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Engineering Design Principles of Biomass-Derived Porous Carbon for Adsorption–Antibacterial Synergy

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Abstract

Porous carbon obtained by biomass has gained great interest as an eco-friendly highly versatile material due to its renewable source, controllable pore structure, and modifiable surface chemistry. Although BDPC has found extensive application in the adsorption-based removal of organic and inorganic impurities, recent reports suggest that rational structural and chemical engineering can be used to confer intrinsic antibacterial activity to BDPC, thus giving rise to a synergistic adsorption -antibacterial platform. This paper offers an overall engineering design strategy of BDPC that incorporates the biomass precursor choice, regulated carbonization, and activation, optimization of hierarchical pore architecture, and heteroatom-mediated surface functionalization concurrently to amplify the contaminants adsorption and bacterial inactivation. The effect of the micro mesoporous structures on adsorption capacity and mass transfer and how surface defects and heteroatom doping may promote the bacterial membrane disruption and oxidative stress are systemically discussed. Key mechanistic pathways that control the adsorption kinetics, electrical interactions, reactive oxygen species formation, and contact-centred bacterial inactivation are discussed critically to explain the root causes of multifunctional performance. Moreover, uniform measures of adsorption efficiency, antibacterial performance, reusability, and structural stability are defined so that meaningful comparison of their performance can be made. Another issue that is approached practically is the challenge of scalability, environmental safety and regeneration strategies. This work has given concrete rules of designing high-performance BDPC materials with the capability of eliminating chemical and biological isobutyls at the same time by integrating relationship of structure, property, and functional aspects. The suggested architecture contributes to the development of the porous carbon systems based on a circular economy and next-generation water purification, environmental cleanup, and anti-bacterial uses.

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Introduction

International issues of water pollution and microbial contamination.

The rapid process of industrialization, urbanisation, and population increase have increased the emission of organic pollutants, toxic heavy metals, dyes, and venomous microorganisms into the water body to threaten the well-being of the population and ecosystem to a high extent. Traditional water treatment technologies tend to treat chemical and biological contaminants independently and therefore contribute to the complex treatment trains, higher operational costs and secondary contaminated water pollution. Besides, the emergence of antimicrobial resistance in the world has revealed the proximity of conventional disinfection approaches, especially those that apply to the use of chemical biocides or metallic-based products. As a result, there is a pressing need of structural materials, which, in turn, can eliminate chemical pollutants and, at the same time, destroy pathogenic microorganisms in a sustainable, efficient, and environmentally harmless way.

Shortcomings of Traditional Adsorbent and Anti-bacterial Matters.

Activated carbon is still the standard in adsorption with a large surface area and chemical stability but most of the commercially produced activated carbons use raw products that are fossil-based which means they are energy-intensive, expensive, and environmentally strainful. More importantly, standard activated carbon does not have inherent bactericidal properties and will be prone to biofouling, blockage of pores and performance loss over time when used. Even though there have been the introduction of antibacterial additives like silver or copper nanoparticles to adsorbents, the issue of metal leaching, cytotoxicity, and the accumulation of the metal in the environment in the long-term remain of concern. These restrictions incite the necessity of other carbonaceous materials which must be efficient in adsorption but have inbuilt antibacterial properties without undermining their sustainability and safety.

Biomass-Derived Multifunctional Porous Carbon.

Due to its renewable feedstocks, low cost of production and remarkably high structural tunability, Biomass-derived porous carbon (BDPC) has become a promising alternative. Agricultural remains, forestry wastes and food by-products offer a lot of carbon sources which can be processed to form porous carbons with specified pore structures and surface chemistries through an efficient process of controlling carbonization and activation reactions. Recent investigations prove that BDPC has the potential to attain high adsorption capacities in a large variety of contaminants at the same time presenting antibacterial properties due to defect-rich surfaces, heteroatom doping, and hierarchical porosity. This multifunction allows an adsorption/antibacterial synergist to inhibit microbial growth, biofouling, extend the lifetime of the material which makes BDPC very appealing when it comes to purifying water as well as remediate polluted environments.

Research Gap and Scope of Present Study.

