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Review Article

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Preparation, types, and applications of one- and two-dimensional nanochannels and their transport properties for water and ions

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Abstract: Biological ion channels play an important role in living processes, such as maintaining osmotic pressure, signal transduction, and transmitting nerve impulses, and can selectively regulate the transmembrane transport of substances. Inspired by the structure and function of biological ion channels, researchers have prepared a variety of biomimetic nanochannels using advanced nanofabrication techniques to study the mechanism of ion transport in the nanoconfined space. In this study, we mainly introduce the current materials and preparation methods of nanochannels; compare the advantages and disadvantages of the current mainstream theoretical models and simulation software; clarify the influence of confinement effect and surface interface effect on the hydrogen bond structure characteristics and phase transition behavior of confined water in graphene nanochannels, revealing the driving effect of separation pressure in nanochannels on water transport, the micromechanical nature of the water flow boundary slip of nanochannels, and the dominant micromechanical mechanism behind the confined mass transfer phenomenon of nanochannels at different scales; and expound the regulation of nanomaterials based on ionic bond modification and the influence of ion transport properties in industrial desalination, energy enrichment, and detection. The future applications of nanochannel bionic design and regulation, ion-exchange filtration membranes, and ultra-high-speed water transport mechanisms are prospected.

Keywords: GO nanochannel, preparation and modification method, ion transport, confinement effect, mechanical mechanism

1 Introduction

When exploring the boundaries of nanotechnology, the ion transport phenomenon of nanochannels has become a hot topic in research due to its unique confinement effect. The confinement effect refers to a phenomenon in which a substance's physical and chemical properties change significantly when its size is reduced to nanometer level. This effect is particularly pronounced in the ion transport of nanochannels, where the nanochannel's size is comparable to the scale of motion of the ions, which greatly affects their transport behavior.

The ion transport mechanism in nanochannels is mainly influenced by confined domain effects, which alter the migration rate, selectivity, and conductivity of ions. According to Siwy and Fuliński [1], ion transport in nanochannels can be described by a single-ion transport mode, which depends on the size of the channel, the surface charge, and the concentration of the electrolyte solution.

The key to the design of nanochannels is to manipulate the chemistry and geometry of their internal surfaces to achieve specific ion selectivity and transport efficiency. By adjusting the diameter, length, and surface modification of the channels, researchers can design highly selective ion channels, which are of great importance in the fields of biomedicine, energy storage, and environmental monitoring. For example, Karnik *et al.* [2] demonstrated a high selectivity for ionic species by nanochannels in their work in 2007.

The influence of the confinement effect on ion transport is mainly reflected in two aspects: one is the enhanced ion selectivity, and the other is the change of transport kinetics. In the confined space at the nanoscale, the interaction between ions and the channel surface is enhanced due to the influence of surface effects and quantum effects,

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which leads to the improvement of ion selectivity. At the same time, the diffusion behavior of ions in the confined space is different from that in the macroscopic level.

With the continuous progress of nanotechnology and materials science, the research on nanochannel ion transport in China will be further deepened, especially in understanding and utilizing the confinement effect. Xia Fan, a professor at the School of Materials and Chemistry at China University of Geosciences (Wuhan), and his research group have focused on the surface functionalization and ion regulation mechanisms of nanochannels and have published three related articles in *Nature Communications*. These articles discussed the role of nanochannels in the regulation of ions by external functionalized molecules at different stages: first, the synergistic effect of external functionalized molecules and internal functionalized molecules to regulate ions [3]; second, the resistance of external functional molecules to environmental disturbances and their regulatory effect on ions [3], and finally, the study turned to the independent regulation of ions by external functionalized molecules without the participation of internal functionalized molecules [4]. Through the in-depth study of the "spatial confinement" effect of nanochannels, Prof. Xia Fan's team has opened up a new field of ion regulation on the outer surface of the channel in the "macroscopic environment," revealed a new mechanism of matter transport in the confined space, constructed a new interface that can be accurately functionalized and characterized, and developed efficient new technologies for a wider range of application scenarios. By precisely controlling the structure and surface properties of nanochannels, other scholars can design more efficient and selective ion transport systems in the future, which will revolutionize areas such as energy conversion, biosensors, and drug delivery.

2 Nanochannel preparation

A nanochannel is defined as having at least one dimension in the cross-section of a nanochannel, such as a length or width in the range of 100 nm. According to the structure and dimension of the cross-section, nanochannels can be divided into one-dimensional (1D) nanochannels and two-dimensional (2D) nanochannels.

2.1 Preparation of 2D materials

2D materials, including elemental and compound, can be divided into two types according to the way they are bonded between the layers of 2D materials: layered materials and non-layered materials. The controlled preparation of 2D materials and the exploration of their physical properties and new functional applications on this basis not only have important scientific research value, but also promote their wide application. At present, there are three main types of controlled preparation methods for 2D materials: micromechanical exfoliation, chemical vapor deposition (CVD), and liquid exfoliation.

2.1.1 Micromechanical stripping method

Micromechanical stripping is a routine method used to peel off layered bulk crystals using scotch tape to create thin flakes [5–7]. The original idea of the technique was to apply mechanical force through scotch tape to attenuate van der Waals interactions between the sheets. Without breaking the covalent bonds within the sheet layer, a single layer or a few layers of 2D materials are obtained. A typical example is graphene stripping: large crystals, such as graphite, are first attached to an adhesive on scotch tape and then peeled into thin sheets using another adhesive surface. The aforementioned process is repeated, and then, the tape is glued to the silicon wafer, and a single layer or a few layers of graphene are left on the target substrate. The crystals of 2D materials obtained by the micromechanical stripping method are of high quality, and the physical properties of all aspects are close to the theoretical eigen values, so they are widely used in the study of physical properties and devices. The efficiency is low, the yield is low, and the randomness is large.

2.1.2 CVD

CVD methods too have continued to evolve over the past few decades and are considered a reliable technology for mass production of large-area, ultra-thin 2D materials. In a typical preparation process, a pre-selected substrate is first placed into the furnace chamber and one or more gas/vapor precursors are passed through the furnace chamber, where the precursors can react or decompose on the substrate surface for modification purposes. By optimizing the experimental conditions, ultra-thin 2D materials, such as graphene [8], transition metal dichalcogenides, and heterojunctions [9–11], can be obtained on substrates. The 2D materials prepared by the CVD method have the characteristics of large area and high quality and are suitable for applications such as optoelectronic and flexible devices, but they face challenges such as high cost, room for improvement of crystal quality, and urgent need to solve the transfer method.

2.1.3 Liquid-phase stripping method

In the liquid-phase exfoliation method, a nanosheet dispersion of 2D materials is prepared by overcoming the interlayer adhesion of 2D materials through a certain external force in water or organic solvents [12]. The liquid-phase exfoliation method mainly includes the following methods: ion intercalation method, ion selection method, and ultrasonic-assisted exfoliation method.

Ion interpolation uses ions in the liquid phase to be inserted into the layers of bulk materials to increase the spacing between crystal layers, thereby weakening the interlayer interactions, and finally completely exfoliates them with the assistance of applied external fields (such as shear force, ultrasonic, or thermal expansion) to form a 2D material nanosheet dispersion, such as the preparation of graphene oxide (GO) by the Hummers method [13] and the electrochemical intercalation of molybdenum sulfide (MoS_2) by *n*-butyllithium intercalation or quaternary ammonium molecules [14]. Ion intercalation exfoliation is often accompanied by the creation of vacancies or functionalization, and the resulting 2D nanosheets are uniformly dispersed in water or organic solvents. For MoS_2 exfoliation, macromolecular quaternary ammonium salt molecules (such as tetraheptylammonium bromide) were first inserted into the bulk MoS_2 layer by electrochemical methods, and then, a 2H-phase MoS_2 nanosheet dispersion was prepared by exfoliation, with a concentration of up to $10\ \text{mg ml}^{-1}$.

In the ion displacement method, some layered bulk materials carry ions between the layers, which can be displaced in the liquid phase and assisted agitation to obtain a dispersion of 2D material nanosheets, such as peeled vermiculite [15], layered double hydroxides. The ion replacement method mainly selects cations with large, hydrated ion radius (such as Li ions) to replace the intrinsic cations between the layers, and at the same time, more water molecules enter, increase the layer spacing, and complete the peeling. Taking vermiculite stripping as an example, the 2D vermiculite nanosheet dispersion was obtained by two-step cation substitution, Li ions were selected to replace the Mg ions contained in the interlayer of the block, and the 2D vermiculite nanosheet dispersion was obtained through ultrasonic treatment. Or select anions with small binding force (such as Cl ions), replace the anions with strong binding force in the bulk material, and select suitable solvents to complete the peeling. Before and after peeling, the surface structure and charge distribution of the 2D material sheet remain unchanged, because they can be evenly and stably dispersed in the solvent due to the electrostatic repulsion of each other.

In the ultrasound-assisted exfoliation method, high-energy ultrasound is used to weaken the adhesion between the sheets. One method is to select a solvent with suitable surface energy to prevent the aggregation and precipitation of the peeled 2D material nanosheets, and directly ultrasonic peeling to obtain the dispersion of the 2D material nanosheets. Another method is to use surfactants, which are homogeneously dispersed in water with nanosheets of 2D material. For example, sodium cholate was used as the surfactant to directly ultrasound the bulk 2D materials, WS_2, $MoTe_2$, $MoSe_2$, $NbSe_2$, $TaSe_2$, and boron nitride (BN), to prepare the corresponding 2D nanosheet dispersions [16].

The preparation of 2D materials by liquid-phase exfoliation method has the characteristics of a wide sourcing of raw materials, simple process, low cost, and can obtain a large amount of 2D materials, which is suitable for industrial production. The exfoliated 2D materials are dispersed in water or organic solvent in the form of liquid phase, and the concentration is adjustable, the yield is high, and different three-dimensional macroscopic structures can be constructed by liquid-phase treatment. Saikam *et al.* [17] synthesized exfoliated graphite (EG) using liquid-phase exfoliation by changing the heating source or by changing the intercalation compounds, and the general synthesis process and some potential applications are depicted in Figure 1.

2.1.4 Non-covalent bond modification

During his doctoral dissertation, van der Waals studied the dynamics of gasses (including noble gasses) in a high-pressure environment from the gaseous phase to the liquid phase and found that the behavior of the gasses did not correspond to the ideal gas equation. Therefore, van der Waals had hypothesized that there is a mutual attraction between these gas molecules, so the ideal gas equation cannot accurately describe the gas behavior, and there will always be a deviation between experiment and theory. Finally, he combined experimental research with the

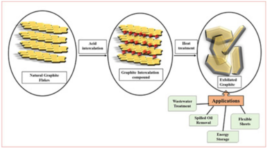

Figure 1: Schematic diagram of synthesis and applications of EG [17].

equation of state of non-ideal gases: the van der Waals equation of state [18]. van der Waals was awarded the Nobel Prize in Physics in 1910 for his outstanding work on the gaseous and liquid equations of state, and the weak interaction between molecules was named van der Waals force, or non-covalent bonding. After decades of development, with the in-depth research of the scientific community on the weak interaction between molecules, as well as the establishment and development of quantum chemistry theory, it was found that the van der Waals effect between molecules is a quantum mechanical phenomenon. In 1931, Pauling [19] proposed the concept of hydrogen bonding, stating that hydrogen bonds are formed when a hydrogen atom is placed between two electronegative atoms, and the position of hydrogen is biased toward the more electronegative atom. Hydrogen bonds were the first non-covalent bonds to be defined. As research progresses, π–π bonds and ionic bonds are also defined as non-covalent bonds.

