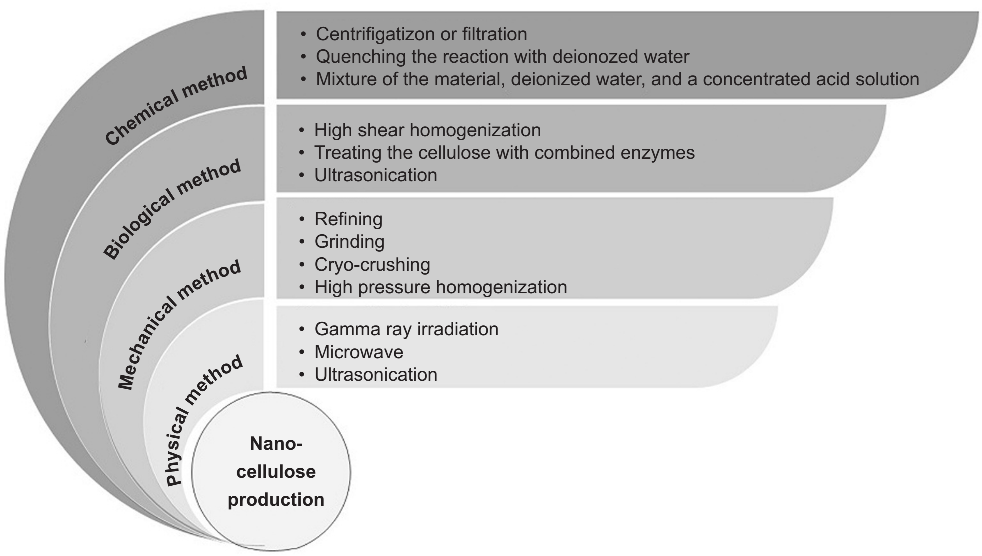

Figure 2. Producing methods of nanocellulose from agriculture waste and plants.

Consequently, there's an urgent need to further utilize this practical computational tool for a profound understanding of dynamic phenomena and the design of polymeric systems before resorting to expensive laboratory methods. In line with this objective, the present work provides valuable insights into the MD simulation of nanocellulose.

2. Properties of cellulose nanoparticles

Cellulose has a multi-molecular structure composed of highly oriented cellulose chains organized in orthogonal layers. When cellulose microfibrils are reduced to the ultrafine and nanoscale, the result is known as nanocellulose, an exceptional material for a variety of advanced applications. To date, the primary categories of nanocellulose based on their structure include cellulose nanocrystals (CNC) and cellulose nanofiber (CNF). Nanocellulose exhibits a wide variety of properties, depending on both its source material and the methods used to produce it (Table 1). Cellulose nanocrystals typically have diameters in the range of 5 to 70 nm and lengths in the range of 100 to 250 nm. Cellulose nanofibers are characterized by particle diameters in the range of 5 to 60 nm and lengths up to several micrometers. These dimensions are closely related to the cellulose source and the processing methods employed [6, 21, 22]. The properties of natural fibers are influenced by numerous factors, including chemical composition, location within the plant, stage of maturity, separation methods, and microscopic and molecular characteristics such as pits and knots. In addition, the type of soil and prevailing weather conditions also play a significant role in determining the final properties of these fibers [1, 23].

Due to the unique properties of nanocellulose such as high specific area, biodegradability, sustainability, low density, high absorbency, water adsorption up to 99%, moldability, excellent mechanical properties and porous network, it stands out as a preferred choice for various applications. Its robust nature, coupled with its natural and environmentally friendly attributes, positions it as a strong competitor to other commercial fibers.

2.1. Mechanical properties

The structure of cellulose consists of two components: the crystalline region and the amorphous region. Certain factors, such as the production process and impurities, such as lignin and hemicellulose, can exert a negative direct effect on cellulose crystallinity, morphological structure, and consequently the quality of cellulose [21]. The modulus of nanocellulose is derived from a mixing rule involving the modulus of the crystals, the amorphous fraction, and the defects/air present in the sample. The crystalline regions of cellulose act as physical cross-links and fillers, increasing the modulus due to their finite size. The physically cross-linked network of cellulose nanofibers, which are randomly distributed, can actually act as an excellent water absorber. The Young's modulus of crystalline regions is a critical property directly related to reinforcement in composites. For example, the elastic modulus of CNC is approximately 105–168 GPa [1, 24, 25]. Similarly, the specific elastic modulus is another parameter that indicates the relationship between elastic modulus and density. The mechanical properties of CNC have contributed to additional outstanding characteristics, such as a Young's modulus ranging from 20 to 50 GPa and an exceptionally low density, making it highly versatile and applicable in various fields [14]. In research comparing the properties of CNCs with other materials such as glass fibers, steel wire, Kevlar, graphite, and carbon nanotubes (CNTs), the results showed that CNCs exhibit exceptional strength and superior properties such as Young's modulus, tensile strength, specific Young's modulus, strength-to-weight ratio, specific stiffness, and coefficient of thermal expansion compared to the aforementioned

Table 1. Classification of nanocelluloses.

Sources	Type of cellulose	Extraction process	Crystallinity [%]	Dimensions [nm]	Aspect ratio [–]	References
Different parts of plants	CNC	Hydrolysis	54–88	$100 < L < 250$ $5 < d < 70$	10–50	[2, 3, 5]
Tunicin	CNC	Hydrolysis Bleaching	73–89	$1374 < L < 1567$	80–90	[22]
High plants such as sugar beet	CNF	Mechanical treatment	68.5	L: Several mm $5 < d < 60$	30–300	[2, 3, 5]
Bacteria	CNF	Biosynthesis	75–80	$20 < d < 100$	50	[2, 3]

materials [26–28]. For example, partial replacement of silica with modified CNC in a rubber compound resulted in significant improvements. Specifically, the Payne effect, heat buildup, and compression set were reduced; while the 300% modulus, tear strength, and hardness were significantly increased [29]. These specific properties have made nanocellulose a suitable material as a reinforcing agent for use in polymer composites.

The mechanical properties of nanocellulose are determined by structural factors, including crystal structure, morphology, geometric dimensions, crystallinity, anisotropy, and defects induced by the starting material and production processes. When comparing the different types of nanocellulose, it is clear that variations in feedstock and processing techniques have a significant impact on their mechanical properties [27–32]. For example, this suggests that the choice of source and processing method plays a critical role in determining the mechanical performance of nanocellulose-based products. In addition, the presence of lignin and hemicellulose in nanocellulose derived from botanical sources influences its mechanical properties, although further research is needed to fully understand this relationship. Overall, this comparative analysis highlights the need for careful selection and optimization of nanocellulose production processes to tailor their properties for specific applications.

The value ranges of mechanical properties for CNC, CNF and bacterial nanocellulose come in the published papers are presented in Table 2.

2.2. Rheological properties

Rheological properties, such as viscosity and shear stress, indicate the deformation of the material and its response to external forces over time. In the nanoscale, both external and internal specific surfaces play a critical role in determining the rheological behavior of dispersion. Nanostructures have the ability to immobilize significant amounts of water on both external and internal surfaces, leading to the formation of gel-like water systems. For example, NFC suspensions exhibit remarkable gel-like behavior, which is mainly due to two factors. First, their large specific surface area, approximately 900 m^2/g, facilitates enhanced interaction with surrounding molecules. Second, the abundance of hydroxyl groups on the NFC surface promotes gel formation through the formation of hydrogen bonds, resulting in the formation of a reticular three-dimensional structure [33–35].

The studies conducted on CNC suspensions have shown that the shear thinning behavior of these suspensions within a 'dilute' regime intensifies with increasing concentration. This dependence is mainly observed for CNC suspensions in the low shear rate range [13]. The rheological properties of CNC aqueous suspensions were investigated, with a particular focus on evaluating the influence of CNC concentration, temperature variation, and ionic strength [36]. In this study, CNCs were extracted from cotton using an alkaline pretreatment followed by concentrated sulfuric acid hydrolysis.

At a concentration of 0.4 wt%, the suspension exhibited a Newtonian plateau at low shear rates, followed by a shear thinning region at intermediate shear rates, and another plateau at high shear rates, indicating isotropy. However, concentrations between 3 and 10 wt% showed a three-region viscosity profile characteristic of polymer liquid crystals or amorphous cellulose suspensions. Beyond 10 wt% concentrations, the distinct regions disappeared and only shear thinning behavior was observed, likely due to CNC gelation at elevated concentrations. Besides the amount of CNCs in a suspension, the concentration of salt influenced the rheological properties of the CNC suspensions. A decrease in viscosity with increasing NaCl concentration was observed, which is attributed to the shielding of electrostatic repulsion between CNC particles, a common phenomenon in polyelectrolyte systems with added salt. The storage modulus showed an increase with higher ionic strength in chitin nanocrystal dispersions. Despite the low sample concentration (1.0 wt%), which prevents gel formation with added salt, a decrease in

Table 2. Mechanical properties of nanocellulose.

Type of nanocellulose	Source	Young's modulus [MPa]	Tensile strength [MPa]	Strain at break [%]	Degree of polymerization	References
NCC	Wood fibers	145 000	7 500	–	10 000–15 000	[12, 30]
NFC	Cotton	4 980–10 920	264–654	3.0–7.0		
BNC	*Gluconacetobacter Xylinus*	15 000–35 000	200–300	1.5–2.0	2 000–6 000	[27, 30]

storage modulus was observed with increasing NaCl concentration. This decrease is attributed to the shielding of electrostatic repulsion resulting in weakened interactions within the CNC suspensions.

The final section of the discussion deals with the temperature-dependent behavior of viscosity and storage modulus in CNC suspensions. It was observed that the viscosity remains largely unaffected by temperature at low and medium shear rates but shows a slight decrease at high shear rates [36]. The effect of temperature on viscosity is found to be dependent on shear rate, temperature range and CNC concentration. This finding differs from the results of Ureña-Benavides *et al.* [37], where viscosity decreased with increasing temperature, suggesting potential differences in microstructural properties. Notably, the behavior of the experimental sample is consistent with other nanocylinder dispersions that exhibit minimal temperature dependence at steady shear viscosities. Conversely, the decrease in storage modulus with temperature is attributed to the attenuation of intermolecular interactions within CNC suspensions at elevated temperatures. In contrast, chitin nanocrystal dispersions exhibit an opposite trend, characterized by a significant increase in elastic modulus with increasing temperature, which is attributed to enhanced associative forces between nanocrystals.

2.3. Optical properties

Nanocellulose exhibits a distinct optical response compared to other cellulosic materials due to its nanoscale size, anisotropic individual structures, and liquid crystalline behavior. In addition, the thickness of the nanocellulose plays a significant role in determining its optical properties. Birefringence in cellulose-based particles is expected due to the inherent anisotropy of cellulose structures at different length scales, from cellulose chains to wood fibers. This anisotropic structure can be maintained during the fibrillation of wood or pulp fibers into CNCs. In the case of CNCs, the orientation of the cellulose chains is preserved, resulting in birefringence. CNCs have refractive indices of 1.618 and 1.544 in the axial and transverse directions, respectively. A thin layer of boron nitride nanosheets was coated on the CNF-nano paper, achieving optical transparency of 70% [15, 38].