Although there is an increasing trend in the study of BDPC-based multifunctional materials, much of the current literature only addresses the adsorption and antibacterial performance of the materials in isolation with little regard to the principles of integrated engineering design that can connect processing parameters and structural characteristics with synergistic functionality. An organised structure aligning the selection of biomass precursors, the ability to engineer pores, tune surface chemistry and anti-bacterial systems is not well established. To bridge this gap, the current research paper puts forward a holistic engineering design viewpoint of BDPC, that is, rational co-optimization of the adsorption capacity and antibacterial efficacy. In explaining the structure-property-function relationships and mechanistic pathways, this piece of work will be used to offer clear indications on designing the next-generation, sustainable porous carbon materials as multifunctional water treatment units.

Literature Review

Porous Carbon-Based Biomass Adsorption.

Biomass-based porous carbon (BDPC) is a promising option that has got extensive research as an alternative to fossil-based activated carbon based on its renewable feedstock, low production cost, and controllable physicochemical properties. A wide range of agricultural and forestry wastes containing rice husk, coconut shell, corn cob, bamboo and sawdust have been transformed into porous carbons that have large surface areas and highly developed pore structures that facilitate easy adsorption of dyes, pharmaceuticals, antibiotics, pesticitives and, heavy metal ions.[1, 5, 6] BDPC adsorption activity depends mostly on specific surface area, size distribution of pores, surface functional group and charge characteristics of surfaces. KOH and H 3 PO 4 have been reported to chemically activate surfaces to form ultrahigh surfaces that were as high as 1500 m 2/g, resulting in a high adsorption capacity and faster adsorption kinetics.[5] However, microporosity can limit mass transfer in aqueous system when it is too high, highlighting the potential of combating it with hierarchical pore structures to incorporate a combination of micro- and mesopores that can be more accessible and enhance mass adsorption efficiency.[11]

Antibacterial Properties of Carbon-Based Materials.

Activated carbon, graphene-based structures, carbon nanotubes and heteroatom-doped carbons, which are carbon-based materials, have been found to have intrinsic antibacterial effect over a variety of physicochemical mechanisms. The reported antibacterial signalling is physical membrane disruption of the bacteria, oxidative stress caused by reactive oxygen species (ROS), interruption of cellular respiration, and nutrient deprivation effects.[3, 4] The heteroatoms include nitrogen, sulphur, and phosphorus donor carbons derived from biomass with superior antibacterial activity as the number of defects increases, the redistribution of charges is more localised, and the molecular surfaces become more polarised.[12] When compared to antibacterial agents based on metal, metal-free carbon materials perform better with respect to chemical resistance, fewer cytotoxic effects, and less chances of developing antimicrobial resistance, hence can be applied to long-term water treatment systems.[4]

Adsorption-Antibacterial Synergistic.

Recent studies have paid more attention to multifunctional materials that have the potential to eliminate chemical contaminants and destroy pathogenic microorganisms at the same time. Porous carbon scaffolds offer a special adsorptionantibacterial synergy with a high-level of contaminant uptake combined with direct microbial inactivation.[2] Antibacterial metals or metal oxides including silver, copper, zinc oxide or photocatalytic constituents supported on BDPC have been demonstrated to exhibit increased bactericidal activity in hybrid systems.[3] Nevertheless, its extensive use is limited by its disadvantages associated with the possible leaching of metals, secondary pollution and the environmental toxicity in the long term. Consequently, intrinsic antibacterial pore engineered that have been developed using BDPCs on the basis of surface defect modification, heteroatom doping, and surface defect modulation is becoming popular.[7, 8] In spite of these developments, the majority of the research still considers evaluating adsorption and antibacterial properties in isolation and therefore it can be argued that there is a need to incorporate engineering design ideals that interrelate both the structure and surface chemistry as well as the combined multifunctionality.

Methodology

Biomass-Derived Porous Carbon Synthesis.

To produce customised both pore structures and surface features, a regulated carbonization activation pathway to produce biomass derived porous carbon was used. As a first step, chosen biomass precursors were diligently washed with deionized water so as to remove the sticking impurities, soluble biomass, and the organics as well as the inorganic contaminants after which they were dried in the oven at temperatures of between 80 and 105°C in order to remove the remaining moisture. A uniform particle size was then mechanically broken and sieved to obtain the dried biomass to make sure of uniform thermal treatment in further processing.

Carbonization was conducted in a tubular furnace in an atmosphere of constant nitrogen pressure to stop the natural loss of oxidants. Heat was incrementally applied on the biomass until it reached a desired temperature, which is commonly approximately 500-800 o C, and held at a certain residence time to transform the organic materials into carbon filled biochar. This process helped in the breakdown of cellulose, hemicellulose, and lignin keeping the carbon skeleton and original pore structure.