To increase the dispersion of carbon nanotubes (CNTs), Sapalidis *et al.* [20] synthesized hydrophilic and biocompatible CNTs grafted with polyvinyl alcohol and GO linked to polyvinyl alcohol (PVA) using non-covalent π–π interactions. These multi-walled carbon nanotubes (MWCNTs) contain the poorly soluble drug camptothecin (CPT) and are used as anti-cancer drugs for chemotherapy for breast and skin cancer. PVA-modified MWCNTs loaded with CPT drugs are more cytotoxic than CPT alone. This method successfully loaded modified CNTs and graphene-based nanostructures onto aromatic drugs, making them suitable water-soluble nanocarriers [21]. Conjugated block copolymers composed of polyethylene oxide-polyaniline modify MWCNTs by π–π interactions. For the agglomeration of graphene, researchers use the method of combining π electrons with substances with large π bond-conjugated systems, which can change the original function of graphene and add new functions to graphene.

This method is often used for substances with aromatic structures and organic small molecules added to the molecular structure of graphene. Graphene can autonomously form agglomerates, which can reduce the free energy on the molecular surface due to the van der Waals force action caused by the π–π stacking between the sheets, resulting in a very low concentration of graphene dispersions [22]. Among organic molecules containing conjugated structures, pyrene (PyS) and its derivatives are often used to form π–π bond interactions with graphene, thus effectively modifying the graphene surface. Su *et al.* [23] present an approach to noncovalently functionalize graphene with large aromatic donor and acceptor molecules, in order to exert a rational control over the electronic properties of graphene sheets and fabricate graphene sheets in a feasible way. Liu *et al.* [24] prepared functionalized graphene by reacting with graphene by poly(*N*-isopropylacrylamide) (PNIPAAM). Graphene is dispersed in water to make an aqueous solution of graphene, and then, the PNIPAAM with PyS end is dissolved in water and added to the aqueous solution of graphene, and the modified graphene is prepared by stirring in an ice water bath. The functionalized graphene can have good dispersion ability and can produce high hardness and ductility when mixed with polymers.

As a type of chemical bond structure, ionic bonds can also functionalize non-covalent bonds of materials through their interaction with each other. At present, there are two main methods: one is to directly use the material to make its surface charged, in this way to reduce the molecular force and optimize it. The other is to add opposite charges to the surface of the material through the interaction force between the charges, changing the original structure and exhibiting new material properties. Lotya *et al.* [25] developed a method for dispersing graphite in an ultrasonic-assisted surfactant-aqueous solution. A large number of multilayer graphene was prepared by the reaction of the surfactant sodium dodecyl benzene sulfonate with graphene. Experiments have shown that only a few defects or oxides are present on the surface of graphene. These films have reasonable electrical conductivity and can be made translucent, and improved surfactants can significantly improve their performance. Yue *et al.* [26] performed non-covalent bond modification of GO by L-cysteine (L-Cys). L-Cys, as an environmentally friendly chemical agent, is a weak reducing agent containing amino groups, sulfhydryl groups, and carbonyl groups. GO was dispersed in ultrapure water, and a certain amount of L-Cys was added, stirred, and freeze-dried to form three-dimensional functionalized graphene oxide (3DGOL). Experiments show that with the increase of L-Cys, the pore size of 3DGOL gradually increases, and the pore size decreases from a few microns to several hundred nanometers. Through the reaction of L-Cys with GO, L-Cys is oxidized to cystine, which inhibits the aggregation of the graphene layer.

The functionalization of hydrogen bonds is mainly to make the surface of GO with oxygen-containing functional groups such as carboxyl groups and hydroxyl groups, which is similar to the modification of ionic bonds. These functional groups are easy to form hydrogen bonds with hydrophilic polymers, biological macromolecules, medical antibiotics, *etc.* It has been found that there is a strong energy between hydrogen bonds, and the breaking of intermolecular hydrogen bonds is conducive to the recombination of new substances. Mann *et al.* [27] reacted DNA with graphene to create graphene with novel properties. In this process, GO is first obtained by oxidizing natural graphene, and then, newly despiraled single-stranded DNA is added, and hydrazine is used to reduce it to develop a new type of graphene, which has extremely high stability. Experiments have found that agglomeration occurs without the addition of DNA. In terms of medical drug gene vectors, GO can be modified by modifying it with polyethylene glycol (PEG) to make the surface of GO loaded with PEG.

2.1.5 Covalent bonding modification

Covalent bonding is when an atom's electrons are delocalized around the entire molecule, resulting in a strong covalent bond interaction.

Polymers can be used as modifiers to achieve graphene functionalization. The experimental principle is assisted dispersion by the introduction of polymer chains. Shen *et al.* [28] produced graphene functionalized with amphiphilic polymers. In this process, the method of chemical oxidation and ultrasonic exfoliation was used for the first time, and the reducibility of sodium borohydride was used to copolymerize styrene and acrylamide with graphene through the catalytic action of dibenzoyl peroxide, and finally, the modified graphene was obtained, which improved the dispersion of graphene. Ma *et al.* [29] functionalized graphene using vinyltrimethoxysilane coupling agent. Polysiloxane composites were prepared by the chemical reaction of vinyl in silane graphene and silicone resin, and the dispersion study showed that the modified graphene had good dispersion and showed relatively active chemical properties. Salavagione *et al.* [30] modified GO by a direct esterification reaction between GO and PVA under conditions of *N*,*N*-O-dicyclohexylcarbodiimide and 4-dimethylaminopyridine catalysts. It is reduced by hydrazine hydrate to obtain reduced graphene hybrids, which are soluble in water and dimethyl sulfoxide under mild conditions. The degree of esterification of the experiment mainly depends on the stereostructural regularity of the PVA, which changes the glass transition temperature, crystallinity, and thermal stability of the polymer.

The functionalization of small-molecule covalent bonds is the functionalization modification of hydroxyl groups and epoxy groups on the surface of organic substances by chemical reactions, such as isocyanates, amphiphilic GO, and sulfonic acid groups. Bai *et al.* [31] first prepared GO and then modified the surface of GO with toluene-2,4-diisocyanate (TDI), and the modified GO (TDI-GO) was characterized by fourier transform infrared spectroscopy and X-ray photoelectron spectroscopy, and they found that TDI was successfully grafted with modified GO, and the modified GO could be dispersed uniformly and stably in anhydrous dimethylformamide (DMF) and could remain stable for a long time, indicating that TDI-GO could be well dispersed in organic solvents. Bekyarova *et al.* [32] added nitrobenzene to the graphene molecule through continuous research and innovation, giving it new chemical properties, and infrared spectroscopy can be observed whether nitrobenzene is added to the graphene molecule. Yu *et al.* [33] used the Hummers method in the preparation of GO. After a redox reaction with mercaptoethanol, the modified graphene was obtained. It is found that it has good electrical conductivity and strong sensitivity to heavy metal Cd^{2+}, which can be used for the detection of heavy metals in water and plays an important role in the detection of heavy metals.

2.2 1D nanochannels

Nanomaterials are classified into three different types according to their size and morphology: zero-dimensional nanoparticles, 1D nanotubes, and 2D nanosheets. The cross-sectional length and width of 1D nanochannels are less than 100 nm, and they mainly include 1D nanopores and nanotubes [34]. In terms of preparation methods, 1D nanochannels can be divided into 1D nanochannels formed by bottom-up assembly of monomers, and 1D nanochannels formed by physical or chemical etching of materials, such top-down preparation methods include polymer nanochannels prepared by ion beam etching technology and solid-state nanopores formed by electron beam exposure [35].

2.2.1 Bottom-up approach

The bottom-up method for the preparation of solid-state 1D nanochannels usually uses small building blocks such as atoms, molecules, or ions to assemble materials with nanoscale 1D channels through strong chemical bonding, including covalent bonds, ionic bonds, and coordination bonds. To put it simply, the "bottom-up" method is that 2D materials are synthesized by molecules or atoms through chemical or physical methods, and the bottom-up method mainly includes CVD and molecular self-assembly methods.

CVD is a common method for the preparation of CNT solid-state 1D nanochannels, which has a wide range of applications in the laboratory and industrial fields, with high preparation efficiency, through the carrier gas to carry the gasified catalyst precursor, growth promoter, and carbon source to the surface of the substrate material; at high temperature, these compounds undergo gas-phase chemical reactions, including thermal decomposition, hydrogen reduction, oxidation and displacement reactions, *etc*., and finally grow on the substrate material to form CNT solid-state 1D nanochannels. CVD-grown CNT solid-state 1D nanochannels have atomic-scale sizes similar to those of actual biological ion channels, which are suitable for simulating the function or role of biological ion channels.

The self-assembly method is a typical method for the preparation of solid-state 1D nanochannels by the bottom-up method. The self-assembly method is defined as the process by which different parts are arranged in order to achieve disorder to order by adjusting the internal interaction in an initially disordered system. Through the self-assembly method, researchers have successfully prepared covalent organic frameworks (COFs) with clear structure, high porosity, adjustable pore size, and periodic arrangement, and they applied them to many fields such as selective separation, ion conduction, electrochemical energy conversion, and storage. Given the precisely tailored ordered 1D channels and uniform pore size distribution of COF materials, COF nanochannels exhibit excellent size sieving performance for molecules/ions [36,37]. Moreover, the organic monomers and side chain groups that make up COFs have strong designability, and the size and surface charge of COF nanochannels can be effectively modulated, so the molecular/ion-selective transport performance of COFs has room for extensive adjustment.

In conclusion, the bottom-up approach provides an excellent solution for the design of solid-state 1D nanochannels with precise sub-nanometer size and ordered channel structure, and it lays a foundation for the design of nanochannels with excellent molecular/ion selective transport capabilities, which is of great significance for promoting the application of 1D solid-state nanochannels in the fields of biosensing, selective separation, energy conversion, and collection.

2.2.2 Top-down approach

The top-down method of preparing 1D nanochannels uses mainly various chemical or physical means to treat substrate materials, such as polymer films, metal films, and atomically thin 2D materials, and introduces single or multiple nanochannels throughout the entire film into the substrate materials, which can be divided into ion path etching and electron/ion beam lithography.