The optical properties of cellulose-based materials are influenced by several key parameters that significantly impact their optical applications. These parameters include the birefringence of cellulose, which typically ranges from 0.05 to 0.10, affecting its ability to create differences in the refractive index of polarized light. Quantum yield, which ranges from 0.01 to 0.15, indicates the efficiency of photon emission. The chiral luminescence *g*-factor also plays a crucial role, typically falling between 0.01 and 0.1. The size of cellulose nanoparticles, with diameters ranging from 5 to 20 nm and lengths from 100 to 500 nm, along with crystallinity degrees between 40 and 70%, and the luminescence emission bandwidth (50 to 100 nm) and absorption and emission wavelengths (300 to 400 and 400 to 600 nm, respectively), all impact optical performance and scattering [39]. The birefringence and intrinsic/polarized luminescence of CNC made it a marvelous component to be used in photonic films, sensors, circularly polarized luminescence and cluster luminescence materials.

The optical properties of cellulose are employed in a range of applications. Notably, in biological imaging, cellulose's suitable luminescence and biocompatibility facilitate cell observation. In anti-counterfeiting and optical encryption, cellulose-based photonic films enable the creation of complex and unique optical patterns. Biocompatible chemical sensors based on cellulose are designed to detect various substances such as TNP and copper ions. Additionally, cationic cellulose derivatives are utilized for producing antibacterial and hydrophobic materials. In optoelectronics, cellulose's optical properties and mechanical flexibility are applied in devices such as light-emitting diodes (LEDs) and displays. Moreover, tunable biosensors based on cellulose are developed for detecting biological and chemical changes, such as pH and substance concentration.

These applications underscore the significant role of cellulose in advanced optical and biological technologies. In a study conducted by Niskanen *et al.* [26], the optical properties of thermally modified cellulose nanofibers (TO-CNF) were investigated. This research focused on the impact of various parameters on the optical characteristics of cellulose, including color changes, complex refractive index, birefringence, and the dependence of these properties on temperature. At room temperature films exhibited a complex refractive index with a real part (n) of 1.454 and an imaginary part (k) of 0.0001. As the temperature increased to 200 °C, the real part of the refractive index increased to 1.598, which indicates changes in light absorption and optical behavior. The birefringence values, which were 0.035 at 0 °C, decreased to 0.0075 at 200 °C, reflecting a reduction in the structural order of the nanofibers due to thermal treatment. Additionally, significant color changes were observed in the films with increasing temperature, with the films becoming much darker at 200 °C, resulting in increased light absorption and decreased light reflection. These results clearly illustrate the impact of parameters such as temperature and crystalline structure on the optical properties of cellulose, highlighting the importance of these parameters in tuning optical properties for various applications [26].

Cellulose has garnered significant attention in scientific research due to its unique optical properties, which arise from its nanofibrillar structure. These optical properties are influenced by their molecular and electronic characteristics, including electron affinity, ionization energies, and optical absorption spectra. Various cellulose molecules, such as benzoquinone and naphthoquinone derivatives, have been investigated using density functional theory (DFT) and time-dependent DFT calculations. These studies have demonstrated that even minor changes in molecular structure can significantly impact the optical properties of the material. Specifically, Kumar *et al.* [40] studied an in-depth analysis of cellulose's optical properties and revealed that nanocellulose with smaller dimensions (approximately 100 nm) can exhibit up to 90% transparency in visible wavelengths, whereas larger NC particles show a decrease in transparency to around 70%. Furthermore, the results indicate that chemically modified cellulose can reduce light reflection by up to 20% and significantly improve light transmission to 85%. These characteristics are particularly useful in optical applications such as anti-reflective coatings and transparent films. Additionally, the study showed that incorporating nanoparticles into the cellulose structure can enhance optical properties, including increased light intensity and reduced light attenuation, facilitating novel applications in various fields such as historical paper preservation and tissue engineering.

2.4. Electrical properties

Given the wide range of morphological forms of cellulose, composites offer the opportunity to develop materials with high electrical conductivity, electrical and optical ON-OFF switching capabilities, and electrochemical redox properties. It is important to note that NC by itself is not electrically conductive. However, when combined with other conductive substances, it can acquire this property [38]. Nanocellulose has the ability to enhance thermal insulation, thereby improving energy efficiency and reducing heat loss in devices. It increases the power factor and improves charge transfer by increasing the electrical conductivity, a property induced by various chemical or physical modifications to produce conductive NC materials. In addition, NC contributes to increased stability by inhibiting electronic oxidation and degradation. In particular, the high aspect ratio and ease of surface modification make NC an excellent material for the fabrication of various carbon electrodes. This is due to (1) the abundance of hydroxyl groups on reactive surfaces, which allows versatile hybridization possibilities with various active materials to fabricate nitrocellulose-based composite electrodes and separators, and (2) its high aspect ratios coupled with commendable mechanical properties, which make nanocellulose highly attractive for flexible electrodes. The Table 3 describes the properties of nanocellulose relevant to its suitability for electrical applications [28].

The conductivity of adding some conductive materials to cellulose is investigated by different researchers [41–43]. Various conductive materials exhibit unique properties, such as conductive polymers (*e.g.*, PPy, PANI, PEDOT/PSS, PEDOT) with conductivity ranging from 10^{-5} to 10^{2} S/cm [41]. The conductivity of graphene and carbon nanotubes, including both single-walled (SWNTs) and multi-walled (MWNTs)

Table 3. Characteristics of nanocellulose for electrical applications.

Characteristics	Description
High aspect ratios	Nanocellulose exhibits high aspect ratios, making it conducive for the production of various carbon electrodes.
Ease of surface modification	The ease of surface modification allows for versatile applications, including the fabrication of nitrocellulose-based composite electrodes and separators.
Flexibility	Nanocellulose's good mechanical properties and high aspect ratios make it highly suitable for flexible electrodes.

variants, also come in a range of 10^{-4} to 10^{2} S/cm. Inorganic nanoparticles, including ZnO, SnO_2, TiO_2, I, Au, Ag, and Cu, exhibit a conductivity range of 10^{-6} to 10^{3} S/cm. Ionic liquids, with a conductivity range of 10^{-8} to 10^{-4} S/cm, complete the spectrum of conductive materials [42]. Pure CNF aerogels have no conductivity, whereas pure few-walled carbon nanotubes (FWCNT) aerogels exhibit an electrical conductivity of 1.8 S/cm when freeze-dried with liquid nitrogen, and an order of magnitude lower conductivity when freeze-dried with liquid propane. In hybrid aerogels, the electrical conductivity increases with higher FWCNT weight fractions. A CNF/FWCNT 80/20 w/w aerogel freeze-dried with liquid nitrogen shows a relatively high electrical conductivity of 10^{-2} S/cm [41]. The electrical conductivity of the RGO-CNF (20%) hybrid aerogel film, measured using a four-probe method, is approximately 100 S/m [43].

3. Nanocellulose applications

Due to its unique properties, nanocellulose finds numerous applications in various industries, such as paper making, medical and biomedical engineering, electrical engineering, food engineering, civil engineering and water treatment, and so on [6–9, 24, 44–49]. The named applications, as depicted in Figure 3, will be discussed separately in this paper.

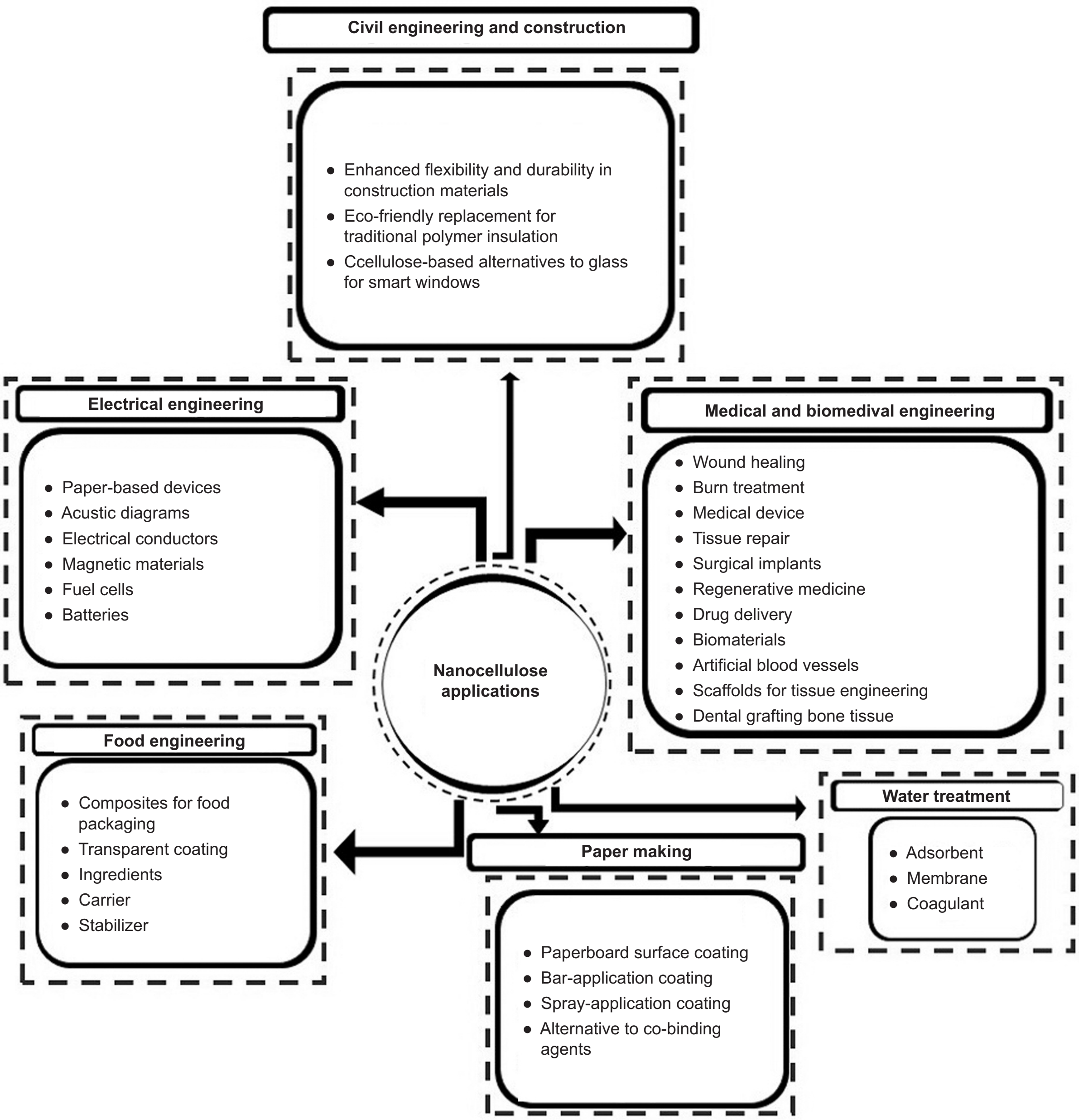

Figure 3. Nanocellulose applications.

3.1. Papermaking

Growing environmental concerns advocate the use of biodegradable and environmentally friendly products derived from natural materials such as bamboo (as a non-wood source) and rice straw (as an agricultural waste) in order to reduce the cost of paper production and cause less environmental problems, thus increasing the demand for paper consumption [50–54]. Nanocellulose, recognized as a green and environmentally friendly nanostructure, offers a viable solution. It readily integrates with other polymers and additives, using its hydroxyl groups to facilitate cross-linking with pulp fibers, thus providing synergistic effects. CNF can play a pivotal role in the paper industry as an important additive, contributing to the production of high-quality papers with remarkable properties such as improved dry strength, low thermal expansion and reduced surface roughness [55–59]. However, improving the mechanical properties of such products often requires functionalization with additives. The characteristics of NC that make it a promising material for the paper industry are tabulated in Table 4.

