Effect Pore Structure of Nanoporous Material and Prospect on Daily Applications

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Abstract. Nanoporous materials with tunable pore structures and exceptional physicochemical properties become a pivotal component in material science, driving advancements in filtration, catalysis, and environmental remediation. This study focuses on the intrinsic relationship between pore structure (size, shape, connectivity, and distribution) and the macroscopic performance of nanoporous materials. Key research indicates that micropores could improve small-molecule adsorption, mesopores (2–50 nm) optimize catalytic efficiency, and macropores (>50 nm) facilitate rapid mass transport. Ordered pore structures improve directional diffusion, while disordered pores offer abundant adsorption sites. Advanced methods such as template-assisted synthesis and microwave heating allow for precise arrangement over pore structures achieving high specific surface areas (up to 3000 m^2/g) and tailored functionalities. Challenges in pore uniformity, scalable synthesis, and mechanical stability were identified, alongside solutions like interdisciplinary optimization and eco-friendly techniques. This work provides theoretical insights and practical guidelines for designing high-performance nanoporous materials, fostering their application in addressing global energy and environmental challenges.

Keywords: Materials; Structure; Efficiency; Remediation.

1. Introduction

Materials science is booming, nanoporous material plays a significant role in the field of material science and has become the focus of research because of its particular structure and potential application. Nanoporous materials exhibit unique characteristics that distinguish them in various applications. Firstly, they possess an exceptionally high specific surface area due to the presence of numerous nanoscale pores, which provide a vast number of active sites. This feature is particularly advantageous for applications such as adsorption and catalysis. For example, activated carbon can achieve a specific surface area exceeding several thousand square meters per gram, enabling efficient gas and impurity adsorption. Secondly, the pore sizes of these materials are tunable. By modifying preparation methods and process conditions, pore sizes can be precisely controlled to meet the requirements of diverse application scenarios. In gas separation, for instance, materials with pore sizes tailored to specific gas molecules can be designed for efficient gas separation. Thirdly, nanoporous materials exhibit low density. The internal structure, rich in pores, results in a low overall density while preserving adequate mechanical properties. This characteristic makes them ideal for fabricating lightweight components in industries such as aerospace and automotive, where weight reduction is crucial without compromising performance. Lastly, these materials demonstrate excellent permeability. The abundance of channels facilitates rapid substance transport, enhancing the penetration and diffusion of gases and liquids within the material. This property is highly beneficial for applications including separation, filtration, and battery technology. Recent research in the field of nanoporous materials has been quite diverse. The traditional method of synthesizing porous materials via conventional electric heating is energy-intensive and time-consuming. However, microwave heating, which is commonly used in homes for heating food, has emerged as a powerful alternative in the synthesis of nanoporous materials. This microwave-assisted synthesis offers a more

straightforward, rapid, efficient, and cost-effective way to produce advanced nanomaterials such as silicas, carbons, metal-organic frameworks, and metal oxides. These materials typically have high specific surface areas and show great potential in applications like gas adsorption, water treatment, and more [1]. In terms of studying the physical properties of nanoporous materials, demonstrates a technique based on Monte Carlo resolution of the Boltzmann transport equation related to the Green - Kubo autocorrelation of the phonon heat flux. This method, which evolved from a prior study, is utilized to predict the thermal conductivity tensor of nanoporous structures, for instance, in Si porous matrices and Si phononic membranes at room temperature, taking into account various porosities and pore network arrangements and comparing results with existing data and models [2]. Additionally, points out that despite the well-documented confinement and surface effects in nanoporous hosts, the transport of nanoconfined fluids remains complex and not fully understood. With phenomena like memory and intermittent dynamics challenging traditional theories, especially for molecular-sized pores, and lacking a microscopic theory for collective diffusion, the concept of "De Gennes narrowing" is introduced. Molecular simulations reveal an important connection between wavevector-dependent collective diffusivity and the fluid's structural ordering imposed by the nanoporous host, and it is shown that the fluid collective dynamics can be accurately characterized using this concept [3].

Although there has been some progress in the research of nanoporous materials, a comprehensive and systematic review is still lacking. On the one hand, while the applications of nanoporous materials in different cases have been demonstrated, there is a lack of in-depth analysis of their commonalities and differences, which is not conducive to summarizing the rules to guide more extensive applications. On the other hand, the research on the pore structure, characteristics and preparation methods of nanoporous materials has not been closely integrated with practical applications, resulting in a low efficiency of converting research results into practical applications. Therefore, this paper focuses on exploring the intrinsic connection between pore structure and macroscopic properties and will rely on the study of the influence law of pore structure parameters on material properties. This paper aims to conduct a comprehensive and systematic study of nanoporous materials, deeply analyze their structure, performance, application and development direction, provide theoretical support and practical guidance for the further research and application of nanoporous materials, and promote the development of this field.