The ion track etching technology consists of three continuous processes: high-energy heavy ion radiation, ultraviolet sensitization, and chemical etching. Using this technology, researchers have successfully fabricated nanochannels with size distributions ranging from tens of nanometers to hundreds of nanometers in polymer film substrates such as polyethylene terephthalate (PET), polycarbonate, and polyimide [38]. Theoretical calculations have shown that the size and geometry of nanochannels have an important impact on the molecular/ion transport behavior of nanochannels [39]. By improving the process parameters and preparation process of ion path etching, researchers have developed an asymmetric ion track etching technique to expand the shape of nanochannels from cylindrical and conical channels to cigar-shaped, hourglass-shaped, bullet-shaped, and asymmetric hourglass-shaped [40]. The study of the molecule/ion transport process of channels of different shapes shows that the narrow opening of the nanochannel can significantly affect the transport behavior of the nanochannel.

For example, when separating with size sieving, narrow openings in the channel can effectively impede the passage of molecules/ions. For charged nanochannels, the charge effect of molecules or ions at the opening is most significant due to the highest charge density at the narrow opening location. The high-energy ions used in the ion path etching process cause the C–H bonds around the nanochannel wall to be oxidized to carboxyl groups, so the etching process introduces many negative charges on the surface of the polymer nanochannels, which makes the nanochannels have good ion selectivity. Hsu *et al.* [41] fabricated funnel-shaped nanochannels in PET membranes using ion path etching techniques, which contain abundant surface negative charges to convert Gibbs free energy generated by salinity gradients into electrical energy. By introducing an asymmetric pH environment into polymer nanochannels of different shapes, the researchers have effectively controlled the surface charge at both ends of the narrow opening of the nanochannel, endowing the nanochannel with a variety of ion-selective transport behaviors. However, the charge density and charge type introduced by ion trace etching on the surface of nanochannels are limited, and the size of nanochannels obtained by etching is usually large (>50 nm), and the surface charge has limited effect on the selective transport of molecules/ions in solution. Therefore, researchers have attempted to effectively control the surface charge and charge density of nanochannels by modifying various charged molecules and functional polymers on the surface of nanochannels [42]. At present, researchers have successfully used chemical covalent modification of solutions, electrostatic self-assembly, and plasma modification to modify various charged molecules and monolayer or multilayer polymer molecules on the surface of nanochannels. Wu *et al.* [43] modified two thermally responsive polymers, PBOB-PNIPAM and PMan, in conical nanochannels formed by PET etching, using a dynamic covalent interaction-driven layer-by-layer (LBL) self-assembly method. The

LBL assembly of PBOB-PNIPAM and PMan on the surface of the nanochannel effectively adjusted the size of the nanochannel, and then adjusted the ion charge density on the surface of the channel, and realized the effective control of the cation selectivity of the nanochannel. In addition, the conformation of the polymer can be adjusted by adjusting the ambient temperature, so as to effectively control the charge density on the channel surface.

Electron/ion beam lithography is a means of precision etching of substrates using the electron/ion gun cathode generated by the discrete electrons/ions by the high-voltage (25–300 kV) electric field acceleration and electrostatic lenses convergence formed by the dense high-speed electron/ion flow (0.3–0.7 times the speed of light). At present, electron/ion beam lithography is widely used in the manufacture and processing of microelectronic devices, microfluidic chips, and mask molds. In view of the advantages of small diffraction radius, concentrated beam current, and high energy intensity, researchers have tried to use electron/ion beam lithography to prepare nanoscale and even sub-nanoscale pores in nanoscale silicon nitride (Si_3N_4) and atomic-thin layers of BN, MoS_2, and graphene [44,45].

The top-down method not only shows significant advantages in the preparation of selective nanochannels, but also indicates a broad application prospect. The abundant functional groups introduced by the high-energy ion bombardment technology can be used to precisely control the molecular/ion transport characteristics of nanochannels. Despite the cost and scale challenges, simplification and efficient fabrication techniques are critical to the scaling up of nanochannel applications. Compared to bottom-up methods, top-down etching technology offers greater application possibilities due to its wide range of material applicability and dependence on process equipment.

2.3 Preparation of 2D nanochannels

2D nanochannels are 2D structural channels formed in materials, which are characterized by having a height or thickness in the nanoscale, while the length and width can be larger, forming a 2D confined space. These channels enable the selective transport of molecules or ions and therefore have a wide range of application potential in areas such as sensors, energy storage, and separation technologies. For example, rapid, selective, and sensitive detection of contaminants can be achieved by integrating ordered 2D COFs into nanofluid channels [46]. The self-assembled films of 2D materials have a typical layered structure, which is characterized by a parallel arrangement of highly oriented nanosheets. The 2D material film's uniqueness is that it has many 2D nanochannels inside, and the channel size is comparable to that of the 2D material nanosheets. These 2D nanochannels are connected to each other, resulting in a complete nanopathway that runs through the entire film. Methods for assembling 2D layered membranes mainly include a variety of combination methods, such as suction filtration, coating relying on substrate smoothness and solution surface tension, and LBL self-assembly with alternating deposition of different 2D materials on the substrate.

2.3.1 Suction filtration

Pressure/vacuum filtration is one of the most commonly used and effective methods for the preparation of 2D lamellar membranes, in which the vertical downward force provided by pressure/vacuum filtration drives the 2D nanosheets to assemble into a parallel layered structure on a porous substrate. The whole device is very simple, mainly composed of a filter bottle, a filter base, and a pump; between the filter bottle and the base, there is a porous and good mechanical strength substrate as a support; the area of the membrane is determined by the effective area of the contact between the filter bottle and the base during the suction filtration process. In 2014, Joshi *et al.* [47] prepared micron-thick membranes by filtering the aqueous solution of GO and showed by ion permeation test that only ions with ion diameters smaller than the layer spacing of GO nanosheets could pass through, showing excellent ion sieving performance, showing the potential of lamellar membranes. This method can effectively adjust the thickness of the membrane from nanometer to submicron by changing the volume, concentration, *etc.*, of the suction filtration solution. In addition, other ions, molecules, or nanoparticles can be easily embedded into the interlayers, which facilitates flexible adjustment of the nanochannel structure [48].

2.3.2 Coating

A variety of coating methods have been reported to assemble 2D nanosheets into lamellar films, including drop, spray, spin, and scraping. However, it is difficult to guarantee the uniformity and thickness of the film by the coating method. In order to prepare thinner lamellar films, spin-coating and spray-coating methods have been developed. The spin-coating method can provide centrifugal and shear forces to control the assembly of 2D nanosheets, resulting in a well-cross-linked, parallel, and ordered lamellar structure [49]. The general process of spin-coating method is to evenly coat the dispersion system containing 2D nanosheets on the substrate under the action of centrifugal force, and the rotation speed of the substrate, the coating time, and the viscosity of the solution will affect the morphology and thickness of the film. Due to the advantages of easy operation, adjustability, and fast speed, spin-coated film has been widely used in the preparation of layered films. Compared with the GO membrane (GOM) prepared by vacuum filtration, the GOM prepared by spraying technology has more pronounced and denser external folds. In addition to this, scraping technology is currently being used to prepare highly ordered lamellar films. The scraping process is continuous and scalable, and the shear forces generated by the lateral movement of the scalpel blade promote the alignment of GO liquid crystals during the scraping process [50]. This method can produce large-area (>100 cm^2), homogeneous, and continuous lamellar membranes.

2.3.3 Layers of self-assembly (LBL)

LBL self-assembly represents the process of alternating the deposition of different 2D materials on the surface of the substrate. This method relies primarily on interactions between adjacent layers, including electrostatic, hydrogen bonding, and even covalent bond interactions. The LBL method allows for precise control of the thickness of the selective layer by varying the number of deposition cycles and facilitates the precise introduction of stabilizing forces between the layers, so that the synthesized film remains stable in aqueous or organic media. In 2013, Lee *et al.* [51] first synthesized a polyamide (PA) film on a polysulfone substrate by interfacial polymerization and then obtained a composite film with GO deposited on the surface by soaking the film sequentially in a GO solution and an aminated GO (AGO) solution. Since the GO surface is negatively charged and AGO is positively charged, the electrostatic interaction between the GO sheets allows the adjacent sheets to be tightly bonded to act as a protective layer, significantly improving the chlorine resistance and antifouling ability of the composite film. However, the implementation of this method requires strong interaction, and the preparation process is time-consuming. At present, processes such as the combination of covalent LBL and electrochemistry have become new options for the preparation of membranes with higher stability and better structure.

2.3.4 Combination of multiple methods

Relying on one of the aforementioned methods to prepare a layered membrane, it is difficult to synergistically adjust the structure of the membrane in the horizontal and vertical directions. In general, the vertical arrangement of the nanosheets can be adjusted by vacuum filtration, while the horizontal arrangement can be adjusted by spin coating or scraping. Xu *et al.* [52] reported on a method combining pressure filtration and spin coating, which realized the synergistic regulation of GO lamellar film in the horizontal and vertical directions. In this method, highly ordered lamellar membranes were prepared, and nanochannels with a height of 0.4 nm were formed in the membranes, and the efficient separation of H_2/CO_2 and H_2/C_3H_8 was realized.

The scalability of the membrane preparation method is an important consideration for real-world applications. Methods such as coating are scalable and suitable for industrial production to prepare layered films. For example, 2D nanosheets can be attached to hollow fibers by suction filtration, which can facilitate the transition from laboratory scale to industrial scale [53]. It is important to note that all these methods are based on the homogeneous dispersion of nanosheets in solution. In recent years, new methods for the preparation of 2D nanochannels have emerged, providing more possibilities for the construction of 2D layered nanomaterial films. Liu *et al.* [54] proposed a wet-spinning assembly technique for continuous and rapid generation of GO films. In the first step, the GO dispersion is injected into the coagulation bath using a rotating channel. Subsequently, the GO dispersion is converted into a wet film by coagulation, which is simultaneously attached to the PET film, resulting in a GO film that can be up to 15 cm wide and 20 m long.

3 Applications of nanochannels

The wide variety of intelligent organisms that have evolved over millions of years in nature have brought endless inspiration for the design of biomimetic materials. From small biological ion channels to large oil pipelines, “pore” and “channel” structures can be seen everywhere: ion channels at the nanoscale in living organisms play an important role in maintaining the balance of physiological states and are the “smart” doors to ensure the selective transport of ions, while micron-scale pipelines are commonly used as material transport channels in chemical, food, agricultural, energy, petroleum, and other industries. Multi-scale pore systems have been widely explored and are now applied to materials science, membrane science, and technology and have made outstanding contributions in the fields of micro/nanotechnology for analytical, biomedical, and energy applications. Although the research results of multi-scale pore system have great application prospects, more and more detailed research work is still needed, including the development of pore systems with energy saving, anti-fouling, anti-corrosion, anti-clogging, integration of system channel switching performance conversion and controllability, and confined space stability. Inspired by the pores in living organisms, we introduce the bionic liquid gating mechanism and the dynamic nanopore transport mechanism into the multi-scale pore system, design and develop new functional composite micro- and nanopore materials, extend the traditional scientific problems of solid–gas and solid–liquid systems to solid–liquid–gas and solid–liquid–liquid systems, and at the same time explore the influence of dynamic deformation of pores on material transport in nano-confined space, which will promote the application of bionic multi-scale pores in energy materials, environmental governance, practical applications in biomedical fields, and more.