The papermaking and recycling industries are challenged by the difficulty of removing short fiber lengths and contaminants, which can result in reduced water dewatering performance of the pulp. Nanocellulose additives, with their superior properties, offer a solution by acting as paper retention aids to minimize the loss of fine fibers. In addition, they can act as paper filter aids to improve the dewatering performance and dewatering rate of wet paper during the papermaking process. Cationic nanofibrillated cellulose (CNFC) was used as a precipitated calcium carbonate (PCC) retention additive in a study focused on the production of reconstituted tobacco sheets/papers (RTS) for conventional hand sheet production. The addition of 7 wt% CNFC increased PCC retention from 32.71 to 44.74%. In addition, parameters such as air permeability and RTS index were improved by 15.1% and approximately 28.0%, respectively, compared to cases where CNFC was not added [55]. Merayo *et al*. [56] investigated the synergistic effects of combining CNF with various retention additives such as polyvinylamine, chitosan, cationic starch, C-PAM, and C-PAM-B to improve paper strength while mitigating negative effects on drainage. The results showed that the incorporation of CNF resulted in a reduction in drainage time of 30 to over 40%. Furthermore, the combination of CNF with C-PAM-B or chitosan showed the most favorable results in terms of increased paper strength and a significant reduction in drainage time.

In research on the reinforcing effects of nanocellulose to improve the mechanical properties of paper, it was found that increasing the amount of NFC as a reinforcing agent in the polylactic acid (PLA) latex matrix resulted in improvements in the elastic modulus, tensile strength, thermal stability, and elongation at break of the biocomposite material [57]. Hydrogen bonding plays a critical role in establishing inner fiber contacts in papermaking, where direct fiber-to-fiber interactions are essential. NFC, characterized by nanoscale diameters and lengths of several micrometers, has a strong tendency to self-associate. They effectively fill the gaps between fibers and facilitate direct contact through robust hydrogen bonding [58]. Nanodispersed cellulose can serve as a substitute component for traditional co-binding materials in coatings and improve the whiteness, opacity, smoothness, and print clarity of new papers [59].

In summary, the use of nanocellulose in the papermaking industry presents a significant advancement with the potential to reduce production costs and environmental impacts. Nanocellulose, derived from biodegradable materials such as bamboo and rice straw, offers several benefits due to its nanoscale dimensions, high mechanical strength, and effective interaction with cellulose fibers. It also acts as an efficient retention aid in recycling processes, which

Table 4. Key features of nanocellulose for papermaking applications.

Reason	Description
Nanoscale lateral dimension	Expands specific surface area
Lengths in the micrometer scale	Provides substantial length
Semi-crystalline structure	Composed of extended cellulose chains
High intrinsic mechanical strength	Demonstrates robust mechanical properties
Good flexibility	Demonstrates robust mechanical properties
Potential to interact with fibers	High ability to form hydrogen bonds with cellulosic fibers
Inherent tendency to form strong networks	CNFs naturally form strong, entangled networks

helps in improving drainage rates and reinforcing paper quality. Functionalized nanocellulose can enhance the mechanical properties of paper, reducing issues such as wrinkling and improving overall strength. Its application extends to enhancing the barrier properties and durability of packaging materials, contributing to the development of more sustainable and environmentally friendly fiber-based products. This topic will be more discussed in the Section food engineering. Overall, integrating nanocellulose into papermaking and packaging processes supports the creation of high-performance, eco-friendly products, demonstrating its valuable role in advancing sustainability within the industry.

3.2. Medical applications

Various therapeutically active substances (TAS), such as peptides, amino acids, proteins, enzymes, *etc.*, are used in both the cosmetic and medical industries for the effective treatment of the skin. In order to minimize their side effects, provide low release and increase efficacy, it's essential that these therapeutically active substances are chemically attached to suitable reactive nanocarriers. Nanocellulose particles are an excellent choice for biocarriers due to their nanosize, compatibility with various organic ingredients, insolubility in water, oils and organic solvents, and other outstanding properties. Natural polymers, including cellulose pastes, hydrogels and CNF, play an important role in cosmetic manufacturing. The characteristics such as high hydrophilicity, aspect ratio, mechanical strength, and elasticity make nanocellulose a prominent candidate in formulations as a thickening or stabilizing agent in emulsions, masks, carriers, and so on [60–72].

Due to its unique properties such as biocompatibility, nanocellulose finds numerous applications in cosmetics and biomedicine. In the pharmaceutical industry, NC is used as a binder, filler and excipient in tablets and powders. It is also used in medical suspensions to stabilize phase separation and prevent sedimentation of heavy ingredients. Due to their biocompatibility and reduced rejection upon contact with blood and cells, nanocellulose composite scaffolds hold potential for applications in wound dressings and tissue engineering scaffolds aimed at regenerating damaged organs. A comparative analysis of conventional treatment methods for wound healing with the use of nanocellulose-based products, presented in [60], is summarized in Table 5.

Cellulose nanocarriers may contain ingredients such as proteolytic enzymes composed of amino acids, which may have a beneficial effect on facial skin, especially in the treatment of skin burns, wounds, and postoperative cars. Due to its immediate pain relief, promotion of autolytic debridement, reduced infection rates, accelerated granulation, absence of microbial activity, high water absorption capacity and large surface area, bacterial cellulose serves as an ideal healing dressing for the treatment of wounds in large and difficult to cover areas of the body. Wound healing requires a supportive environment and there are several types of wound dressings available. An ideal wound dressing should have properties such as non-toxic, non-adherent, absorbent and antimicrobial, while also being transparent, capable of removing exudates and providing a moist wound environment conducive to healing.

With the high thickening capacity of therapeutically active substances when combined with NC-based carriers, the need for synthetic thickeners is reduced, and the phase stability in liquid pharmaceutical formulations is enhanced. The excellent compaction properties of NC are useful in formulating densely packed, drug-loaded tablets. Drug release refers to the process by which a drug exits a drug product and

Table 5. Comparative analysis of medical approaches for wound treatment: conventional *vs*. nanocellulose-based bioadhesives.

Aspect	Conventional medical approach	Nanocellulose-based bioadhesives
Treatment methods	Suturing, splinting, surgical incisions	Direct adhesion to wounds, sutureless surgery
Limitations	Susceptibility to infection, lengthy procedures	Reduced risk of infection, faster treatment
Wound healing	May result in tissue damage	Promotes healing with minimal tissue damage
Material properties	Limited customization	Customizable properties, *e.g.*, antioxidant, antibacterial effects
Applications	Primarily used for hemostasis, fracture treatment, surgery	Versatile applications including drug delivery, wound dressing, hemostasis, and surgery
Safety	Variable safety depending on procedure and material used	Safer treatment with reduced risk of complications
Innovation	Limited innovation in recent years	Significant advancements and ongoing research

undergoes absorption, distribution, metabolism and excretion. The disintegration rate of CNC-based tablets and their drug release can be regulated by various methods, including microparticle entrapment, excipient layering, or tablet coating [35, 67]. Several combinations of cellulose with other particles, such as CNCs-reinforced core-shell gelatin hydrogel, carboxymethylcellulose (HS-CMC)/polyvinyl alcohol (PVA) hydrogel, and polydopamine (PDA)/cellulose nanofibrils (TOCNFs) hydrogel, have demonstrated efficacy in drug delivery and wound healing applications. Hydrogels based on chitosan and cellulose, as well as hydrogels incorporating CNCs, have been investigated for their potential applications in bone tissue engineering and as inhibitors [69].

Aqueous suspensions with controlled concentrations of CNCs indicated the potential to form hydrogels that serve as a supportive matrix to create a suitable environment with favorable mechanical properties for cell differentiation and growth [70]. Nanocellulose-based hydrogels can also act as drug carriers, facilitating the controlled release of drugs into the body. The combination of CNC with various types of functional groups can significantly enhance essential properties critical for medical applications, such as drug loading and targeting capabilities. For example, the incorporation of CNC, cyclodextrin, and curcumin has shown promise as an effective drug in the treatment of cancer, exhibiting anti-proliferative effects on rectal cancer cells and colonies [22, 65–69].

Nanostructured BC, characterized by its high degree of hydration (99% water content), is suitable for application in moisturizing masks and as an ingredient in moisturizing creams in cosmetics [34, 35, 62]. BC, especially when produced by the bacterium *Gluconacetobacter xylinus*, has several properties that make it highly suitable for medical device applications in the healthcare industry. These characteristics include compatibility with biological systems, high degree of polymerization, excellent mechanical properties, insolubility in solvents, and formability. This unique combination of properties makes bacterial cellulose a versatile biomaterial for use in various medical devices. Bacterial nanocellulose exhibits higher crystallinity, greater water-holding capacity, a finer reticular network, and thinner thickness compared to cellulose fibrils derived from plants [31]. BC has been recognized for its ability to improve skin hydration and increase skin luminosity by approximately 7–28% [54]. In particular, BC has been investigated as a drug release carrier and has shown high efficiency in facilitating the rapid release of both hydrophobic and hydrophilic drugs [61]. They can effectively clean the skin's pores and penetrate through the lipid layer and epidermis to the deeper layers of the skin, helping to treat and regenerate damaged skin tissues [65]. Bacterial cellulose also was investigated to be incorporated in masks or support for skin care applications [62–65].

Nanocellulose has attracted attention for its use in bioassays [70, 71]. One of the key advantages of cellulose-based nanomaterials is their high specific surface area, which facilitates the immobilization of advanced bioreceptor units. Through direct functionalization, surface modification or polymer coating, cellulose nanomaterials can be tailored to improve their properties without compromising their inherent properties. This customization allows reproducible immobilization of bioreceptor units while maintaining biocompatibility. Biosensors are measurement devices in which immobilized biological components interact with analytes and produce diverse signals that span physical, chemical, or electrical domains. The basic concepts of biosensors are reviewed in [27]. NFC shows great potential for diagnostic applications due to its unique properties, including low porosity, high surface area, and strong hydrogen bonding capability. Research has demonstrated the creation of water-resistant and non-porous substrates suitable for biosensors through surface activation methods such as carboxylation and EDC/NHS coupling chemistry. Activated MFC films with suitable conjugation sites have been used for antibody immobilization using techniques such as inkjet printing and physical adsorption of molecules such as polyclonal anti-human IgG and bovine serum albumin (BSA) [70]. Biosensors play a critical role in healthcare by rapidly and accurately detecting biological molecules, enabling early diagnosis, disease monitoring and personalized treatment. These devices integrate a biological component (such as enzymes, antibodies or DNA) with a transducer to convert the biological response into a detectable signal. Because of their ability to provide rapid and reliable diagnostics, biosensors are playing an increasingly important role in modern medicine and disease management. Among biosensors, those based on BC have shown promise for healthcare and medical diagnostics. BC-based biosensors offer several advantages, including high sensitivity, rapid response, precision, and affordability. BC and its derivatives are versatile materials that provide excellent substrates for immobilizing biologically active compounds in biosensors. As a result, BC-based biosensors exhibit desirable properties such as accuracy, sensitivity, ease of use and rapid response. BC has attracted attention in various biomedical applications due to its unique combination of properties. Its potential in biosensor applications is particularly noteworthy, and ongoing research is exploring its suitability for various healthcare diagnostic and monitoring scenarios.