Potassium hydroxide was subsequently used as the activating reagent in order to do chemical activation in order to come up with a well-defined porous structure. The optimization of mass ratios of biochar and KOH was carried out by impregnating the biochar with KOH, then thermal activation at high temperatures in a nitrogen atmosphere was done as shown in Figure 1. In the activation, KOH favoured redox reaction and pore expansion by the presence of gases and led to the formation of interconnected micro- and mesopores. The same procedure was reiterated after the activation process to wash the carbonised product with dilute acid, and deionized water to achieve neutral pH, and eliminate any residual activating agents and inorganic by-products. Lastly was the collection of biomass-porous carbon which was dried and stored to be characterised and evaluated in terms of performance.

Structural and Surface Characterization

Combined textural, mo0rphological, and spectroscopic methods and analysis of the structural and surface

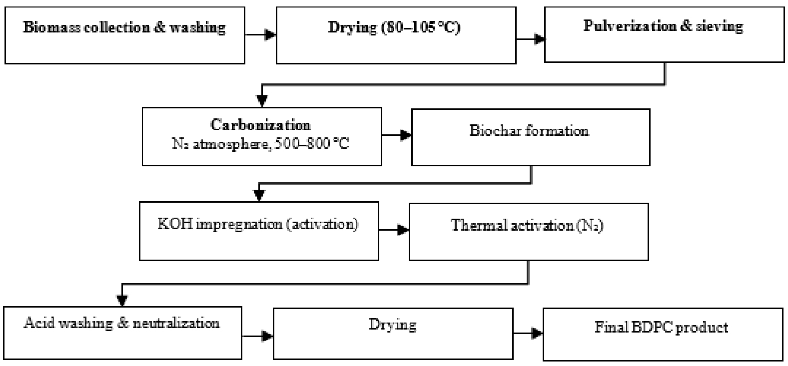

Fig. 1: Schematic illustration of the synthesis process of biomass-derived porous carbon via carbonization and KOH activation.

features of the biomass-derived porous carbon (BDPC) were explored systematically to determine structure-property correlation. To measure the textural properties of the texts the Nitrogen adsorption-desorption measurements were conducted at 77 K. Specific surface area was determined through Brunauer-Emmett-Teller (BET) method, the total pore volume and the size distribution of pores was determined through Barrett-Joyner-Halenda (BJH) and density functional theories (DFT) models. The form of the adsorption desorption isotherms and the existence of the hysteresis loops were studied to determine co-existence of micro-, meso-, and macroporous structures.

Surface roughness, pore opening and particle morphology was observed by scanning electron microscopy (SEM) looking at surface morphology and pore architecture. To measure the formation of hierarchical porosity at nanoscale inside the tissue, transmission electron microscopy (TEM) was utilised to give high resolution images of internal pore networks and to ensure the formation of a network of pores. These studies allowed the direct correlation of the conditions of synthesis and the formation of pore structures.

The structural order and the density of defects in the carbon framework were assessed with the help of Raman spectroscopy. The ratio of the intensity of the disorder induced D band to the graphitic G band (ID/IG) was summed up to determine the extent of graphitization and the occurrence of defect sites, which are linked with the inclusion of the heteroatoms and the formation of pores. The spectroscopy using the Fourier-transform infrared (FTIR) was performed to determine the surface functional groups, hydroxyl, carbonyl and carboxyl functionalities that are important in adsorption as well as antimicrobial interactions. The X-ray photoelectron spectroscopy (XPS) was also utilised to infer elemental compositions, chemical bondings of elements, and heteroatom doping configurations offering an in-depth analysis of the surface chemistry and functionalization.

Adsorption and Antibacterial Performance Evaluation.

The effectiveness of the biomass-derived porous carbon (BDPC) in adsorption was tested by carrying out batch adsorption tests on representative organic dyes and metal heavy ions as a model pollutant. Determined amounts of BDPC were sprinkled in contaminant solutions of known concentrations and swirled in a constant temperature to have equal contact. The impact of the key functional parameters that are the contact time, the initial contaminant concentration, and the pH of the solution was systemically examined. The number of contaminants present as residues was also measured by the corresponding analysis methods and the adsorption

Table 1: Experimental conditions for adsorption and antibacterial performance evaluation of BDPC