3.1 Desalination

Rapid social progress, especially industrialization and urbanization, has exacerbated the problem of water pollution. Population growth and climate change are increasing the demand for fresh water, and there is an urgent need to address freshwater scarcity. Considering that 97% of the planet's water resources are seawater, desalination offers a potential solution that has a broader prospect than the development of groundwater. At present, in the industrial field, distillation and reverse osmosis technology are mainly used for seawater desalination. Distillation (including multi-stage flash and multi-effect distillation) is an energy-intensive, environmentally significant, large-scale, and costly process for hot seawater desalination. In contrast, reverse osmosis uses external force or osmotic pressure to pass seawater through a specific polymer membrane, effectively separating ions to produce fresh water, which is both energy-saving and environmentally friendly. However, it is difficult for traditional polymer membranes to balance water permeability and ion selectivity. Low-dimensional nanomaterials have opened up a new research direction for seawater desalination technology due to their excellent water permeability and ionic selectivity after special treatment and have great commercial potential.

Corry [55] used classical molecular dynamics (MD) simulations to show that the hydrophobic and smooth (6, 6) CNT can completely intercept ions and achieve 100% desalination rate under the action of 200 MPa hydrostatic pressure. The desalination rate of (7, 7) CNT, which is larger, can also reach 97%, and the water permeability is significantly higher than that of (6, 6) CNT at the same pressure. At present, the industry still encounters significant challenges in the large-scale synthesis of defect-free, high-density, and high-orientation CNTs. With the advancement of sustainable development strategies, energy costs and environmental pollution have become the focus of attention. The high energy consumption of seawater desalination may be a better solution by removing ions from seawater. By applying an external voltage, ions are temporarily stored in an electrical bilayer formed by porous carbon nanomaterials, which can significantly reduce the energy consumption of the desalination process compared to reverse osmosis [56]. Some researchers have also found that the interaction between alkali metal cations and large bonds will block ion channels and seriously reduce the permeability of water, resulting in uncertainty about the application prospect of CNT in water desalination [57]. Using classical MD, Cohen-Tanugi *et al.* [58] revealed the mechanism of desalination of single-layer graphene through pore size, as shown in Figure 2. Their research discovered that nanopores in a single graphene layer can filter NaCl salts from water. By adjusting the pore size, they allowed water to pass through while blocking ions, thus achieving desalination. At present, the industry has not been able to synthesize high-orientation, high-density, and defect-free nanotubes on a large scale. Although experiments can produce nanoscale pore sizes by ion or electron bombardment, precise control of hole shape and size is still very difficult.

3.2 Ion separation

Biological ion channels play an extremely important role in cell transport. The process and selectivity mechanisms

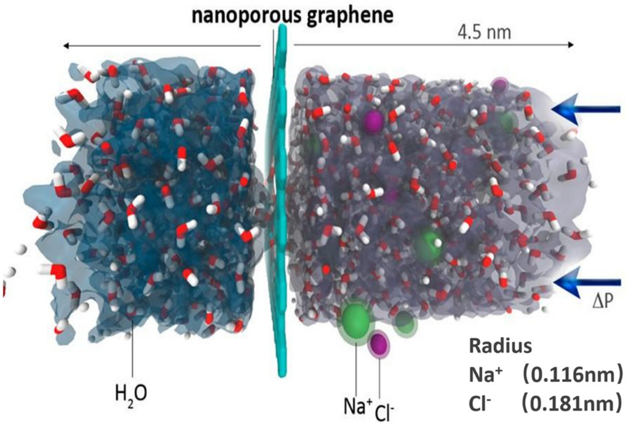

Figure 2: Schematic diagram of MD simulation of water desalination [58].

by which ions pass through membrane protein channels are complex, especially for biological protein channels, which are affected by factors such as steric hindrance, Coulomb interactions, charged amino acid arrays, and ion dehydration. Biological ion channels are essential for cell transport. The process and selectivity mechanism of ions passing through membrane protein channels are particularly complex, especially in biological protein channels, which are affected by multiple factors such as steric hindrance, Coulomb interaction, charged amino acid arrangement, and ion dehydration. Although biochannel proteins have excellent ionic selectivity, their industrial applications are significantly limited due to their fragile mechanical properties and bioenvironment-dependent activity. The synthetic nanochannels are narrow and hydrophobic, with excellent mechanical properties and large specific surface area. The chemical stability, mechanical strength, and electrical conductivity in the structure give it the potential for a wide range of applications in ion separation devices. Researchers have conducted a lot of theoretical and experimental studies on the application of CNT in ion separation, explored the ion selectivity mechanism of CNT, and analyzed the influence of steric hindrance, Coulomb coupling, and other factors on ion transport and separation.

The charge on the surface of CNTs has a significant effect on the selectivity and transport of charged ions. Aluru *et al.* [59] demonstrated that asymmetrically functionalized (16, 16) CNTs pass significantly higher chloride ions than potassium ions through MD simulations. Majumder *et al.* [60] placed negatively charged functional groups at the nozzle of the CNT and found that this could significantly improve the cation transport efficiency. Gong *et al.* [61] showed that (9, 9) the inner surface of CNTs can be modified with different carbonyl functional groups to achieve the separation of Na^+/K^+ ions. Siria *et al.* [62] fabricated a hierarchical nanofluidic device consisting of a single boron nitride nanotube (BNNT) that connects two reservoirs across an impermeable solid-state membrane to study diffusion and osmosis, as shown in Figure 3.

With the development of nanotechnology, the area and quality of graphene prepared experimentally are getting larger and higher, and the method of generating pores on a porous matrix has been developed, which makes porous graphene have a good application prospect in the field of ion separation. Thanks to the development of industrial technology, layered graphene nanochannels with precise layer spacing have been successfully prepared experimentally, which has expanded the application of nano-flow devices in the field of separation.

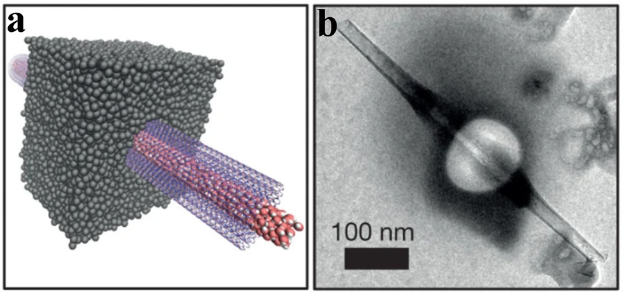

Figure 3: Nanotube with smooth inner walls used as an ion transport channel [62]: (a) sketch of the transmembrane BNNT for nanofluidic measurements and (b) its experimental realization, imaged by transmission electron microscopy.

3.3 Energy harvesting

Since the beginning of the Industrial Revolution, fossil fuels (mainly coal, oil, or natural gas) have been the main source of energy for humanity. However, burning fossil fuels is a serious pollution to the environment, and burning fossil fuels produces a large amount of greenhouse gasses, causing global warming, melting glaciers, rising sea levels, abnormal climate, and frequent El Niño phenomena around the world. Therefore, access to sustainable, abundant, and affordable energy is one of the major challenges facing modern society. Potentially available renewable energy sources include sunlight, wind, tidal, and geothermal. However, so far, none of these energy sources have been able to replace fossil fuels, mainly because of the limited efficiency of generating and storing electricity, medium availability, unsustainability, and high cost. Scientists and engineers are also exploring tidal energy, wave friction power generation, and blue energy. Using the difference in salinity between seawater and river water (salinity gradient) to generate clean energy, known as blue energy or osmotic energy, is a promising, challenging, accessible, clean renewable energy source.

At present, pressure-retarded osmosis and reverse electrodialysis (RED) are two possible methods for extracting and converting osmotic energy (Gibbs free energy). The differential pressure permeation method uses the osmotic pressure generated by the different salinities on both sides of the semi-permeable membrane to drive water molecules from the freshwater tank to the seawater tank, and the flowing water can drive the connected turbine generator to generate electricity. However, the average power ($1\ \mathrm{W\ m^{-2}}$) of the separation membrane produced by this method in actual industry is much lower than the target power ($5\ \mathrm{W\ m^{-2}}$) [63], so the development of this project has been suspended. Electrodialysis (RED) refers to the direct generation of electrical energy by a salinity gradient-driven ion through a selective nanofluidic device of cation or anion. In models using silica nanochannel configurations, this power can even reach ~8 W m^{-2}. The Dutch company REDS take is currently experimenting with this approach to generate electricity on a large scale, and the membranes are now achieving conversion efficiencies in the range of a few watts per square meter, which is close to commercial targets.

Feng *et al.* [64] developed a monolayer porous MoS_2 membrane with a pore size of 10 nm, which can optimistically estimate a power density of 106 W m^{-2} in the case of massive parallelization. Siria *et al.* [65] discussed current technologies for converting blue energy. Specifically, the membrane serves as an ionic current generator, as illustrated in Figure 4. The generated electric power is collected by connecting electrodes in the reservoir to an external load resistance. However, unlike seawater desalination or ion separation, electroosmotic energy-enrichment nanochannels do not require strict ion separation, and the pore size of nanochannels can reach tens of nanometers without precise pore size regulation [62,65], which greatly increases the possibility of their industrial applications.

Although highly conductive electrodes and ion-exchange membranes have been developed for energy recovery, practical applications still face several challenges. For example, the interaction between the nanopore ion-exchange membrane and the salt solution may affect the storage of ions during subsequent desalination, reducing the efficiency of energy recovery. Therefore, optimizing the interfacial properties of ion-exchange membranes can help improve the efficiency of energy recovery.

3.4 Single-molecule detection

In 1953, Coulter invented the Cooler counter and was the first to develop the resistance pulse method based on the ion transmission principle to achieve the analysis and detection of single particles. When a single particle enters a micron-to-millimeter-sized pore under electric field migration, the current decreases due to the blockage of the ionic current, and when it moves out of the pore, the current recovers, resulting in a resistor-pulse signal in the I–T curve. By analyzing the frequency, peak width, and amplitude of the ionic currents during perforation, information on particle size distribution, concentration, shape, and surface charge can be obtained [66,67]. In recent years, solid-state nanopores have become a versatile alternative to biona-nopores due to their clearly adjustable geometry and pore size, high mechanical strength, ease of modification, and compatibility with various devices and technologies. DNA is composed of repeating units of nucleotides, and only one nucleotide can reside in ultra-thin graphene pores at a time, so sequencing can be performed by observing the translocation of successive nucleotides through the nanopores [68].