Bone diseases present challenges to healing and often require bone grafting to facilitate the process. Autologous bone grafts have limitations, particularly in repairing large bone defects. Loss of alveolar bone is another challenge. BC provides biocompatibility, allowing endothelial cells, smooth muscle cells and chondrocytes to adhere. Cellular studies have demonstrated enhanced cell migration, particularly of smooth muscle cells, in microporous BC materials. Microporous BC is created by introducing porogens into the fermentation process of *A. xylinum* to enhance cell infiltration into BC scaffolds. Subsequent removal of these porogens after fermentation leaves a network of interconnected pores that promotes bone regeneration [68].

Table 6 presents the comparative importance of NC-based composite scaffolds versus conventional counterparts.

When artificial surfaces come into contact with blood and cells during procedures such as dialysis, cardiopulmonary bypass, and blood transfusion, there's a risk of clotting, thrombus formation, and increased susceptibility to microbial infection. The use of nanocellulose, a natural and biocompatible material with unique properties, is proving beneficial in long-term implant applications such as cardiovascular devices, including vascular grafts, venous catheters, and artificial heart valves [8]. Bacterial cellulose has been evaluated for its potential use as blood vessel substitutes in microsurgery and for the development of novel cardiovascular or bypass implants [8]. Targeted nanoparticles offer the potential to mitigate serious side effects associated with the selective delivery of chemotherapeutic drugs, including low blood cell counts, mouth ulcers, hair loss, kidney and heart damage, and the relief of nausea and vomiting. The geometry of the particles plays a critical role in the efficacy of drug nanocarriers. Modified CNCs with elongated geometry and specific surface chemistry are recommended for targeted delivery of chemotherapeutic drugs, such as folic acid delivery for targeting brain cancer tumors in mammals [72]. The properties of nanocellulose and their medical applications are depicted in Figure 4. The excellent biocompatibility of NC, including non-toxicity and non-irritating, coupled with supportive characteristics, such as high mechanical strength and elasticity, and water-holding capacity,

Table 6. Comparative significance of nanocellulose composite scaffolds *vs.* conventional materials.

Aspect	Nanocellulose-based scaffolds	Other scaffold materials
Characteristics	Water retention, optical clarity, enhanced mechanical, thermal, and swelling properties	Variable properties, including biocompatibility and mechanical strength
Pore structure	Interconnected pore structures, enlarged with increasing CNC concentration	Variable, often less uniform pore structures
Equilibrium swelling ratio	PVA/CNC with 4 and 6 wt% CNC showed greater swelling ratios compared to pure PVA	May exhibit lower swelling ratios
Hydrophilicity	Enhanced by CNC, provides an ideal microenvironment for cell adhesion, growth, and metabolism	Variable, may not offer ideal conditions for cell behavior
Biocompatibility	Excellent, suitable for tissue engineering applications	Variable, some materials may exhibit poor biocompatibility
Mechanical strength	Strong, suitable for neural tissue engineering	Variable, may require reinforcement to achieve desired mechanical properties
Cell affinity	Promotes cell adhesion, growth, and metabolism	Variable, some materials may exhibit poor cell affinity
Fabrication technique	Electro spun cellulose/CNC nanocomposite nanofibers (ECCNN)	Variable, may involve different fabrication methods
Performance	Increased elastic modulus and tensile strength, improved thermal stability	Variable, may exhibit lower mechanical properties and thermal stability
Cell structure alignment	Benefited from aligned nanofibers, crucial for neuronal tissue engineering	Variable, may lack alignment leading to less directed cell structure

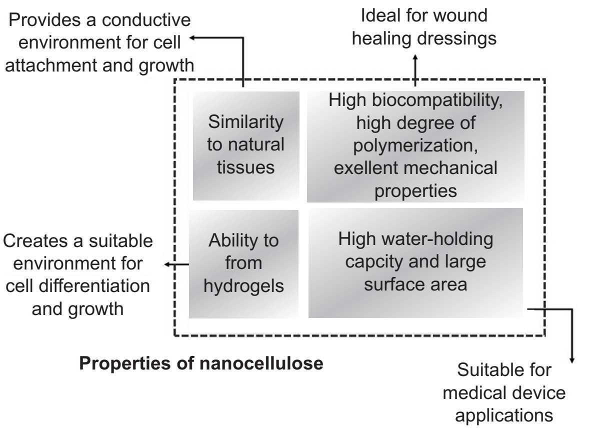

Figure 4. Properties of nanocellulose and biomedical applications.

make it a valuable component for diverse biomedical applications. NC can be used as

- Binders, filler, and stabilizing agents in drug formulations and drug delivery systems.
- Bio-adhesives or in wound dressings for the treatment of burns and diabetic ulcers.
- Implants in cardiovascular systems such as vascular grafts, heart valves.
- Hydrogels for wound healing and skin regeneration as well as bone tissue engineering and drug delivery systems.
- Skincare products that improve skin hydration and luminosity due to its superior hydrophilicity.

3.3. Electronic and electrical applications

In addition to its biodegradability, nanocellulose has several specific properties, including good contrast, flexibility, and reflectivity, which make it suitable for electronic applications [73–78]. Figure 5 illustrates the application of nanocellulose in electronics. Cellulose can be used as a component in conductive composites. When combined with conductive coating polymers or conductive nanoparticles like carbon nanotubes, these composites exhibit moderate electrical conductivity [74]. By combining cellulose nanofibers with other conductive functional materials, the pore structure, Young's modulus, specific surface area, and mechanical properties of electrodes can be tuned. This enhancement contributes to improved electrochemical and mechanical performance of the electrodes, making cellulose nanofibers a preferred material for supercapacitor electrodes. However, due to their insulating nature, cellulose nanofibers alone often fail to meet the requirements of supercapacitor electrodes and exhibit poor electrochemical properties. Therefore, creating conductive composite materials by incorporating cellulose nanofibers with conductive substances such as conductive polymers and carbon materials has proven to be an effective approach. This process simplifies the preparation of composite materials while retaining the advantageous properties of cellulose nanofibers, such as their flexible three-dimensional network, high flexibility, and good hydrophilicity.

Supercapacitors offer advantages such as rapid energy charging and discharging, better power density than batteries, and resistance to chemical degradation from rapid power surges. Nanocellulose, with its high surface area and active sites, is being explored for use in supercapacitor electrodes and separators [73]. It enhances ion transfer and provides an ideal diffusion channel for electrolyte solutions. In addition, nanocellulose can improve mechanical strength and capacitive performance when used as an electrode, especially when combined with conductive carbonaceous materials such as carbon nanotubes and graphene. Researchers have experimented with nanocellulose-derived materials in the construction of supercapacitors, achieving improved electrochemical performance due to their unique structural properties. In addition, nanocellulose is being incorporated into automotive applications to develop lightweight and sustainable materials in response to regulatory requirements and environmental concerns in the automotive sector. Based on their research, these advances demonstrate the potential of nanocellulose to revolutionize electric vehicles and automotive materials for a greener and more efficient future. Detailed information about supercapacitors and their potential to overcome the energy storage challenges are outlined in [38, 43, 74]. Table 7 illustrates the applications and benefits of nanocellulose in the automotive industry.

Nanocellulose papers, with diameters typically in the tens of nanometers, offer high transparency, smoothness, and mechanical strength, making them suitable

Table 7. Applications and advantages of nanocellulose in the automotive industry.

Specific applications	• Lightweight car parts • Improved supercapacitors for electric cars • Enhanced lithium-ion batteries • Improved energy gadgets
Benefits	• Improved fuel economy • Reduced CO_2 emissions • Enhanced strength and sustainability in automotive materials

for various flexible energy and electronic devices. Nanocellulose can serve as an environmentally friendly substrate in optically transparent plastics, enabling applications such as bendable displays and flexible organic light-emitting diodes (OLEDs) or in transparent, insulating or semiconducting substrates for transparent paper transistors. These paper-based transistors have applications in disposable microelectronics, including biosensors and smart packaging. In addition, cellulose can be used not only as a non-conductive substrate for printed circuits, but also in the fabrication of conductive substrates, which includes dielectric, conductive, semiconductor, and photovoltaic applications. Nanocellulose-based films, which have a low dynamic loss and high sound velocity compared to aluminum or titanium films, offer potential applications in ultrafine acoustic headphone diaphragms [8].

A novel nanocomposite was developed by integrating nanocellulose with inorganic fillers such as kaolin and precipitated calcium carbonate (PCC). The filler-NC combination offered several advantages over oil-based plastic sheets, including compatibility and favorable physical properties such as smoothness, porosity, density, and wettability. This smooth and flexible film also demonstrated improved printability and lower thermal expansion compared to the reference plastic film, Mylar. In addition, they exhibited good dimensional stability and low surface roughness, making them promising candidates for printed electronics applications [75]. Organic photovoltaic devices typically use substrates such as polyethylene terephthalate (PET) and polyethylene naphthalate (PEN). The cells composed of CNC exhibited higher efficiencies compared to those including CNF. This is attributed to the fact that CNC films are smoother, have a more uniform fiber distribution, and exhibit less roughness.

CNC-derived papers can serve as both substrate and electrolyte in the photovoltaic components of solar cells [76–78]. These papers can achieve transparency levels of up to 90% through various methods such

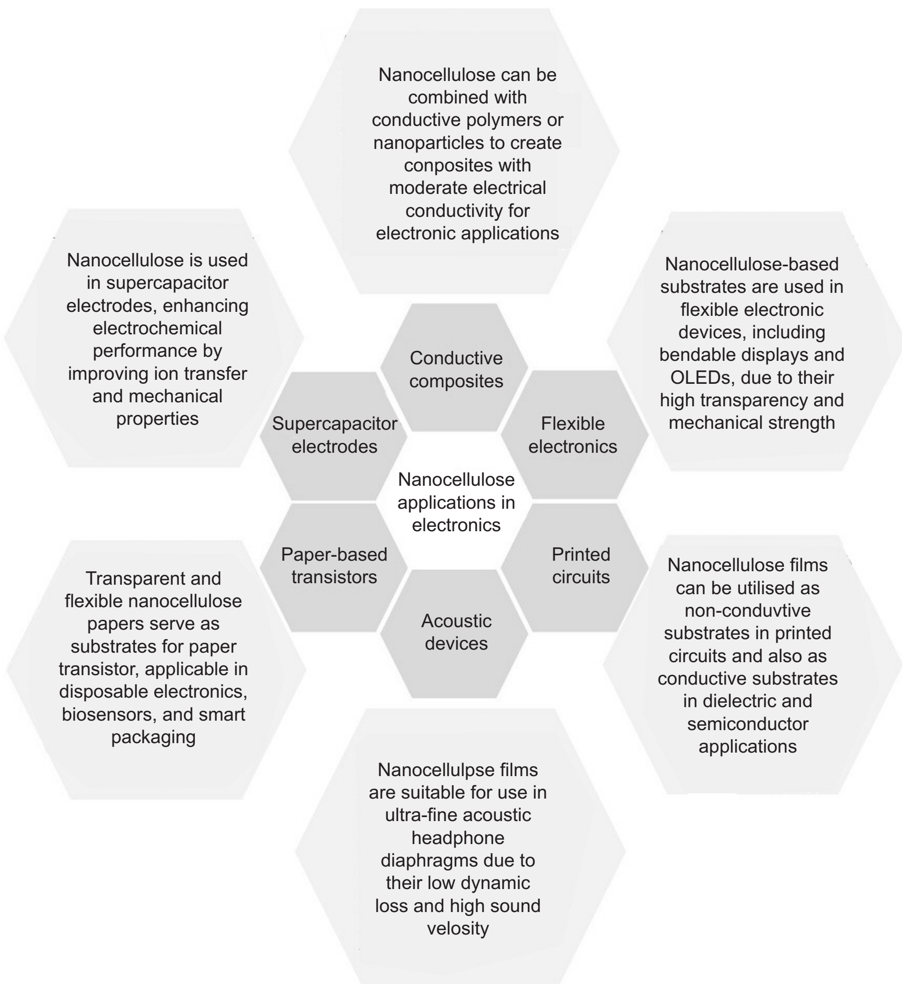

Figure 5. Nanocellulose applications in electronics.