Category	Parameter	Demscription / Conditions
Adsorption Experiments	Adsorbent dosage	Fixed mass of BDPC added to contaminant solution
	Model contaminants	Organic dyes and heavy metal ions
	Initial concentration	Predetermined concentration range
	Solution pH	Systematically varied using acid/base adjustment
	Contact time	Monitored over defined time intervals
	Temperature	Maintained constant during experiments
	Agitation speed	Continuous shaking to ensure uniform mixing
	Analytical method	Residual concentration measured using standard analytical techniques
	Adsorption capacity	Calculated using mass balance equations
Adsorption Modeling	Kinetic models	Pseudo-first-order and pseudo-second-order models
	Isotherm models	Langmuir and Freundlich isotherms
Antibacterial Evaluation	Bacterial strains	Gram-positive and Gram-negative bacteria
	Exposure conditions	BDPC contacted with bacterial suspension
	Viability assessment	Colony-forming unit (CFU) counting
	Membrane integrity	Live/dead fluorescence staining
	Damage mechanism	Permeability and intracellular leakage assays
Reusability & Stability	Number of cycles	Multiple adsorption-disinfection cycles
	Regeneration method	Washing or desorption treatment
	Performance metrics	Retention of adsorption capacity and antibacterial efficiency

capacity computed on the basis of the mass balance principles. The pseudo-first-order and pseudo-second-order adsorption models were used to understand the adsorption mechanisms, the rate-limiting stages, and equilibrium data were modelled to Langmuir and Freundlich isotherms so as to learn about adsorption behaviour, homogeneity of surfaces, and adsorption maximum capacity.

The efficacy was evaluated with reference to the Gramme-positive and Gramme-negative bacterial strains commonly used to determine the broad-spectrum effect. BDPC was subjected to a bacteria suspension under controlled conditions, and the efficiency of bacteria was measured using colony-forming unit (CFU) counting in the assessment of bacterial viability. The relative membrane integrity and cell viability were visually assessed by using live/ dead fluorescence staining with permeability and leakage being used to further investigate membrane damage. These complementary methods allowed me to obtain mechanical understanding of the mechanisms of inactivating bacteria, such as membrane disruption and oxidative stress.

The stability of BDPC in terms of reusability and operational stability Table 1 was tested by using several adsorption-disinfection cycles. The material was then recycled following the proper desorption or washing procedures and reused under the same conditions after each cycle. The durability, structural integrity, and long-term performance were important measures that were observed by evaluating how changes in adsorption capacity and antibacterial efficiency changed with successive cycles, which is appropriate to practical water treatment processes.

Results and Discussion

Structural Properties and Surface Chemistry.

According to the nitrogen adsorption desorption analysis and electron microscopy, the developed biomass porous carbon (BDPC) had hierarchical pore structure with interconnected micro pores and mesopores. Micro pores helped to achieve high specific surface area which offered large numbers of adsorption sites whereas the mesopores offered high efficiency in mass transport and accessibility to the internal surfaces. The regulated chemical activation production was a defect-ridden carbon frame with a balanced distribution of pore networks to avoid collapse of the pores in the frame, thereby improving structural stability. The surface analysis showed there were some oxygen-and nitrogen-containing functional groups, which enhanced surface polarity and hydrophilicity. Raman spectroscopy also verified a high density of the defects as the ID/IG ratio was high that suggested the successful incorporation of the structural defects and other active sites supported by the heteroatoms, which is beneficial to adsorption and antibacterial interaction.

Adsorptions Behaviour and Mechanical insights.

BDPC showed a good adsorption capability to organic and inorganic pollutants in batch mode and fast uptake was recorded at the first contact mode. Such a tendency may be explained by the synergistic action of hierarchical porosity and surface functionalization, which simultaneously decreased the resistance to diffusion and increased the adsorbate-adsorbent interactions. Kinetic analysis showed that the adsorption behaviour was pseudo-second-order that is chemisorption prevailed in the whole process with exchange or share of electrons between surface functional groups and contaminant molecules. Equilibrium isotherm analysis was indicative of desirable adsorption characteristics of high affinity towards the target contaminants. It also increased adsorption selectivity by incorporating heteroatoms (nitrogen) to generate localised charge positions, initiated electrostatic interactions and surface complexation reactions, especially with charged organic molecules and metal ions.

Mechanisms of Antibacterial Performance and Inactivation.