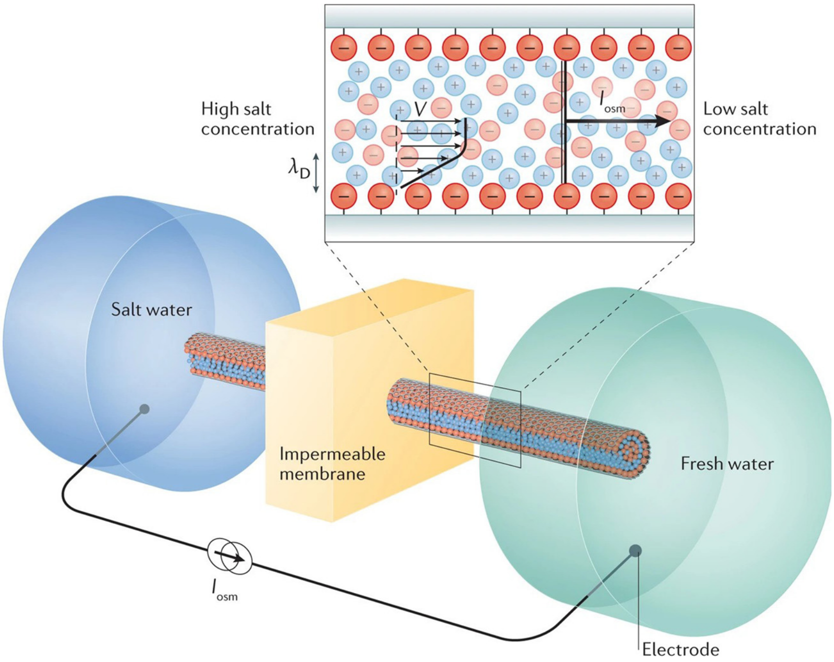

Figure 4: Diffusion–osmotic process for osmotic energy conversion [65].

The research team of Jiang *et al.* [69–71] summarizes recent progress in artificial solid-state nanochannel-based sensing systems for detecting various types of biomarkers. Artificial solid-state nanochannels with probes on the outer surface not only contribute to the *in situ* detection of large analytes but also provide promising opportunities for ultra-high sensitivity detection with a clear mechanism. They developed a set of intricately designed supersandwich DNA probes and fabricated wettability-controllable nanochannels to explore the mechanism of nanochannels with regional wettability modification. Their research shows that this single set of probes can effectively facilitate both reliable on-site qualitative detection and ultra-sensitive quantitative analysis, all while minimizing error propagation. They consider that designing solid-state nanochannels with functionalized outer surfaces and achieving quantum-confined superfluid would effectively overcome the challenge of universal single-molecule detection and ultra-high-precision spatiotemporal resolution. These pioneering nanochannels will expand the scope of biosensor applications and facilitate the exploration of mass transfer mechanisms.

In 2021, Gao *et al.* [72] reported a protocol to explicitly divide the regional and functional elements at the outer surface and inner wall of solid-state nanochannels (SSNs) in order to achieve the highly specific ionic output in complex matrices. This will contribute to the fundamental understanding of substance transport in SSNs and provide high specificity and sensitivity in SSN-based analyses. In other works, in order to study the signal mechanism, Wu *et al.* [73,74] used electroneutral peptide nucleic acid and negatively charged DNA to quantitatively analyze the individual contributions of the space charge and steric effects of charged targets on the outer surface to the ionic signal in order to demonstrate the signal mechanism and used the rolling circle amplification (RCA) process to synthesize DNA amplicons to enhance the ionic signal through the space charge effect. Their research shows that the ionic signal increases with the local surface potential per nanochannel and is further enhanced by decreasing the porosity density of nanochannels.

In 2022, Si *et al.* [75] reported a method using polydopamine (PDA) to modify the highly charged surface in nanoconfinements in order to fix the electrostatic repulsion in nanoconfines, which limits ion current rectification (ICR) manipulation. Their research found that the charged properties of PDA change the ICR effect of the nanochannel due to property changes in the ion-depletion zone from PDA modification.

Meller's team [76] improved the DNA capture rate of SiN nanopores by establishing a transmembrane ion concentration gradient, and a 20-fold salt gradient could detect picomolar concentrations of DNA at high throughput. Thakur and Movileanu [77] discovered that specific and nonspecific interactions in a heterogeneous solution can be distinguished using a protein bait-containing biological nanopore in mammalian serum, as shown in Figure 5. Wu developed an analytical strategy-based nanochannel system modified with RCA amplicons on the outer surface, which provides a highly sensitive and specific sensing platform for identifiable molecules using nucleic acids.

4 Transport properties in nanoconfined space

The confined domain of the 2D space is generally only a few molecules in diameter, and the hydrogen bonding configuration between the confined water molecules is very different from that of the bulk water/ice system, and a quasi-2D special hierarchical structure will be formed in this highly confined space. In early MD simulation studies, hard-sphere models were used to simulate confined liquid molecules, where a quasi-2D confined space consisted of two parallel virtual sheets. Schmidt and Löwen [78] found that the confined space has a great influence on the condensation phase transition of water molecules, and the phase transition temperature and structure are very different from the bulk phase space, and gave a variety of quasi-2D phase structures, such as single-layer rhombic structure, single-layer triangular structure, double-layer triangular structure, double-layer AB stacking structure, *etc.* In 1997, Koga *et al.* [79] found for the first time in MD simulations that confined water was transformed into a 2D ice structure by condensation phase transition, based on the TIP4P model. Subsequently, the rigid water molecular

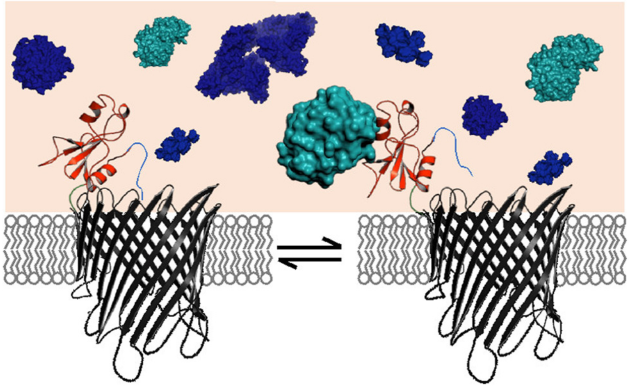

Figure 5: Single-molecule protein detection at single-tethered receptor resolution [77].

models such as TIP3P, SPC, TIP4P, and TIP5P, and their modified models, were used to study the phase behavior and transition of quasi-2D confined water. Under different confined spaces and different thermal conditions such as temperature and pressure, quasi-2D confined water can form a variety of ice phases.

4.1 Graphene nanochannels

In the 2D confined channel, scholars have prepared graphene nanochannels based on the material properties of graphene, and their dimensional accuracy can be controlled at 0.34 nm channel, and the channel wall has the characteristics of atomic-level smoothness, which has extremely high water transport properties. In GO films, oxygen-containing functional groups on GO sheets are used as supports to form graphene nanochannels with atomic-level smoothness in the layers of unoxidized sheets stacked on top of each other. MD studies have shown that the mechanism of the rapid passage of water molecules through GO films is not driven by traditional differential pressure, but by the combined effect of capillary pressure and evaporation to drive water molecules to enter graphene nanochannels [80].

Experimental studies have shown that GO films are size-selective in terms of ion screening. The graphene nanochannels in the film are only a few layers of aqueous molecules perpendicular to the wall and are therefore capable of precise size selectivity for ions in aqueous solutions as well as other solute molecules. MD structural simulations verify this phenomenon – allowing water and small ions to pass through quickly and large ions to tissue to pass through. And the experimentally measured ion diffusivity is several thousand times higher than the value estimated using the classical concentration diffusion theory. Through simulation studies, researchers have discovered the phenomenon of "ion sponge effect" [47], *i.e.*, the interaction between graphene and ions causes ions to aggregate in the nanochannels, forming a higher concentration gradient, which further promotes the ion diffusion process. Shi *et al.* [81,82] *via* the drop-casting method to prepare freestanding reduced GO (rGO) from an rGO suspension in order to observe Na_2Cl and Na_3Cl as 2D Na–Cl crystals on reduced GO membranes (rGOM), and they used the MD simulations method to incorporating cation–p interactions to classic all-atoms force fields in order to show that Na^+ has a clear enrichment on a carbon-based p electron-rich surface in NaCl solutions. Their research found that Na^+ is the p electron-rich structures in aqueous salt solutions, and the cation–π interactions between the ions and the aromatic rings in the graphitic surfaces would promote the ion adsorption on the surface to form crystals and help to make 2D Na–Cl crystals of stoichiometries.

Li *et al.* [83] found that there are strong electrostatic, van der Waals, and hydrogen bond interactions between water/ions and oxygen-containing groups in GO nanosheets, which largely hinder mass transport of species. Therefore, the rapid water/ion transport in GO membranes mainly occurs in the non-oxidizing region adjacent to the GO nanosheets. Gu *et al.* [84] showed that the electrostatic interaction of ions with the surface of fluorinated graphene (F-GRA) results in ideal ion repulsion on the surface of F-GRA and ultra-low water friction mediated by its hydrophobicity, resulting in good water permeability. Esfandiar *et al.* [85] prepared graphene electrodes with a thickness of nearly 100 nm by mechanical exfoliation, constructed a single sub-nanometer channel with a bilayer of graphene as a spacer, and found that the conductivity of the chloride solution in the sub-nanometer channel was much lower than that of the bulk solution, and the water molecules tended to face the outward direction of the –OH functional group in the hydrated layer of Cl– ions, and the surface of graphene was found to promote the polarization of water molecules and strongly attract water molecules, resulting in a strong force between the two, making Cl– ion transport characteristics are greatly reduced.

GO flakes have both oxidized and non-oxidized bands. According to slip theory, water molecules exhibit frictionless, ultra-fast flow in the non-oxidized zone of the GO layer, resulting in a very fast water permeation rate. The oxidized band, containing abundant oxygen functional groups, undergoes strong hydrogen bonding interactions with water molecules, hindering their rapid slip [86]. The transport mechanism of ions is mainly due to steric hindrance and cation–π interactions on GO nanosheets. Researcher [87] shows that by controlling the interlayer spacing between GO flakes, the size of nanochannels can be adjusted, allowing for precise separation of different ions and molecules. Additionally, GO films with nanochannel sizes larger than the ionic hydration radius exhibit good ion repulsion performance. The primary component of cation–π interaction is electrostatic, inducing a cross-linking effect that helps control interlayer spacing in GOMs. The cation–π interaction was first proposed by Sun *et al.* [88], who prepared GO films using a drip method. Metal cations (including K^+, Na^+, Ca^{2+}, Li^+, Mg^{2+}) can reduce the interlayer spacing of GO films to 0.1 nm [89]. The interaction between cations and π is very strong in non-covalent interactions. Chen *et al.* [90] used the drop-casting method to prepare GO GOM in order to separate ions from bulk solution or for sieving ions of a specific size range from a mixed salt solution. Combining experimental observations and theoretical calculation, their research found that cations (K^+, Na^+, Ca^{2+}, Li^+ and Mg^{2+}) themselves can determine and fix the interlayer spacing of GOMs at sizes as small as a nanometer and the variable range of this spacing can be controlled to within one ångström.