as TEMPO oxidation, while effectively scattering light in desired directions [3]. Perovskite solar cells (PSCs) are known for their low cost and high energy conversion efficiency, making them promising for portable electronics applications. In particular, the power conversion efficiency (PCE) of metal hydride perovskite cells reaches up to 23.3%, which is close to that of crystalline silicon cells at 26%. Traditionally, PSCs have been manufactured using oil-based polymer substrates, which can pose contamination problems. However, the nanocellulose paper-based perovskite solar cells have shown that PSCs have a remarkable power-to-weight ratio of 0.56 W/g, coupled with an energy conversion efficiency of 4.25%. Impressively, these cells can maintain their efficiency at over 80% even after 50 bends, highlighting their durability and suitability for flexible applications [76]. Both crude cellulose and CNC were used as precursors for carbon nanoparticles [77]. These nanoparticles served as light sensitizers in dye-sensitized solar cells (DSSC). CNC yielded a higher percentage of carbon nanoparticles (54.6%) compared to crude cellulose (37.2%). A novel approach was introduced for the development of dye-sensitized solar cells (DSSC) by replacing oil-derived polymer matrices with environmentally friendly gelling agents, such as carboxymethylcellulose (CMC) [78]. This innovation aimed to address issues related to moisture and water degradation in solar cells. The DSSC achieved a photovoltaic yield of 0.72% using 5.5 wt% CMC as the electrolyte and demonstrated good stability even under aging conditions. Despite these advances, several challenges remain before NC can be widely adopted for solar device production. Researchers are working to develop cost-effective methods for extracting nanocellulose and integrating it into solar devices on a large scale. In addition, further investigation is needed to improve the durability and stability of nanocellulose-based solar devices in wet conditions.

In addition, nanocellulose is being used as reinforcement in electrolytes and as a binder in electrodes and separators for high-power Li-ion batteries (LIBs) and other energy storage applications. The porosity of nanocellulose-based electrodes facilitates the movement of ionic species between the electrode surfaces, improving battery performance [12].

In conclusion, nanocellulose presents significant potential for advancing electronic and electrical applications due to its biodegradability, flexibility, and exceptional properties such as high contrast and reflectivity. Its ability to be integrated into conductive composites, particularly with conductive polymers or nanoparticles, enhances its electrical conductivity and mechanical strength, making it valuable for energy storage devices like supercapacitors and lithium-ion batteries. The automotive industry benefits from nanocellulose through its application in lightweight car parts, improved supercapacitors, and enhanced batteries, contributing to greater fuel efficiency and reduced CO_2 emissions. Additionally, its use as a substrate in flexible electronics, including bendable displays and OLEDs, highlights its versatility and suitability for advanced electronic devices. Nanocellulose's role in organic photovoltaic devices and perovskite solar cells further demonstrates its utility in improving light scattering, efficiency, and durability in flexible electronics. Overall, while nanocellulose holds promise for numerous electronic and electrical applications, including flexible electronics, energy storage, and photovoltaic devices, challenges such as large-scale integration and stability under various conditions must be addressed to fully realize it's potential. Cellulose nanowhiskers or nanocrystals have the ability to form robust hydrogen-bonded porous films. By employing layer-by-layer deposition techniques while preserving the open pore structure of the nanocrystal films or nanowhiskers and incorporating electronically conductive polymers, it becomes possible to fabricate conductive free-standing porous membranes. These membranes can find applications in electrochemical sensors, separation processes, and catalysis, serving as electrocatalysts or materials for supercapacitors. Transparent coatings made from paper-based materials offer significant potential for use as thermal and/or acoustic insulation. Because of their transparency, these coatings can be applied to windows, serving the dual purpose of reducing energy consumption by improving thermal insulation and providing sound insulation for buildings. This multifunctional application is expected to contribute to improved energy efficiency and enhanced acoustic comfort in indoor environments.

3.4. Food engineering

The versatility and diverse properties of nanocellulose have paved the way for a wide range of applications and the development of new products, especially in the food industry [79–93]. Although research on food applications of cellulose is still limited, several applications have been presented, including stabilization of Pickering emulsions, food packaging, functional food ingredients, food-grade hydrogels, 3D structured hydrogels, and carriers for bioactive factors. Nanocellulose, when used as a functional ingredient in food products, can serve as a fat substitute, reduce fat during frying, increase volume, act as a binder, and serve as a bulking agent. Nanocellulose can extend the shelf life of products, improve texture and flavor, or modify formulations to reduce fat, sugar, or salt content while increasing vitamin levels; ultimately promoting healthier options. Table 8 presents a summary of information from academic research. Specific nanocellulose applications in food industry are illustrated in Figure 6.

Emulsions are colloidal dispersions of two or more immiscible liquids in which one liquid is dispersed as small droplets in another liquid. Simple emulsions typically include oil-in-water (o/w) or water-in-oil (w/o) types, depending on which liquid is dispersed in the other. More complex emulsions can consist of multiple layers, with combinations of oil-in-water (o/w) and water-in-oil (w/o) emulsions occurring simultaneously within the same system. Pickering emulsions offer several advantages over traditional emulsions, including superior stability, controllable permeability, and improved elasticity. In fact, because of their stability andversatility, Pickering emulsions are widely used in a variety of industries, including pharmaceuticals, cosmetics and food. Pickering emulsions are stabilized by solid particles, called Pickering stabilizers, which adsorb to the oil-water interface and prevent droplet coalescence. These emulsions are stabilized by colloidal or solid particles that adsorb at the interface between immiscible

Table 8. Rheological properties and functional applications of nanocellulose in food packaging.

Property	Description
Viscosity	High viscosity at low concentrations
Rheological behavior	Shear-thinning behavior
Application	• Excellent candidate for use as a suspension stabilizer, thickener, and/or emulsifier in various applications • Active substances like antimicrobials and antioxidants can be chemically conjugated to nanocellulose to create active packaging materials and edible coatings • Nanocellulose can serve as a carrier for flavor compounds, enhancing their stability and controlled release in food products.

Figure 6. Specific nanocellulose applications in the food industry.

liquids and prevent droplet coalescence. Various solid particles have been used as Pickering stabilizers, intcluding silica particles, titanium dioxide nanoparticles, and non-degradable microgel particles. CNFs are a type of cellulosic material that can serve as effective stabilizers in Pickering emulsions due to their amphiphilic surface chemistry. Nanocellulose stands out due to its promising properties, including non-toxicity, high surface area-to-volume ratio, amphipathicity, high Young's modulus, high tensile strength, degradability, and biocompatibility. These properties make nanocellulose an attractive option for stabilizing Pickering emulsions in various applications [14, 83–86, 90–92]. The majority of reports focus on cellulose nanoparticles as emulsifiers for oil-in-water (o/w) emulsions due to the superior wettability of cellulose fibrils and microfibrils in water compared to oil. Chemical-modified NFC and CNC were examined as emulsifiers to stabilize oil-in-water-in-oil (o/w/o) double emulsions [83]. These double emulsions exhibited remarkable stability over the course of one month, with the globules showing resistance and maintaining their integrity even under centrifugation at 5000 rpm. Similarly, the stabilization of another type of multiple emulsions, water-in-oil-in-water (w/o/w) emulsions, by MCC has been investigated in separate research efforts [88, 89]. The stability of Pickering emulsions is influenced by factors such as the hydrophobicity, shape and size of the solid particles. While many solid particles used for stabilization are inorganic, there is a growing preference for natural resources to avoid the potential hazards associated with synthetic materials. Natural particles such as nanocellulose offer promising properties for stabilizing Pickering emulsions while ensuring safety and sustainability in various applications [83–86, 89, 91, 92].

He and co-researchers conducted a study on high internal phase emulsions (HIPE) [89]. When the volume fraction of the dispersed phase exceeds 0.74, the emulsion with this unique property is called a HIPE. Such HIPEs stabilized by colloidal particles are specifically categorized as high internal phase Pickering emulsions (HIPPEs). Conventional HIPEs typically require significant amounts of surfactants. However, in the absence of irreversible adsorption of Pickering particles at the interface, conventional HIPEs often struggle to maintain long-term stability due to phenomena such as coalescence and Ostwald ripening, where larger emulsion droplets grow at the expense of smaller ones. In contrast, HIPPEs typically exhibit prolonged stability at lower stabilizer levels due to the high Gibbs free energy required for stabilizers to detach from the liquid-liquid interface. In addition to sharing characteristics with conventional Pickering emulsions such as long-term stability and large interfacial area, HIPPEs exhibit highly flocculated emulsion droplets with polyhedral shapes and unique rheological properties. These include shear thinning behavior with promising shear moduli and thixotropic recovery attributed to the jamming and creaming of emulsion droplets. HIPPEs typically exhibit solid-like or semisolid gel-like properties, indicated by a higher storage modulus (G') than loss modulus (G'') at low shear rates. However, at high shear rates, HIPPEs can exhibit fluid-like behavior due to transient disruption of reversible interactions within the continuous phase. The switchable rheological behavior of HIPPEs in response to different shear rates suggests potential applications in combination with extrusion-based 3D printing techniques. This is because such techniques require the ink to transition between solid-like and liquid-like states before or during extrusion while maintaining the structure of the printed object afterwards.

Studies have progressed towards the use of nanocellulose-based materials for active packaging, including controlled release packaging (CRP) and responsive packaging (RP) [1, 61, 87–89, 93]. Nanocellulose shows a remarkable ability to produce transparent films that are resistant to acid and fat. Therefore, it serves as a viable alternative to conventional non-renewable petroleum-based plastics and aluminum in food packaging, especially in the context of edible coatings. Although NC has no inherent resistance to external stresses, it can be integrated with other nanoparticles to form nanocomposites that exhibit excellent mechanical properties, non-toxicity, renewability, and biodegradability, all of which are critical in food packaging. In addition, nanocellulose possesses properties conducive to the formation of effective crosslinking or grafting bonds, making it well-suited for applications in the food packaging industry [14]. In terms of functionality, nanocellulose transparent films can be combined with various materials as needed, thereby expanding their range of applications. For example, nanocellulose-derived transparent paper exhibits antibacterial properties and remarkable resistance to high temperatures, with a maximum decomposition temperature peak of 353 °C

[93]. In addition, when transparent paper is mixed with other substances, it has the potential to improve packaging materials or give them new capabilities. To solve the problem that nanocellulose transparent paper is not very good at repelling water, scientists have come up with various ways to make it more waterproof. One innovative approach is to use natural polymer materials together with environmentally friendly water-based waterproofing agents as coating layers. This method has resulted in transparent papers with remarkable barriers to oxygen and water vapor. The CN-based coatings also exhibited excellent anti-fog properties, improved oxygen barrier properties of conventional materials, and reduced friction and water vapor permeability [91–93]. The films containing less than 1 wt% NC exhibited improved mechanical and barrier properties, as well as favorable printing characteristics. These films also exhibited a low oxygen transmission rate, as low as 17 ml/(m^2·day), suggesting their suitability as surface layers for modified atmosphere packaging.