2. Fundamentals of Nanoporous Materials and Preparation of Pore Structures

2.1. Definition and Structural Characteristics of Pore Structure of Nanoporous Materials

The pores of nanoporous materials mainly refer to the voids with pore sizes in the nanoscale range, usually between 0.1 nm and 100 nm. This size range gives the material special physicochemical properties that are distinctly different from macroscopic porous and non-porous materials. They can be categorized by pore size into micropores, mesopores and macropores. The pore size of microporous is less than 2 nm, its internal specific surface area is large, the adsorption of small molecules is strong, widely used in gas separation, molecular sieve and other fields, such as zeolite molecular sieve materials in the microporous structure can be realized on a specific size of molecules sieving. The pore size of mesopore is between 2nm and 50nm, mesopore has moderate pore size, which is conducive to the diffusion and transmission of larger molecules, and is commonly used in catalyst carriers and adsorbent materials, such as mesoporous silica materials, which can be loaded with the active components of catalysts to improve the efficiency of catalytic reactions. Macroporous pore sizes greater than 50nm, large pores are conducive to rapid transmission and diffusion of substances, and can be used as a channel for material transfer, in biomedicine, filtration and other fields have important applications, such as macroporous ceramic materials can be used for biological tissue engineering in the growth of cellular scaffolds. Pore sizes are characterized by large size spans and significant nanoscale effects. Nanoporous materials have a wide range of pore size distribution, from micropores smaller than 2 nm to mesopores of 2-50 nm to macropores covering larger than 50 nm, and this large size-spanning pore size range enables nanoporous materials to satisfy the

adsorption, separation, and transport of molecules and ions of different sizes. Due to the nanoscale pore size, the materials have a huge specific surface area that can provide a large number of active sites for various physicochemical processes. For example, the specific surface area of 1 gram of activated carbon can be as high as hundreds or even thousands of square meters, which makes its adsorption performance extremely outstanding.

According to the pore shape classification can be divided into spherical pores, cylindrical pores, slit-like pores and irregular pores. Spherical pores are formed with a spherical template agent as the core, which has unique advantages in gas adsorption and drug encapsulation, such as some nanoporous materials prepared by the template method. Spherical pores can provide uniform space, which is favorable for uniform adsorption of gas molecules and slow release of drugs. Cylindrical pores are cylindrical in shape with regular pore structure, such as some mesoporous carbon materials with cylindrical pores, this pore structure is favorable for the directional transport of molecules in the pores, which is more commonly used in separation membranes, electrode materials and so on [4]. Slit-like pores have pores similar to slits, commonly found in layered materials, such as graphene oxide and other layered materials, interlayer pores can form slit-like pores, which are favorable for the rapid transport and storage of ions, and have potential application prospects in fields such as supercapacitors. There is no obvious regularity in the shape of irregular pores, such as the pores in activated carbon materials, which have complex and diverse shapes, and this irregular pore structure can provide abundant adsorption sites and enhance the adsorption performance of the material, which is widely used in the fields of wastewater treatment and air purification. Pore shapes are diverse and anisotropic[5]. Pore shapes are rich and diverse, including regular shapes such as spherical, cylindrical and slit shapes, as well as a large number of irregular shapes. Irregularly shaped pores can provide more adsorption sites and complex diffusion paths, which are conducive to improving the adsorption capacity and separation effect of the materials. In some nanoporous materials, the shape of the pores may be anisotropic, i.e., the shape and size of the pores are different in different directions. This anisotropy can lead to materials exhibiting different physicochemical properties in different directions, offering the possibility of directional design and application of materials. Pore surface properties are characterized by high surface energy and abundant surface functional groups. Nanoscale pores have high surface energy, which makes the surface of the material have a strong adsorption effect on gases, liquids and other substances, and can quickly adsorb molecules in the surrounding environment, so as to realize functions such as gas purification and liquid separation. The pore surface usually contains a variety of functional groups, such as hydroxyl, carboxyl, amino, etc. These functional groups can be adsorbed with the material to have a chemical reaction or form a chemical bond, thus improving the selective adsorption and catalytic properties of the material[6].

According to the classification of pore connectivity can be divided into connected pores and isolated pores. Connectivity pore pores are interconnected to form a network structure, the material can be freely transported between the pores, such as porous ceramic materials in the connectivity pore structure, which is conducive to the rapid penetration and diffusion of gases or liquids inside the material, so that it plays an important role in the field of filtration, catalytic and other fields[7]. Isolated pores are independent of each other and are not connected, it is difficult for molecules to be transmitted between the isolated pores, some nanoporous materials obtained by special preparation methods may have isolated pores, isolated pores have a certain role in some special applications, such as sound insulation materials, thermal insulation materials, etc., which can prevent the conduction of heat or sound. Pore connectivity is characterized by a complex network structure and a large variation in connectivity. Connected pores usually form a complex three-dimensional network structure, which provides a channel for the transport of substances inside the material, which is conducive to improving the mass transfer efficiency of the material and enables the material to carry out rapid exchange of substances and reactions in the fields of catalysis and battery. The pore connectivity of different nanoporous materials varies greatly, some materials have good pore connectivity, in which substances can diffuse freely; while some other materials have poor pore connectivity, and there may be some isolated pores, which affects the overall performance of the material, and it is necessary to

select materials with appropriate connectivity according to the specific needs in the actual application[8].