Due to the unique spatial arrangement of water molecules in the confined space and the solid–liquid contact area-to-volume ratio much higher than that of macroscopic fluids, the interaction between water and nanochannels is extremely important in phase transition, and the phase transition temperature of water is affected by the structure of the channel pipeline and is different from that of body water, which also has high application value in practical engineering. Experimental studies have shown that when the separation between solid surfaces approaches the atomic scale, fluid properties change dramatically. In particular, the drying transition occurs on the surface of water molecules. This is due to the action of strong hydrogen bonds between water molecules that cause the liquid molecules to retreat. The non-polar surface forms different layers that separate the bulk phase from the surface, so that the hydrogen bonding network of water molecules in the confined space exhibits multiple phase transition states when the hydrogen bonding network is broken [91]. Simulation studies have found that water molecules can freely enter the nanochannels formed by two graphene sheets with a gap of only about 0.35 nm and spontaneously form a 2D crystalline solid structure, *i.e.*, a single layer of square ice, which is a new form of water at room temperature. MD simulations have revealed that the van der Waals force interaction between graphene sheets exerts a confined pressure of up to the order of GPa on the confined water, which changes the hydrogen bonding network of the water from a 3D to a 2D plane, and the orderly arrangement of water molecules results in a 2D square crystal structure [92]. Raju *et al.* [93] studied the phase transitions of water in 2D graphene nanochannels at scales of 5.5, 8.5, and 11.5 Å and observed that water forms an ordered hexagonal phase at low densities and an ordered square phase at high densities. Through the analysis of structural properties by radial distribution function and transverse density profle, it is observed that the double-layer hexagonal ice has the characteristics of the first-order phase transition, while the double-layer (three-layer) square ice structure has no phase transition, which is a continuous structural change without a clear transition temperature.

4.2 Micromechanical nature of separation pressure and boundary slip

The separation pressure caused by the solid–liquid interface at the nanoscale [94–96] provides an additional driving force for fluid transport, which is essentially the embodiment of various intermolecular forces between the solid–liquid interfaces. Intermolecular forces at the nanoscale are key to explaining the rapid transport of nanofluids. The nanoscale has an ultra-high specific surface area; there is a strong surface interface effect; incompressible Newtonian fluid, wall no slip, and other conditions may no longer be applicable; and the microscopic transport process cannot be described by classical theory.

The flow behavior of non-viscous liquids without kinetic energy loss is superfluidity, which is typically characterized by the fact that the substance is not viscous, there is no friction with the contact surface, and it can be transported in the channel without resistance. Superfluidity was first discovered in liquid helium by Kapitsa [97] and Kim and Chan [98], and a theoretical model was established. When the fluid flows on the solid wall, the fluid atoms at the solid–liquid interface will be limited to the equilibrium position of the solid lattice structure due to the force from the solid surface, the liquid–liquid interaction force inside the fluid will cause the fluid atoms on the surface to deviate from the equilibrium position, and the fluid atoms will gradually deviate from the equilibrium position of the solid surface when the liquid–liquid interaction is greater than the solid–liquid interaction, showing the slip phenomenon. Existing studies have shown that the graphene nanochannels in GO films can allow water molecules to pass through quickly, and nano-water droplets can quickly diffuse on the surface of graphene with regular morphology; thanks to the long boundary slip length (60–100 nm) of the graphene channel wall and the hydrogen bonding network of water in the confined space, the coupling of wall action and surface charge in the nanochannel is the key to affect material transport and ion screening. In smooth-walled nano-sized channels, the transition of water molecular configuration enhances the flow, and the frontage effect due to channel roughness is enhanced. Defects and functional groups, for example, can eliminate the flow-enhancing effect [99]. The water molecules flowing between the GO sheets are hydrophilic groups in the oxidized region, which hinders the rapid transport of water molecules, while the water molecules in the non-oxidized graphene sheets form a 2D network structure between them, and the fluidity is significantly enhanced [80]. Crystals with unconventional stoichiometries hold promise for the design of novel transistors, magnetic devices, and catalyzers, Xia *et al.* [100] reported a highyield synthesis of 2D abnormal Na_2Cl crystals base on applying a a negative potential on a rGOM which not only promoted the ion adsorption on the surface to form crystals but also helped to stabilize 2D Na_2Cl with an excess of sodium. Their research expand crystals with unconventional stoichiometries research interest both in the laboratory and in applications. Their research found that with the cation–π interaction that can be directly strengthened in a crystallization process, the adsorption capacity and stabilization of the crystals will be greatly enhanced. Wu *et al.* [101] from China University of Petroleum comprehensively analyzed the MD simulation results and experimental data from 53 studies and found that in nanochannels with different wettability and pore size, the viscosity of water is inversely proportional to the contact angle, and the contact angle in the hydrophilic pipeline is small, the viscosity is large, and the flow velocity is smaller than that of body water. Hydrophobic pipes have large contact angles, low viscosity, and flow velocities that are even seven orders of magnitude larger than bulk water. Chen *et al.* [102] linked the layered structure formed by water molecules confined to the interlayer voids of graphene with their rapid transport characteristics, and they believed that this special layered structure was the main reason for the rapid transport of water molecules between layers. Falk *et al.* [103] from France studied the relationship between friction coefficient and radius in water flow between graphene sheets, inside armchair CNTs, and outside these CNTs. They discovered that the flow velocity was enhanced in confined spaces. Additionally, the narrower the layer spacing, the more pronounced the enhancement, as illustrated in Figure 6. Jiao and Xu [104] found that when the temperature was lower than 315 K and the interlayer distance was 0.65 nm, a single layer of water appeared between the graphene sheets, and due to the reduction of wall friction, the water diffused in the graphene layer was discontinuous and collective, which was conducive to the rapid transport of molecules. Suk and Aluru [105] used MD simulations to study the flow of water in graphene nanopores and found that the pressure in the channel showed a linear downward trend while the rate of the fluid along the axial direction barely changed, confirming the heterogeneous structural properties of water in confined spaces, as well as the corresponding changes in density and viscosity.

Although scholars have conducted a lot of theoretical simulation research in the field of water transport, it is difficult to obtain a unified self-consistent conclusion due to the differences in simulation methods and parameters. However, due to the shielding of CNTs to the internal fluid, the experimental data for the study of fluid transport in CNTs are extremely limited, and it is difficult to systematically explain the physical mechanism of high-flux transport characteristics.

4.3 Size effect of nanochannel-confined mass transfer

Due to the influence of solid–liquid interaction and spatial confinement effect, the density distribution of the fluid along the radial direction of the nanochannel is not uniform, but the density near the channel wall is significantly higher than that in the center of the channel. Similar to the density distribution, the shear viscosity distribution within the nanochannel may also be non-monotonic. Solid–liquid interactions increase the local shear viscosity of fluids close to the wall, resulting in slow flow. The overlap and mutual interference of the two boundary layers close to the wall in a confined space further lead to a complex change in the viscosity of the fluid with the size of the channel. Based on its special size effect, nanochannels make it possible to separate substances, and the separation of molecules or ions of different sizes can be realized using the difference in the migration velocity of molecules of different sizes in the channel, and the limiting size effect of nanochannels makes it easier for substances to interact with the wall surface after passing through the nanochannels.

Studies have shown that when the size of nanopores or nanochannels is large at the micrometer scale, the transport characteristics of transmembrane ionic molecules are

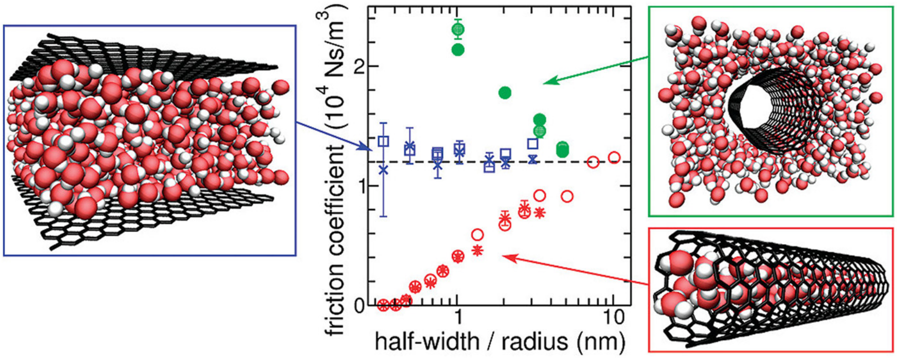

Figure 6: Effects of confinement and curvature on friction in nanochannels [103].

mainly related to their mobility in bulk solution. However, when the size of nanopores or nanochannels decreases sharply to the nanoscale, the transport characteristics of ionic molecules are changed by the action of the pore wall or channel wall. In addition, the proportion of transmembrane ionic molecules interacting increases with the decrease in pore wall or channel wall size, which means that the interaction of ionic molecules through nanoscale pores or channels cannot be ignored. Ions are present in solution in the form of hydrated ions, and when faced with smaller channels, more energy is required to remove the water molecules from the hydrated shell, which determines whether the ions can pass through or not. The use of spatial bits to block the passage of larger substances is an important feature to reflect the selectivity of nanochannels. Generally speaking, the hydrated ion structure formed by the combination of ions and water molecules is divided into the first water shell and the second water shell, and the number of water molecules contained in it is defined as the first coordination number and the second coordination number. When the pore size of the electrically neutral nanochannel is close to or smaller than the diameter of the ionic water shell, a huge energy barrier is formed for the ions that will enter it, preventing the ions from entering. A series of studies by Sun *et al.* [106] showed that for neutral sub-nanochannel ions, the dehydration of the first water shell is the origin of the ion transmembrane energy barrier. However, the recent separation of Mg^+/Li^+ ions in salt solution by Liu *et al.* [107] showed that the dehydration of the ionic second water shell is also the origin of the ion transmembrane energy barrier, and the dehydration of the second water shell should not be ignored. Gao *et al.* [108] also confirmed that the dehydration of the second water shell of the ion is the origin of the ion transmembrane energy barrier. Dai *et al.* [109] developed a class of GOMs from GO suspensions using vacuum filtration without drying treatment in order to have high water permeance when the ion rejection rate is at a satisfactory level and stable performance. Their research found that the ions can control and fix the interlayer spacings in the GOMs, and the distorted hydration structures of the multivalent ions due to the strong hydrated cation–p interaction, resulting in the higher rejection rates of undistorted hydrated ions in solutions through the GOMs. Wei *et al.* [110] prepared rGOM by the amino-hydrothermal method and the modified Hummers' method from GO suspensions in order to separate of radioactive ^{90}Sr from other radioactive ions efficiently. Their research found that the distort energy barrier of Co^{2+} is significantly higher than that of Sr^{2+}, making it difficult for hydrated Co^{2+} to distort and enter the internal space between GO sheets from the bulk solution due to the large energy barrier of dehydration.