In conclusion, nanocellulose exhibits considerable promise in the food industry, offering a range of benefits due to its unique properties. The versatility of NC-based products, including stabilizing agents, Pickering emulsions, active food packaging, and functional food ingredients, has already been demonstrated in several applications. Besides, NC can effectively function as a fat substitute, bulking agent, or binder, contributing to reduced fat content, improved texture, and extended shelf life of food products. Its ability to modify food formulations allows for the reduction of unhealthy components like fat, sugar, and salt while potentially increasing the nutritional value by incorporating vitamins. Furthermore, its potential for chemical modification enables the incorporation of active substances like antimicrobials and antioxidants, enhancing its role in active packaging materials and edible coatings. Its capability to act as a carrier for flavor compounds also improves the stability and controlled release of these compounds, which can enhance the sensory qualities of food products. The rheological properties of NC, such as its high viscosity at low concentrations and shear-thinning behavior, make it an ideal candidate for use as a suspension stabilizer, thickener, or emulsifier. Overall, the integration of nanocellulose into food industry applications holds significant potential for improving food product quality and safety while supporting healthier food formulations.

3.5. Water and wastewater treatment

The primary and overriding goals of water treatment are to improve global health standards and mitigate environmental pollution and water scarcity issues. Several strategies are used for water treatment, including membrane filtration, precipitation, flocculation, ion exchange, evaporation, distillation, and electrolysis [94–98]. Among these methods, membrane-based filtration stands out for its simplicity and effectiveness (Table 9). This approach places special emphasis on aerogels, which play an important role in the purification process.

In general, various methods, including physical, chemical, and biological approaches, have been successfully developed to remove contaminants from wastewater. Occasionally, a combination of these methods is used to enhance the effectiveness of water treatment processes. Hydrogels, primarily used in adsorption-based physical methods, have gained widespread use in wastewater treatment [94–96]. In hydrogel-based techniques, contaminant removal occurs through mechanisms such as hydrogen bonding, π-π interactions, surface adsorption, electrostatic attraction, and ion exchange, depending on the nature of the contaminants present (*e.g.*, dyes, heavy metals,

Table 9. Analysis of wastewater treatment technologies.

Wastewater treatment technologies	Characteristics
Advanced oxidation processes	Techniques to degrade organic pollutants and remove contaminants using advanced oxidation methods
Hybrid water supply systems	Integration of multiple water sources for sustainable water management
Cellulose hydrogel	Environmentally friendly, biodegradable, and renewable method using cellulose for efficient wastewater treatment
Novel membranes	Development of innovative membrane technologies for improved filtration and separation processes in wastewater treatment
Disinfection techniques	Utilization of various disinfection methods such as chlorination, UV irradiation, and ozonation to eliminate pathogens and microorganisms from wastewater
Adsorption-based processes	Application of adsorption technologies using high-performance adsorbents to effectively remove pollutants and contaminants from wastewater streams

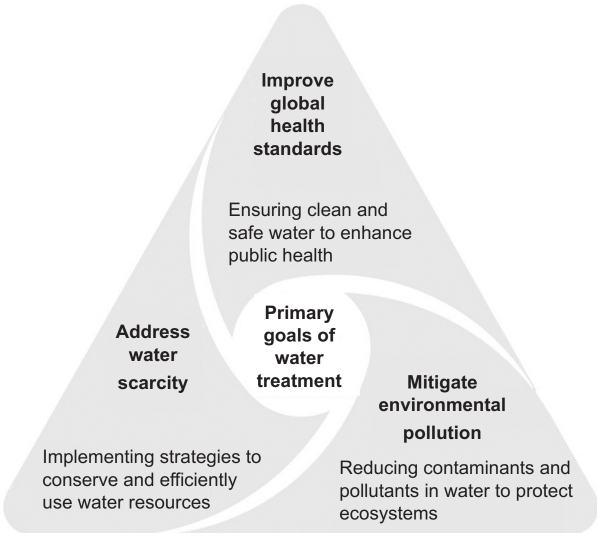

Figure 7. The primary goals of water treatment.

oils, pharmaceuticals). The surface functionality and three-dimensional network structure of hydrogels also play a key role in determining their adsorption efficiency. Various water and wastewater treatment processes utilize adsorbents, membranes, flocculants, and catalytic degradation. Improving the efficiency of these techniques can be achieved through the use of green aerogel materials such as NC, chitosan (CS), and starch. These materials offer environmentally friendly, biodegradable and flexible polymer solutions that are characterized by sustainability and robust mechanical strength. They also have a reduced carbon footprint compared to traditional activated carbon and petroleum-based polymers. The primary goals of water treatment are presented in Figure 7 and strategies for water treatment are summarized in Figure 8.

3.5.1. Adsorbent

The adsorption capabilities of nanocellulose are due to electrostatic interactions and chemical bonds present on its surface. These properties allow it to effectively capture heavy metals, dyes, pollutants, and oils from various solutions [21, 94–126]. To achieve an effective adsorbent, factors such as network hydrophilicity, surface charge, pore size, and surface area need to be optimized. For example, reducing cellulose to the nanoscale and increasing its specific surface area justifies the improvement of its adsorption capacity. In addition, the ability of adsorbents to be recycled and reused is a crucial factor considered for their potential applications in industry. The adsorption properties of nanocellulose are presented in Figure 9.

Water from natural sources and industrial effluents often contain heavy metal ions such as cadmium, zinc, copper, nickel, lead, mercury, and chromium, all of which pose serious risks to ecosystems and human health due to their toxicity. Therefore, it's imperative to remove these heavy metal ions from aqueous solutions. Recently, there has been considerable research on the efficiency of biologically based nanomaterials in removing heavy metals. These materials offer strong selectivity, low cost, temperature adaptability, biocompatibility, and degradability, and possess fluffy, porous surfaces with large specific surface areas. Among these materials, biochar, starch, and cellulose are particularly popular. However, these adsorbents have some limitations, as depicted in Figure 10. Zhang *et al.* [108] developed a bio-adsorbent, known as thiol-functionalized cellulose (TFC),

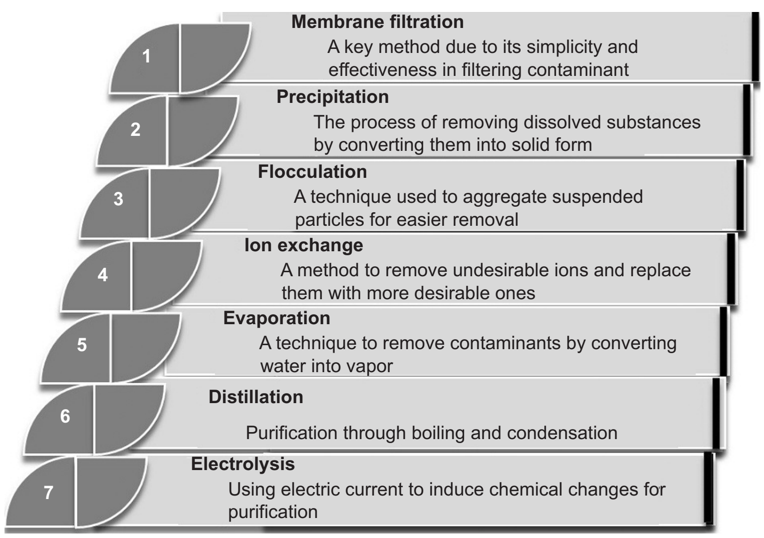

Figure 8. Water treatment strategies.

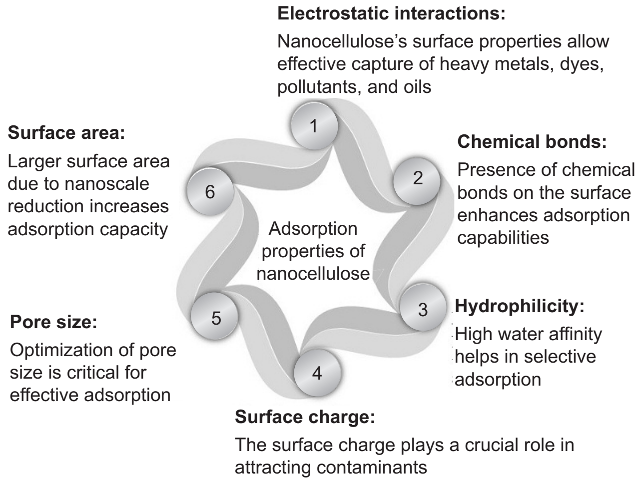

Figure 9. Summary of adsorption properties of nanocellulose.

through chemical modification to remove Hg (II) from aqueous solutions. Their results showed that TFC exhibited a remarkable adsorption efficiency of 99% for Hg (II) using a fast and simple preparation method. In similar work, researchers synthesized mercerized and succinic anhydride-modified cellulose at the nano- and microscale to serve as adsorbents for the removal of Zn (II), Ni (II), Cu (II), Co (II), and Cd (II) ions from aqueous solutions [99]. The pH dependence, adsorption kinetics, and regeneration potential were investigated using different concentrations of acids or ultrasonic treatment. The results showed that succinic anhydride-modified mercerized nanocellulose exhibited metal removal capacities of 2.062, 1.9, 1.610, 1.338, and 0.744 mmol per gram of adsorbent for Cd, Cu, Zn, Co, and Ni, respectively. In addition, ultrasonic treatment of the modified nanocellulose after exposure to 1 M HNO_3 resulted in regeneration efficiencies of 95.28% (Zn), 95.76% (Ni), 106.25% (Co), and 95.52% (Cd). Trimethylammonium chloride-functionalized CNF was used to remove arsenic from aqueous samples, with an arsenic removal efficiency of more than 85% within 2 h. Furthermore, the functionalized CNF was evaluated for its efficacy in treating real contaminated samples containing co-existing anions. The results demonstrated a removal efficiency of up to 94% for Asas (V) from contaminated water [101].

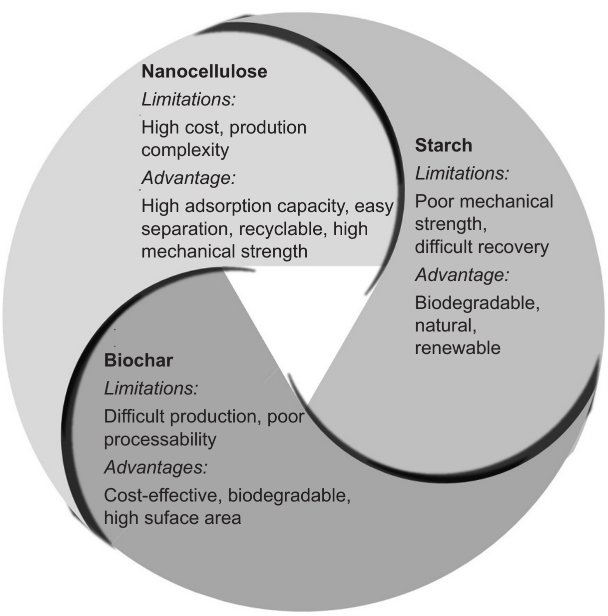

Figure 10. Comparison of nanocellulose with biochar and starch in adsorption applications.