The pore distribution characteristics are categorized as ordered pores and disordered pores. Ordered pores are regularly arranged inside the material with periodicity and symmetry, such as ordered mesoporous materials SBA-15, MCM-41, etc., whose pores are arranged in a hexagonal pattern, and this ordered pore structure is conducive to the directional transport and diffusion of substances, which has excellent performance in the fields of catalysis and separation. Disordered pore is the irregular distribution of pores inside the material, such as some natural nanoporous materials or porous materials prepared by simple methods, the distribution of pores is random, although the performance of disordered pore materials may be slightly worse than that of ordered pore materials, but due to their simple preparation and low cost, they are still widely used in some fields that do not require particularly high performance, such as ordinary activated carbon adsorption materials. The pore distribution of nanoporous materials has a highly ordered periodic arrangement, just like ordered mesoporous materials, there are also many materials with disordered pore distribution. Ordered pore distributions facilitate directional transport and precise control of substances, while disordered pore distributions may provide richer adsorption and reaction sites in some cases. By changing the preparation process and conditions, the pore distribution of nanoporous materials can be adjusted to realize different forms of distribution from uniform distribution to gradient distribution to meet the special requirements of material performance in different application scenarios, for example, in the field of drug slow release, the gradient distribution of pores can be designed to realize controlled release of drugs.

2.2. Methods for Preparation of Pore Structure of Nanoporous Materials

2.2.1 Activation methods

The physical activation method usually uses water vapor or CO2 as an activator, which reacts with the carbon material at a high temperature of 800-1000°C to etch the carbon skeleton and generate pores to form micropores and mesopores. The method is simple, low cost and suitable for mass production, but the pore distribution is random and the specific surface area fluctuates greatly. The chemical activation method, on the other hand, uses corrosive reagents such as KOH, NaOH, and ZnCl2 as activators, and the carbon precursor is immersed in the activator to orient the pores through a chemical reaction. The advantages are controllable pore size, accuracy to ±1nm, and specific surface area up to 3000m²/g [9].

2.2.2 Template method

The hard template method uses silica nanorods, polymer microspheres and other materials with certain shapes and sizes as templates, fills the holes or surfaces of the templates with a carbon source or other material precursors, and then forms materials around the templates through carbonization, deposition and other processes, and then removes the templates at the end, leaving behind regular holes corresponding to the templates' shapes and sizes[4]. The soft template method, on the other hand, utilizes self-assembly of surfactants, block copolymers, etc. to form micelles, liquid crystals, and other soft material structures as templates. These soft templates can form a specific ordered structure in solution, guiding material precursors to aggregate and react around them to form nanoporous materials with specific pore structures[10].

2.2.3 Hydrothermal/solvothermal methods

Metal salts, organic ligands and other raw materials are dissolved in water or organic solvents and put into a high-pressure reactor to carry out the reaction at a certain temperature and pressure. Under hydrothermal or solvent-thermal conditions, the reactant molecules have high activity and diffusion ability and are able to undergo complex chemical reactions to form nanomaterials with specific pore structures, such as metal-organic skeleton materials (MOF) and aluminum silicate-based nanoflower porous materials[11,12].

2.2.4 Electrochemical methods

The metal material is used as an anode and placed in a specific electrolyte, and by applying a certain voltage or current, an oxidation reaction occurs on the metal surface to form a nanoporous oxide film structure. The redox reaction in the electrochemical process is utilized to selectively etch the metal or other materials by controlling the electrode potential, electrolyte composition and other parameters to form pore structures[13].

3. Conclusion

Nanoporous materials demonstrate vast potential in filtration, catalysis, and environmental remediation due to their tunable pore structures. This study utilized electrospinning technology to fabricate polylactic acid (PLA) porous nanofiber membranes, revealing that the solvent ratio (DCM/DMAC) significantly influences pore formation, air/moisture permeability, and filtration performance, with the "breathing effect" and thermally induced phase separation identified as key mechanisms for surface pore generation. Optimized porous structures achieved high-efficiency, and low-resistance filtration, making them suitable for applications like mask materials. The diversity in pore size, shape, connectivity, and distribution enables functional design—for instance, ordered interconnected pores enhance catalytic mass transfer efficiency, while disordered high-surface-area pores improve adsorption capacity. However, challenges remain in controlling pore uniformity, scaling up synthesis (e.g., template removal costs), and balancing permeability with mechanical properties. Future work could consider developing environmentally friendly and scalable synthesis methods, e.g., self-assembly of soft templates using green solvents) to reduce energy consumption and cost; secondly integrate 2D materials (e.g., graphene, MOFs) or functional group modifications to enhance selective adsorption, catalytic stability, and multifunctionality (e.g., carbon dioxide capture, energy storage), and thirdly utilizing AI to predict pore structure-property relationships and accelerate the target material design, and finally extend applications to wearable devices, biomedical scaffolds, and degradable systems (e.g., nanocellulose-based materials) to promote sustainability. By optimizing preparation techniques, fostering interdisciplinary applications, and emphasizing environmental friendliness, nanoporous materials are poised to achieve breakthroughs in scientific and industrial fields, addressing global environmental and energy challenges.

Authors Contribution

All the authors contributed equally and their names were listed in alphabetical order.

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