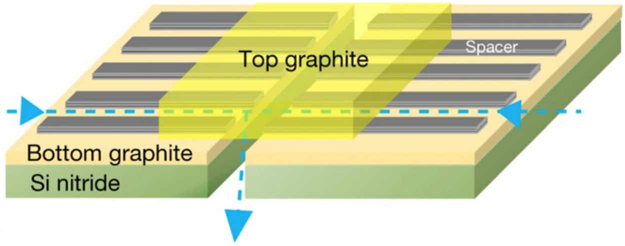

Figure 7: Schematic diagram of the nanoslit channel structure [111].

Radha *et al.* [111] fabricated narrow, smooth capillaries using van der Waals assembly, as shown in Figure 7. Their findings indicate that when the channel height exceeds six atomic layers (2.38 nm), water molecules behave as predicted by classical fluid dynamics. However, when the height is below this threshold, the flow rate significantly surpasses predictions of traditional models. Zhao *et al.* [112] combined non-equilibrium molecular dynamics simulations and first principles density functional theory calculations to study the molecular flux of Lennard-Jones-benzene fluid in nanoslit channels and found a slip length oscillation caused by molecular size effects. Borg *et al.* [113] investigated the structural changes of water molecules within CNTs with diameters ranging from 0.81 to 4 nm. With the gradual increase of the size of the nanochannels, the structure of water molecules transitions from a single-chain structure to an ordered ring structure and finally changes to a structure like that of bulk water.

In the coming decade, the lack of clean water is a formidable challenge because of rapid population growth, extended droughts, and fast growing demands. Nanofiltration membranes (NFMs) are widely used in water purification due to its low energy cost and simple operational process. Generally, most of polymeric NFMs have advantages of flexibility, simple preparation process, and relatively low cost, but also face some problems, such as poor chemical resistance, limited lifetime, and membrane fouling. Thus, researchers proposed CNT-based NFMs, but it is still far away from practical application due to relatively high cost of CNTs, time-consuming, and complex process of obtaining high density of vertically aligned CNTs, and difficulties for achieving large-scale production. Therefore, 2D graphene materials have entered the field of vision of researchers, and graphene can form highly ordered films with 2D nanochannels between two graphene sheets by the facile filtration-assisted assembly method. But Nair *et al.* [80] prepared GOM using Hummer's method in order to investigate molecular permeation through submicrometer-thick GOM. Their research found that submicrometer-thick membranes made from GO can be completely impermeable to liquids, vapors, and gases, but these membranes allow unimpeded permeation of water attribute to a low-friction flow of a monolayer of water through 2D capillaries formed by closely spaced graphene sheets. It seems that NFMs cannot be prepared by dried graphene films. Han *et al.* [114] used chemically converted graphene (CCG) to fabricate ultra-thin graphene NFMs with 2D nanochannels in order to be applied them for water purification. Their research shows that 34 mg of CCG is sufficient for making a square meter of NFM, indicating that this new generation graphene-based nanofiltration technology would be resource-saving and cost-effective.

Unlike the resistance existing in graphene sheets, GO can be easily dispersed in various solvents due to its unique surface chemical composition and amphiphilic nature. In particular, GO has excellent stability in water-soluble dispersion and has been realized in batch production, so GO has been used as the raw material for the production of graphene-based 2D membrane materials in many research works. The study of GOMs is still an emerging field, and research to understand the atomic structure, transport mechanism, and separation mechanism is in progress. Any change in dimensions of the nanochannels would result in dramatically different rates of transport of fluids through the GOMs. Aher *et al.* [115] used the drop-casting method to prepare the GOM in order to measure the permeation and rejection performance of the GOMs with isopropyl alcohol and water as solvents. Their research suggests that water adsorption on the GO surface is a critical factor that controls the flux and sieving effect of the GOM. Huang *et al.* [116] used a novel nanostrand-channeled strategy to prepare nanostrand-channeled GO (NSC-GO) ultrafiltration membranes to meet the growing worldwide demand for pressure-driven ultrafiltration membranes. Their research found that the separation performance of NSC-GO ultrafiltration membranes exhibits an abnormal dependence on applied pressure due to the reversible deformation of the nanochannels.

The rapid development of micro-nanotechnology has brought new challenges to mechanical experiments, and at microscales, the influence of size effects, multi-field (force, electricity, magnetism, heat) coupling, and non-classical forces (van der Waals force, capillary force, electrostatic force, Casimir force, *etc.*) have become factors that need to be considered, and many macroscopic solid mechanics experimental methods are difficult to apply. Therefore, it is of great scientific significance to carry out the research on the analysis method of micro/nanomechanical testing technology and multi-scale correlation. The internal structure of concrete provides a migration channel for medium transport, and the macro-meso-microscale structure characteristics of concrete determine the chloride ion transport behavior. De Vera *et al.* [117] experimentally investigated the effect of water saturation on chloride diffusion in concrete and found that when the water saturation was reduced from 95 to 54%, the diffusion coefficient of chloride ions decreased by about two orders of magnitude. Homan *et al.* [118] confirmed the coupling effect between moisture transport and chloride permeation in concrete by comparing the effects of moisture transport on chloride permeation in partially saturated and fully saturated concrete. Liu *et al.* [119] studied the transport characteristics of multiple groups of separators in the pores of the C–S–H gel under saturation through MD simulation and found that the calcium/silicon ratio had a significant effect on the adsorption of chloride ions on the surface of the C–S–H gel, and the adsorption was strongest when the calcium/silicon ratio was 1.2.

5 MD simulations

In 1957, AdlerAlder and Wainwright [120] tried to apply MD methods to solve the problem of solid–liquid phase transition when studying the hard sphere model system and successfully solved the problem, showing the important role of MD in the study of multi-body problems in the world. In the sixties of the 20th century, Gibson *et al.* [121] proposed that analytical methods are inadequate and that numerical treatment with the aid of a high-speed computing machine is required and adopted the MD method of continuous potential function in the study of crystals, which was the first time that MD simulation emerged in materials science. In the 70 and 80 s of the twentieth century, with the optimization of computing methods, the continuous enrichment of theories, and the increase of theoretical models of MD, which were applied to different fields, but due to the limitation of computer computing power, MD simulation has certain time and space defects, *i.e.*, the number of atoms in the system that can be simulated is limited, and the simulation time step is still at the nanometer level with the rapid development of computer performance and the improvement of computer simulation calculation speed, and the simulation defects of time and space have been greatly improved. In terms of spatial quantities, the micrometer scale has been developed, and new multi-scale algorithms have emerged, which combine nanoscale and macroscopic quantities to achieve more satisfactory simulation results. Nowadays, MD has been widely used in many scientific research fields such as physics, chemical engineering, materials science, nanomechanics, and biochemistry.

5.1 Theoretical model

Molecular simulation is a method of simulating macroscopic matter and system by constructing a microscopic system containing a large number of particles in a computer, solving the equation of motion of particles with the help of computer computing microsystem using the principles of quantum mechanics, and finally using the principle of statistical physics to calculate the various physical and chemical properties of macroscopic system materials at different time and space scales.

MD is a simulation method based on Newton's equations of motion. By deducing the position of atoms and optimizing the interaction force between atoms, the optimal results of the system are obtained. Statistical mechanics is then used to obtain the macroscopic properties of the system, such as binding constants and molecular conformation. The MD method can not only study the static thermodynamic properties of macromolecular systems, but also study the dynamic mechanical properties, obtain various physical and chemical properties, and obtain data that are difficult to obtain under experimental conditions. Using computer-supported theories, the transition states and reaction mechanisms of chemical reactions can be studied, and molecular and material design can be carried out more efficiently, thereby shortening the material development cycle and reducing research costs. However, the details of the atomic-scale simulation of the MD method cannot be described, and it cannot be used to elucidate the chemical reaction process. It is more suitable for analyzing molecular models with fixed molecular species and bond formation.

Monte Carlo (MC) is a research method that transforms practical problems into probabilistic problems, which can also be called random simulations. The core idea of this method is random distribution, which generates a random molecular model from random numbers and makes the particles in the model move irregularly through a computer. Count whether the energy in the newly generated molecular model decreases, if it decreases, the model proves to be valid, and the next iteration is carried out until the final model meets the preset conditions. Compared with the MD method, the MC method does not need to calculate the intermolecular forces, so the simulation is simpler and faster. However, because the motion process of particles cannot be expressed, the dynamic information of the system cannot be obtained, and it is not suitable for large polymer systems.

The quantum MD approach is a density functional theory based on the Koohn–Sham equation and a *de novo* computational MD approach around density functional theory. There are three approximations, namely, the nonrelativistic approximation, the single-electron approximation, and the adiabatic approximation. Scholars usually use quantum MD methods to achieve the accurate solution of the potential energy surface and the determination of the standing point structure of the potential energy surface, and for larger systems, only the local minimum point and transition state on the search reaction path are generally calculated. Purely based on quantum mechanical methods, dynamical simulations are generally only suitable for the dynamic behavior of very small systems on very short time scales, and their high computational costs limit their scope of application, because they are often very computationally large and are not suitable for studying systems with more than 1000 atoms.

Molecular mechanics are mainly based on classical mechanics, also known as force field methods. According to the Born–Oppenheimer approximation, molecular mechanical methods ignore the motion of electrons and express the resulting energy (*e.g.*, bond energy) as an empirical analytical form of the coordinates of the atomic nucleus. These different forms of analytic functions are force field functions, which are at the heart of molecular mechanics. Mechanical parameters can be obtained by experimental measurements or fitting based on quantum mechanical calculations. Since the 80 s of the last century, with the advancement of computer technology, people have developed a variety of force fields with resonant potential energy expressions that contain more details, with similar function compositions and specific expressions. However, because the electron motion is ignored, it is not possible to simulate properties based on differences in electron distribution and phenomena based on changes in electron distribution, so many specialized force fields have also been developed, such as bond level potentials for semiconductors and hydrocarbons [122], ReaxFF force fields for simulating chemical reactions [123], *etc.* The calculation accuracy of molecular mechanics is largely determined by the selected force field form and related parameters, so it is necessary to carefully select and calibrate the force field suitable for the research system before all molecular mechanics simulations.

Deep learning is hierarchical feature learning based on neural network algorithms, as a technology to realize machine learning, which makes artificial intelligence produce revolutionary breakthroughs. From the structural point of view, in the network framework of deep learning, the input layer is used to receive data, the output layer is used to generate the final result, and there are zero or more hidden layers between the input layer and the output layer to learn the nonlinear mapping relationship between the input and output, and deep learning is usually composed of a plurality of hidden layers, which is composed of a deep nested network structure, which can activate a neuron multiple times and automatically discover the features required for the learning task, so the deep learning model is superior to the shallow machine learning model and the traditional data analysis method, and the deep learning can use its automatic feature learning ability to directly complete the modeling task on the high-dimensional original input data into better handle large-scale, noisy, and unstructured data. At present, deep learning has shown excellent performance in the fields of image, language, computer vision, *etc*., and many scholars have applied it to MD simulation.