A challenging problem is cleaning up oil spills and collecting oil from water surfaces. Solving this problem requires a buoyant, reusable, recyclable, and environmentally friendly absorbent capable of absorbing a significant amount of oil without absorbing water. Recent research has focused on achieving this by functionalizing nanocellulose aerogels with a hydrophobic yet oleophilic coating, resulting in a selectively oil-absorbing material that floats on water surfaces. Similarly, ultra-light and recyclable NC-based sponges have been developed that can selectively collect numerous organic solvents and oil spills from water surfaces with high absorption capacity [109]. Surface functionalization techniques such as carboxylation, sulfonation, oxidation, phosphorylation, esterification, and amination of nanocellulose have been examined for waste treatment purposes [94–97, 106, 107, 114, 119, 120]. These methods enhance the binding of dyes, heavy metals, and pollutants from wastewater to the hydroxyl groups present on the surface of nanocellulose. Carboxylation has been used to facilitate cation adsorption [111]. The results indicate that the modification increases the adsorption efficiency, which is likely due to the modification of amorphous domains in the cellulose chain during CNC preparation or leads to greater availability of primary hydroxyl groups on the surface.

3.5.2. Membrane

Typically, membranes serve as one of the primary methods for wastewater treatment. Basically, membrane filtration works on the principle of permeability, allowing certain chemicals to pass through while others are retained during the separation process. The effectiveness of membranes is directly related to their pore size. However, it has been observed that biological and organic fouling pose inherent challenges to membrane technology. To mitigate this problem, researchers have turned to nanocellulose for its hydrophilic nature and have also modified the surface chemistry to enhance its effectiveness in reducing fouling. Commonly used methods for membrane processing include electrospun mat permeation with nanocellulose method, vacuum filtration and coating method, and freeze-drying method [28]. A comparison between traditional polymers such as HDPE, PET and LDPE and NC-based membranes extracted from [97, 120, 121] is summarized in Table 10.

The microstructure and chemical composition of the material play an important role in determining the key properties of membranes and filters, including selectivity and permeability. Cellulose nanoparticles exhibit hydrophilic properties, and their surface properties can be chemically tailored, making them highly suitable for water treatment and purification applications [94, 95, 102, 104]. The functional groups present on the surface of nanocellulose allow for selective adsorption of contaminants from water while mitigating biofouling problems in membrane systems. Cellulose nanopapers are of great importance for nanofiltration and ultrafiltration applications due to the presence of contaminants of various sizes, from microscale particles to nanosized contaminants such as viruses and microbes. This versatility has led to extensive research in the development of cellulose nanopapers and membranes for effective filtration purposes. Researchers are actively investigating ways to improve the structure of nanopaper membranes to achieve a balance between permeability and rejection performance. This balance is critical to effectively address the challenge of size exclusion rejection of nanoparticles (NPs), which has been a concern due to the limited permeance of nanopaper membranes. By improving the structure of these membranes, researchers aim to achieve proportional permeance while maintaining high rejection performance, thus overcoming the limitations associated with size exclusion rejection of NPs [121]. Recent studies have explored various methods to produce nanocellulose-based membranes with high flux and robust mechanical properties. These methods include vacuum filtration, electrospinning, and coating. Through these approaches, researchers aim to develop membranes that exhibit both high flux and mechanical strength, thereby enhancing their applicability in various water treatment and purification applications [97, 120, 121, 123].

The composition of biopolymers like NC and chitosan was investigated for membrane applications. For example, a membrane made of NC and chitosan was used for the removal of three flexographic inks and reported 100% efficiency in reducing turbidity and removing ink from wastewater [98]. In a similar work, a composite of NC and chitosan functionalized with ethylenediamine was examined for the removal of residual diclofenac sodium (DS) from wastewater. The composite showed promising results in terms of adsorption capacity. The improved capacity was attributed to the amino groups of the functionalized nanocellulose-chitosan composite that form ionic bonds with the carboxyl groups of DS. In a separate study, a chitosan/cellulose nanocomposite with activated carbon was developed for the removal of tylosin from antibiotic contamination [119]. The adsorption of tylosin was facilitated by chemical and physical interactions between the hydroxyl and carbonyl functional groups of the composites and tylosin. In addition, Tshikovhi *et al*. [120] highlighted

Table 10. Comparison of traditional polymers and nanocellulose in various applications.

Membrane material	Environmental concerns	Biodegradability	Advantages
HDPE	Toxicity, poor biodegradability	Limited	Widely used, but raises environmental concerns
PET	Toxicity, poor biodegradability	Limited	Commonly utilized, yet poses environmental risks
LDPE	Toxicity, poor biodegradability	Limited	Widely employed, but environmental issues persist
NC	Environmentally friendly	Biodegradable	Promising candidate for membrane fabrication due to natural biodegradability and eco-friendly nature

various studies on nanocellulose adsorbent composites reinforced with other polymers and materials such as activated carbon, carbon nanotubes, graphene oxides, metals, non-metals, and ceramics for the removal of various organic and inorganic contaminants from water.

Mautner and Bismarck [118], conducted a study of bacterial cellulose nanopapersin various organic dispersion media with low surface tension and varying hydrophilicity, such as ethanol, acetone, and tetrahydrofuran. They investigated the membrane performance of these nanopapers and found that those made with organic liquids exhibited significantly higher permeance than those made with an aqueous dispersion medium. This higher permeance contributed to the improved efficiency of the bacterial cellulose nanopaper membranes. Specifically, bacterial cellulose nanopapers in organic dispersion media maintained pore sizes of 15–20 nm, similar to those in aqueous dispersion media, allowing the removal of contaminants as small as viruses.

3.5.3. Flocculent

The purification of wastewater in both municipal and industrial settings often involves the removal of minute suspended solids, metals, colorants, and various organics through a process known as flocculation. In this process, flocculants are added to the solution to promote the collision of colloidal particles, resulting in the aggregation of these particles into larger, less stable formations called flocs, which then settle out of the mixture. In addition, flocculants can sometimes promote the formation of even larger aggregates through mechanisms such as bridging and electrostatic interactions with colloidal particles. Due to their unique properties, CNFs are emerging as promising candidates for use as flocculants in such processes. The majority of studies in this field have highlighted the advantages of using cellulose-based nanocellulose as flocculants. These materials offer safe and environmentally friendly alternatives to petroleum-derived polymers [124–126].

The coagulation-flocculation treatment process is used to reduce turbidity in both industrial and municipal wastewater. However, the synthetic polymers typically used in this process are petroleum-based, non-biodegradable, and may contain neurotoxic and carcinogenic additives.

Suopajärvi *et al*. [124] conducted a study in which they produced anionic decarboxylase cellulose flocculants (DCCs) by nanofibrillation treatment of periodate and chlorite-oxidized cellulose using a homogenizer. These DCCs were then compared to a synthetic reference polymer in a coagulation-flocculation treatment. The results of the experiments demonstrated the prolonged stability of the DCCs and their superior turbidity reduction compared to the synthetic reference polymer at equivalent dosages. In particular, DCC flocculants with higher charge density and nanofibril content showed the best performance. In a subsequent study, sulfonated CNFs were synthesized by sulfonation using sodium metabisulfite [125]. This new generation exhibited higher anionic charge and showed superior performance compared to dicarboxylic acid CNFs in terms of turbidity and COD removal, even at lower dosages. In addition, the efficacy of anionic sulfonated nanocellulose was evaluated against a commercial coagulant with comparable results. Notably, the nanocellulose coagulant resulted in the formation of smaller, rounder, and more stable wastewater flocs compared to the reference polymer. Yu *et al*. [126] conducted a comparative analysis of the flocculation efficiency of CNCs prepared by different hydrolysis methods. They found that CNCs carboxylated by a single-step citric acid/HCl hydrolysis exhibited superior flocculation performance for suspended kaolin clay particles. This improved performance was attributed to the presence of anionic charges on the carboxylated CNCs.

Advanced water treatment technologies are crucial for improving global health, mitigating environmental pollution, and addressing water scarcity. Recent innovations emphasize the shift towards environmentally friendly and biodegradable materials, which offer strong mechanical properties and a lower carbon footprint compared to traditional options like activated carbon and petroleum-based polymers. Research highlights using NC as a promising alternative to conventional polymers for membrane filtration, which offers marvelous advantages such as biodegradability, sustainability and fouling resistance. The hydrophilic properties of NC mitigate the membrane fouling and thus enhance its operation efficiency. Development membranes composed of NC can pave the way for more effective and environmentally responsible wastewater management solutions. Flocculation, a crucial process for removing fine suspended solids, metals, and organics from wastewater, has traditionally relied on non-biodegradable and potentially harmful synthetic flocculants. However, CNFs and CNCs have emerged as effective and environmentally friendly alternatives. For example, carboxylated CNCs exhibited excellent flocculation efficiency, driven by their anionic charges. The advantages of nanocellulose-based flocculants over traditional petroleum-derived synthetic polymers in wastewater purification were addressed. The findings presented here highlight the potential usage of nanocellulose-based flocculants in wastewater treatment that offer greater environmental benefits. Recent research emphasizes the advantages of biologically based nanomaterials, particularly nanocellulose, in environmental applications due to their high selectivity, low cost, and robust mechanical strength. The effectiveness of cellulose in capturing heavy metals, dyes, pollutants, and oils is significantly enhanced when its dimensions are reduced to nanoscale, which increases its specific surface area and then its adsorption capacity. Nanocellulose outperforms other adsorbents, such as biochar and starch, in terms of adsorption efficiency, recyclability, and preparation simplicity. Its application in addressing environmental challenges, such as oil spills and heavy metal contamination, has shown promising results. Its adsorption capability is further augmented by surface modifications that enhance its hydrophilicity, surface charge, and porosity. Functionalized nanocellulose materials offer effective solutions for highly efficient selective adsorption of contaminants. The ongoing advancements in functionalization techniques and material development underscore NC's potential in contributing to more sustainable and effective environmental management solutions.

3.6. Civil engineering and construction

The application of nanocellulose in civil engineering is relatively new [127]. Hisseine *et al*. [128] investigated the mechanical properties of cement systems by incorporating cellulose filaments. Their results showed improvements in compressive strength, Young's modulus, and toughness, suggesting the potential of this material for improved ductility and resistance. The study highlights the exploration of high-performance insulation materials derived from renewable sources to improve the energy efficiency of buildings. Wicklein *et al*. [129] investigated suspensions composed of cellulose nanofibers, graphene oxide, and sepiolitenanosticks with the aim of developing thermally insulating and fire-retardant anisotropic foams as alternatives to conventional polymer-based insulation materials. The results showed promising results, indicating that nanoscale engineering provides a viable approach to producing high-quality foams with favorable properties using renewable nanofibrous materials such as cellulose and others.