The antibacterial assessment also indicated that BDPC had a high bactericidal effect on Gramme-positive and Gramme-negative bacterial strains with a significant reduction in viable cell counts being achieved upon exposure within a very short duration. It is believed that the observed performance with respect to antibacterial activity is based on several synergistic effects, such as the direct physical perturbation of bacterial cell membranes whenever they come into direct contact with the coarse and pitting carbon surface. Also, oxidative stress and electron transfer induced on the surface disturbed the bacterial metabolic activity, which caused permanent cell damage. Contact-mediated antibacterial action was confirmed by live-dead staining and membrane integrity tests which indicated damaged cell membranes and release of intracellular levels. Heteroatom-doped functional groups also reinforced the electrostatic interactions between bacterial adhesion and inactivation to bacterial growth, thereby promoting the broad-spectrum antibacterial activity.

Adsorption Antibacterial Synergy and Reusability.

The major benefit of BDPC is that it has adsorption and antibacterial properties simultaneously and it created

Table 2: Comparative structural, adsorption, antibacterial, and reusability performance of BDPC and baseline carbon

Performance Aspect	Parameter	Baseline Carbon	BDPC	Key Interpretation
Structural Properties	Pore architecture	Predominantly microporous	Hierarchical micro-mesoporous	Hierarchical pores enhance mass transport
	Surface functional groups	Limited oxygen groups	Abundant O- and N-functional groups	Increased surface polarity and activity
	Defect density (ID/IG)	Low	High	Defect-rich structure favors adsorption and antibacterial action
Adsorption Performance	Adsorption capacity (mg g□¹)	Moderate	High	More active sites in BDPC
	Adsorption kinetics	Slower uptake	Rapid initial uptake	Reduced diffusion resistance
	Dominant mechanism	Physisorption	Chemisorption-dominated	Strong surface interactions
Antibacterial Activity	Antibacterial reduction (log CFU)	Low	High	Effective membrane disruption and oxidative stress
	Spectrum	Limited	Broad (Gram ±)	Enhanced surface-bacteria interactions
Reusability & Stability	Performance retention after cycles (%)	Moderate decline	High retention	Suppressed biofouling in BDPC
	Structural stability	Partial degradation	Structurally robust	Stable pore framework

strong synergistic effect in repeated operation cycles. Adsorption of organic constituents decreased the nutrient supply needed by the bacterial growth hence decreasing the proliferation of microbes and biofilm development on the carbon surface Figure 2. At the same time, intrinsic antibacterial activity inhibited bacterial colonisation and blockance of the pore and maintained adsorption efficiency after numerous reuse cycles Table 2.

Regeneration experiments showed that there was a low loss in adsorption capacity and antibacterial activity and this reveals the structural strength and stability of the substance used. Such synergistic action is important in deterring biofouling, increasing the lifespan of the material and upgrading the performance of the treatment over time, which demonstrates the potential of BDPC as multifunctional material in the use of sustainable water purification systems.

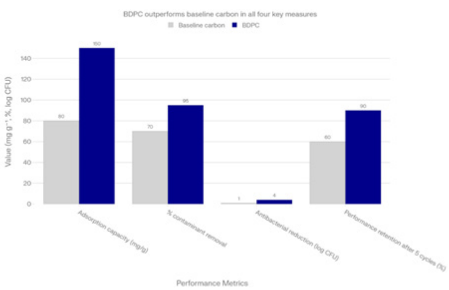

Fig. 2: Comparison of BDPC and baseline carbon performance.

CONCLUSION

This paper includes an in-depth engineering design framework of the creation of biomass-based porous carbon (BDPC) that incorporates adsorption and antibacterial properties. By using the rationale selection of biomass precursors, controlled carbonization, with chemical activation, hierarchical pore architecture, surface chemistry adjustment, BDPC was shown to provide high contaminants capturing efficacy common to the biomass, and successful bacteria inactivation. Their presence in coexistence created high levels of adsorption sites and increased mass transport capabilities through the micro- mesoporous structures, and the presence of heteroatoms as functional groups and high-affinity interactions with the adsorbates and contact-mediated antibacterial capability through discrete defects. Notably, a terrific combination of adsorption and antibacterial processes found effective in reducing biofouling, maintaining adsorption activity in a repeated use, and enhancing the stability of operations. These findings indicate the promise of BDPC as a sustainable, multipurpose material in the future use of advanced water purification and remediation of the environment. The future studies need to focus on scalability of synthesis through environmentally friendly strategies, extensive long-term performance assessment, and testing of BDPC scale when operating in realistic conditions to enable the bridging of the gap between the developed BDPC in the laboratory and in the field.

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