First-principles calculation is a calculation method that directly solves the Schrödinger equation through some basic physical constants, such as electron mass, electron charge, Planck constant, and speed of light, and then obtains the structure and physicochemical properties of materials. There are two approximations, the Born–Oppenheimer approximation and the Hartree–Fock approximation. Since there is no need to provide experimental parameters for calculation, this method can be exempted from the limitation of experimental conditions, and then, the material properties can be explored more deeply from a microscopic perspective, and some phenomena that are difficult to observe experimentally can be obtained. First-principles can be used to calculate the dynamic behavior of atoms at the microscopic scale that cannot be accurately observed experimentally, as well as the complex electronic structure of materials, such as strong correlation and bonding. With the rapid development of computers, first-principles calculations have been widely used in MD simulations and have become an indispensable technical means in simulation research.

5.2 Software environment

In the development of MD computer simulation, the main work has been divided into two aspects. On the one hand, there is a strict theoretical foundation and a suitable mathematical calculation model, and on the other hand, the calculation principle of the mathematical model is written through the computer machine language to realize multi-threaded computing on the computer.

Materials Studio molecular simulation software is an early commercial software that conveniently combines quantum mechanics, molecular mechanics, mesoscale simulation, analytical instrument simulation, and statistical correlation into one easy-to-use modeling environment. It allows people to create and study models of molecular structures, taking advantage of powerful graphical capabilities to present people's results. And the software has corresponding service guidance, has a humanized visual interface, has a high degree of professionalism, and does not require researchers to have high computer ability requirements. However, due to the different systems for which software is developed, the fields of production are different, and they are not comprehensive. Moreover, due to the commercial secrecy mechanism, users cannot understand the core principle, which leads to the limitation of dealing with the problem and, at the same time, has a high cost of use.

Lammps, which stands for large-scale atomic/molecular massively parallel simulator, is a powerful MD calculation program developed by Steve *et al.* of the Sandia National Laboratory in the United States. In the early days, Fortran was written in Fortran, but with successive versions and enhancements, Lammps is now written in C++ code and is updated regularly every month. Lammps does not have a visual interface, and all operations are operated by manually writing IN input files to operate relevant settings and solving problems through computer background processing and calculation. The IN-script code can be used to initialize the simulation system, define the initial state atoms, set the specific simulation parameters, and start the simulation. However, Lammps does not provide intelligent data analysis and data plotting tools for MD simulations, and the maintenance is poor.

VMD software is a powerful molecular visualization and molecular simulation software, which uses OpenGL to provide high-quality 3D molecular graphics for displaying, animating, and processing large atomic simulation systems, and can be used in conjunction with a variety of mainstream MD simulation software. Written in C++ and developed for the interactive graphical display of molecular systems, especially biopolymers such as proteins or nucleic acids, VMD supports the display of dynamic data, can interact with a separate MD simulation application to provide a graphical user interface and visualization console for the simulation program, can display molecules in a user-selectable rendering style, and produces high-quality hardcopy images.

GROMACS is a molecular simulation package based on the GROMOS software package, which was developed to simulate biomolecules in solution. As one of the most widely used open-source MD simulation software, GROMACS has high computational efficiency, wide application range, friendly operation interface, and simple operation. His input file must be readable ASCII text, annotated, and provide an interface to the standard file formats used in the fields of biology, physics, and chemistry. The output file is generic, allowing the user to write their own analysis program or use the analysis tools provided by the gromacs software. However, gromacs software is not compatible with other MD simulation software.

CP2K is an open-source electronic structure and MD software package for massively parallel and linear-scaled electronic structure methods and state-of-the-art *de novo* computational MD simulations. It has a good quantum mechanical approach and can calculate many different properties. But the use of CP2K requires a long and complex input file containing all the required parts, keywords, and atomic types and their sits for the system to be calculated.

The user can obtain the required structure and properties by analyzing the.xyz trajectory file and the.out output file generated by the simulation.

Table 1 lists the commonly used software for MD simulations, describes their performances, and notes their limitations.

6 Conclusions and prospects

In the past few decades, with the rapid development of science and technology, significant progress has been made in the study of the confinement effect of nanochannel ion transport in many fields. This section will focus on the prospects of this field, in order to provide useful references for future research and applications.

6.1 Research status

With the development of nanotechnology, functional nanomaterials have a wide range of application prospects in high-tech fields such as information, biology, energy, environment, and aerospace. CNTs, graphene, and other nanofluidic devices have great application potential in the fields of water desalination, ion separation, energy harvesting, detection, and inspection due to their good mechanical properties, extremely thin thickness, chemical stability, and environmental friendliness. The confinement effect reduces the entropy of the fluid, making its transport properties in the nanochannel different from that of the bulk phase. Factors such as steric hindrance, Coulomb interaction, and pore geometry have an important impact on the transport efficiency of water in nanochannels. In addition, the ions form a stable hydrated shell in an aqueous solution, and the radius of the hydrated ions is greater than that of the water molecules. Choosing the right size of nanochannels can completely block the passage of ions, allowing only water molecules to pass through. Studying the osmotic transport of ions at the atomic scale can help develop effective methods for water filtration and desalination. Biological proteins have good selectivity for ions, but their selection process is complex, and it is difficult to distinguish the role of various factors in ion selection. However, inorganic nanochannels are relatively easy to control the variables, and the roles of ion dehydration, Coulombic interaction, and functional groups in ion selection can be explored. The study of the mechanism of liquid-phase transport and separation has important scientific value and guiding significance for the industrial application of nanofluidic devices in the future.

6.2 Trends

In view of the shortcomings and challenges of the current research, the future research trends of the confinement effect of nanochannel ion transport can be summarized as follows:

1) The behavior of water within the nanoscale channel is significantly different from that at the macroscale, where the motion-governing equations of classical fluid mechanics can no longer account for the flow behavior of water. With the continuous advancement of material preparation technology, we are now able to precisely control the eigenvalue of nanochannels. For example, graphene 2D channels have atomically smooth channel walls, and channel heights can

Table 1: Comparison of commonly used software packages for MD simulation

Name	Advantages	Drawback
NAMD	High level of design, high computing efficiency, compatible with a variety of input and output file formats	The simulation effect of some systems is not good
Amber	The built-in potential energy model is good, and it is convenient to customize new models and new molecules, and the maintenance is good	The operation efficiency is low, and the calculation speed is slow
DL-POLY	The interface is good, the computing efficiency is high, and the maintenance service is good	Compatibility is not good
CHARMM	The potential energy model is updated quickly, and it is convenient to customize the new model and maintain it well	The operation is slow, and the efficiency is low

be reduced to the angstrom level. These angstrom-scale height channels can be directly compared to experiments by simulation. Studying the transport of ions in nanochannel systems has long been of interest to the academic community due to their importance in understanding the properties of environmental, biological, and chemical processes.

2) Several successful studies have shown the potential to construct nanochannels on ion-exchange membranes to achieve selective separation of specific ions. However, how to successfully fabricate selective nanochannels on ion-exchange membranes and the mechanism of their selectivity still need to be further explored. In addition, long-term membrane stability is critical under real-world operating conditions, requiring high chemical, mechanical, and thermal durability, and therefore requires extensive research to achieve stability in membrane structure and performance. Although the membranes studied in these studies have specific ion selectivity at a laboratory scale, upgrading them to a low-cost industrial scale remains a significant challenge. Overall, artificial nano-sized ion channels provide a promising solution for efficient target ion separation and energy conversion.
3) With the deepening of nanofluidics research, the manipulation of fluid transport behavior is gradually developing in the direction of more miniaturization. In nanochannels, the regulation of fluid transport behavior is mainly based on the electrodynamic principle for the regulation of molecular or ion transport behavior inside the fluid. The size of the nanochannel is similar to the thickness of the electric double layer of the channel, which makes it possible to regulate the transport behavior of molecules according to their charged state. According to the structure and function relationship of nanochannels in biofilms, the biomimetic design of functionalized artificial nanochannels has great application potential in regulating the behavior of nanoscale fluids and designing functionalized nanofluid devices.
4) The size of nanochannel materials is small, and it is difficult, costly, and blind to directly control and realize functional design and modification experiments. Therefore, it is necessary to theoretically prove the feasibility of the experiment before conducting it. With the development of computer technology and the enrichment of theoretical models, MD simulation methods have gradually developed into one of the important methods for experimental design and prediction. The simulation results can provide direct guidance for the experiment of materials, improve the success rate of the experiment, and reduce the blindness of the experiment, and the development of MD simulation has great potential in the study of nanochannel experiments.

6.3 Conclusion and outlook

In this study, we introduce the progress of industrial applications of nanochannels, such as desalination, ion selection, energy enrichment, and detection, and explore the phase behavior of confined water in nanochannels, the micromechanical mechanism of confined mass transfer, and material modification in combination with mainstream theoretical models and MD simulation software. Among them, the influence of the nanochannel confinement effect on the confined water structure, shear viscosity, self-diffusion, and hydrogen bonding behavior is revealed, and the micromechanical nature of the confined water flow boundary slip in the nanochannel is clarified based on atomic-scale structure and morphological analysis, which greatly expands the content of the mechanical properties of the nanoscale ion transport confinement conditions. Therefore, future research will seek more breakthroughs in the following channel applications to promote the mechanical properties of nanochannel ion transport confinement conditions to practical applications.

Graphene nanochannels in GO films have the ability to transport water molecules quickly, but are strictly limited by nanochannel size and film stability. How to stably control the size of graphene nanochannels is the key to realize high-flux graphene-based filtration membranes, which provides new ideas for the design of seawater desalination membranes and other separation and mass transfer processes based on size selectivity.

1) Nanochannels are a key component of nanofluid devices, and the function of nanochannels determines the application of nanofluid devices. Therefore, how to design and fabricate functionalized nanofluidic devices is one of the key issues restricting the development of nanofluidics. How to biomimetic the structure of artificial nanochannels based on solid materials, according to the characteristics of biological channel structure, by regulating the interaction between the channel and the transported material (electrostatic interaction, van der Waals interaction, hydrogen bond interaction, *etc.*), to achieve intelligent regulation of the transported substances in the channel.
2) Water under extreme confinement has attracted extensive attention because its structural phase and dynamic behavior are significantly different from those of bulk water. Many researchers have found that the enhancement

of the water transport rate is mainly due to its low-friction flow on graphene. The smooth surface properties of graphene and the interface effect between water and graphene are important factors that lead to low friction. Therefore, the study of the phase state and dynamic behavior of confined water structures is helpful to reveal the mechanism of the high-speed water flow through the graphene nanocapillary channels observed in the experiments.

With the advancement of ion transport mechanism research and biomimetic design of solid-state nanochannels, the industrial application of nanochannels has become an unavoidable topic. Future development should be more diversified and integrated to provide more possibilities for scientific research and technological innovation.

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