Simelane *et al*. [130] conducted a comprehensive investigation of engineered transparent wood (ETW) as a composite material that combines the mechanical properties of wood (the main source of cellulose) with the optical properties of glass. Engineered transparent wood has exhibited a wide range of favorable properties, including thermal insulation, flame resistance, mechanical robustness, electrochromic capabilities, ultraviolet (UV) shielding, flexibility, reduced mass, and exceptional optical transmittance exceeding 80%. With such remarkable properties, ETW holds great promise as a viable alternative to traditional glass windows in smart building applications, with the potential to reduce energy waste and mitigate the effects of global climate change. They are known for their ability to improve emulsion stability and have been investigated as encapsulation materials for phase change materials (PCMs). PCMs are substances that can absorb or release a large amount of latent heat over a range of temperatures as they transition between different phases. Researchers have developed various forms of CNF-encapsulated PCMs, including aerogels, foams, microparticles, paper, and hollow cellulose filaments. Among them, composites of PCMs encapsulated in CNF foams have attracted considerable attention due to their excellent thermal insulation and storage properties. However, the process of synthesizing well-dispersed CNFs can be costly and requires a high level of technical expertise [44].

In conclusion, recent advancements in civil engineering and construction underscore the transformative potential of incorporating nanocellulose and related materials into building technologies. Relevant research have shown:

- Cellulose filaments can significantly enhance the mechanical properties of cementitious materials, suggesting their potential for improving the durability and energy efficiency of construction materials.
- Cellulose nanofibers, when combined with graphene oxide and sepiolite nanosticks, can produce advanced insulating and fire-retardant foams,

offering a sustainable alternative to traditional polymer-based insulation materials.
- Engineered transparent wood (ETW) as a high-performance material with remarkable properties, including thermal insulation, flame resistance, and high optical transmittance, can be a promising alternative to conventional glass in smart building applications, potentially contributing to reduced energy consumption and environmental impact.

Overall, these studies collectively highlight the significant advances being made in integrating cellulose-based materials and novel composites into construction practices. They pave the way for more sustainable, efficient, and high-performance building solutions, reflecting a growing trend toward utilizing renewable and innovative materials to address the challenges faced by modern construction.

4. Nanocellulose computational simulations

MD simulation enables qualitative study of the behavior of large molecules at the molecular scale, providing deeper insights into various physical phenomena, including molecular arrangements, interactions, and mechanisms. Such information is invaluable for the design of systems in various applications. For example, MD simulations can elucidate the trajectory of molecules and chains in various processes, providing structural and dynamic insights, as well as detailing the thermodynamic, thermal, and mechanical properties of the system [20]. Valencia *et al*. [131] investigated the behavior of CNF/graphene oxide (GO) layered membranes during real-time filtration of water and metal ions. Their study utilized in situ small angle X-ray scattering (SAXS) and real-time computational simulations using reactive molecular dynamics (ReaxFF). SAXS analysis confirmed that GO layers effectively limited swelling and structural deformation of CNFs during the filtration of aqueous solutions. Moreover, during the filtration of metal ion solutions, the CNF-GO network bond exhibited increased complexity, with the mass fractal and correlation length increasing. In addition, SAXS data indicated the apparent formation of nanoparticles during the drying phase after ion adsorption, with particle size increasing with time. Molecular dynamics simulations provided detailed insights into the assembly of both components and elucidated the motion of the metal ions, potentially leading to metal cluster formation during adsorption. In addition, these simulations confirmed the synergistic behavior of GO and CNF in water treatment applications. The adsorption properties of GO were demonstrated for various heavy metal ions such as Cd (II), Co (II), Eu (II), and U (VI). This efficient adsorption capacity was due to the hydrophilic nature of GO and the presence of oxygen-containing functional groups, which enabled effective bonding with metal ions. In this study, an ultrathin layer of GO was deposited on a relatively thick, porous CNF lattice by vacuum filtration [133].

Roig-Sanchez *et al*. [132] investigated nanocellulose films integrated with multiple functional nanoparticles distributed in a confined space. Using artificial pathways facilitated by efficient microwaves, mineral nanocrystals were nucleated and grown within cellulose fibers. Subsequently, functional bacterial cellulose layers were assembled into stacked configurations within the fiber structure by simple layering and drying of wet layers at 60 °C, resulting in coarse, thick films. The structural, functional, and mechanical integrity of these sheets was extensively investigated. Molecular dynamics simulations were used to calculate the surface energy of adhesion between two cellulosic fibers, and the results were compared with experimental peeling data to elucidate the separation behavior of the sheets. In a study by Roig-Sanchez *et al*. [132] the feasibility of the method was demonstrated by providing data on different films, each approximately 50 mm thick, containing up to four types of particles regularly distributed across the film cross-section. As a result, flexible nanocomposites of renewable materials with controlled nanoparticle properties were successfully produced. Both the topographic distribution of nanoparticles and the volume fraction of particles within the porous framework were manipulated using simple techniques. This approach sets the stage for the integration of numerous features and geometric configurations into flexible cellulose-based substrates. While the study presents only a few examples of this concept, the potential applications extend to multifunctional sensors, nanostructured devices, and reactors designed for multiple catalytic effects where specific functionalities are confined to well-defined spatial regions.

Chen *et al*. [133] investigated the effects of surface modification on nanocellulose through molecular dynamics simulations using parasitic sampling and computational alchemy. Topochemical modification of nanocellulose particles, particularly acetylation, is a common practice aimed at reducing hygroscopicity and improving dispersion within nonpolar polymers. Despite extensive experimental efforts to modify cellulose surfaces, a comprehensive model that accounts for (a) the specific interactions between nanocellulose particles and the surrounding liquid or polymer matrix and (b) the interactions among the particles themselves is lacking, with the latter often being overlooked. The current approach is based on atomic MD simulations, where computational alchemy is used to quantify changes in the interactions between nanocellulose and the environment (liquid or polymer) after modification. This is complemented by another method based on the average force potential to calculate particle-particle interactions. The results underline the comparable importance of both contributions in the context of surface acetylation effects on nanoparticles. Moreover, the proposed method transcends the confines of cellulose or acetylation and holds potential for specialized applications across a broad spectrum of nanomaterial designs. This excerpt discusses molecular dynamics simulations performed by Kumari *et al*. [134] to study the structural and mechanical properties of a hydrogel composed of cellulose and callose in water. The simulations involve large samples containing millions of atoms ($1.6 \cdot 10^6$ atoms), simulating compositions ranging from pure cellulose to varying ratios of cellulose and callose. The simulated hydrogel closely mimics experimental hydrogels to gain insight into the properties of the plant cell wall. Key findings include the formation of stable networks through cross-links between cellulose, callose and water molecules, leading to hydrogel properties beyond those of a simple polysaccharide-water suspension. However, there are some discrepancies between computational and experimental estimates of mechanical properties such as bulk modulus and Young's modulus, likely due to oversimplified simulation procedures and inadequate relaxation times. The simulations reveal nonlinearity in the stress-strain relationships due to the large number of links connecting nanofibers and chains, which may affect the estimation of mechanical properties. In addition, the role of callose in improving water uptake and slowing dye release suggests potential applications in drug scaffold design. The study also provides a trajectory library for systems with varying cellulose and callose concentrations, facilitating the development of coarse-grained models for larger-scale simulations.

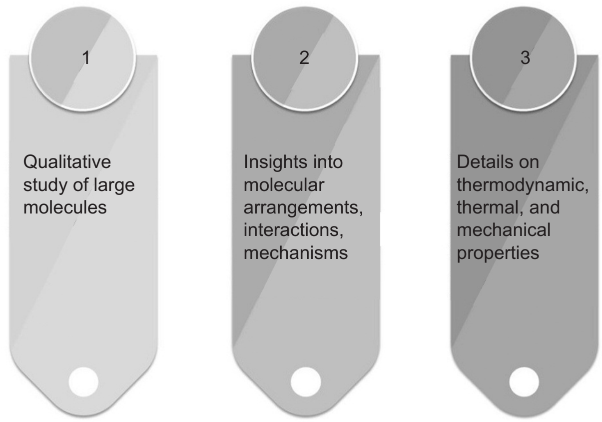

Figure 11. Importance of Nanocellulose Computational simulations.

Future directions include the incorporation of additional polysaccharide types and peptides to better understand plant cell wall dynamics and their implications in various fields such as biology, biomedicine, pharmaceuticals, and nanoengineering. Based on the text, the objective of the simulation can be summarized in Figure 11.

In summary, the recent advancements in MD simulations have markedly advanced our comprehension of nanocellulose and its myriad applications. The ability of MD simulations to offer deep insights into molecular behaviors, interactions, and properties has proven crucial for the development and optimization of nanocellulose-based materials. The research conducted by Valencia *et al*. [131] has demonstrated the enhanced filtration capabilities of nanocellulose-graphene oxide membranes, highlighting their potential for improving water treatment technologies. Roig-Sanchez *et al*. [132] revealed how integrating functional nanoparticles into nanocellulose films can lead to advanced material properties, paving the way for novel applications in sensors and catalytic devices. Chen *et al*. [133] provided a comprehensive model of surface modifications on nanocellulose, which is vital for tailoring nanomaterials for specific applications. Furthermore, Kumari *et al*. [134] underscored the potential of cellulose-callose hydrogels in drug scaffold design, despite some discrepancies with experimental data. These studies underscore the transformative impact of computational simulations on material science, demonstrating that MD simulations are essential tools for exploring and enhancing the properties of nanocellulose. As research continues to evolve, the integration of simulation methods with experimental approaches will further advance the field, enabling the development of innovative nanocellulose materials with tailored functionalities for a wide range of applications.

5. Conclusion

The environmental concerns in this era motivate the researchers who work on the synthesis of functional materials to pay more attention to the sustainability and renewability of the components used. Nanocellulose that can be extracted from cellulosic waste materials can upgrade waste management and waste utilization. It can be also produced by microorganisms, which are sustainable resources. Considering the results described here, the physical properties of NC depend upon the source and procedure used for its extraction from plants or the culture media used for microorganism cultivation. As this review reveals, applications of NC in producing functional materials are diverse and range from the food and cosmetics industry to civil and construction engineering because of their renewability and sustainability. Accordingly, NC plays a significant role in the sustainable development of different science and engineering. NC, as a green nanomaterial, also has potential applications in the field of water and wastewater treatment. Moreover, it has exhibited a high potential for evolving industries like biomedical manufacturing and electrical engineering. It is worth mentioning that the functionalization of NC not only enhances their properties but also gives them new, improved properties. For example, the hydrophilic nature of NC that limits some applications of NC can be overcome by its surface modification. However, the environmental aspects of chemicals and, most importantly, the toxic effects of additives used for this purpose should be precisely studied. From sustainable viewpoints, systematic studies into developing novel applications of NC are all exciting avenues for future researchers.

6. Future aspects

From a sustainable development viewpoint, the usefulness of NC for various applications is clear. However, there is a lack of environmental and economic inspections of the methods used for the synthesis of NC itself and its products. As mentioned in this paper and other reviews, a number of different methods have been introduced for these purposes, and future research should focus on developing scalable and cost-effective methods accompanied by accurate sustainability assessments. In this way a systematic study should be developed for precise inspections of the impacts of chemicals and waste used or generated. Although the application of NC in various areas appears promising, the toxicity effects of NC should be well studied in vivo and in vitro. In these respects, the side effects of NC and its interaction mechanism with cells must be well understood. The in vivo surveys are crucial for broader and unconstrained applications of NC, especially in human health and food products. Novel manufacturing routes like additive manufacturing and self-assembly can offer marvelous advantages for developing the next generation of NC-based products with high performance. Artificial intelligence and machine learning-based algorithms may help in different areas related to NC or NC-based production; for example, optimization, modeling and simulation.

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