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- **Junqiao Zhang**, Tianyang Sun, Lijun Liang, Tao Wu and Qi Wang, Drug promiscuity of P-glycoprotein and its mechanism of interaction with paclitaxel and doxorubicin. ***Soft Matter***, 2014,10, 438-445（第一作者，中科院一区，IF=4.1，已经被引用超过10次）
- Debing Li, Wei Hu, **Junqiao Zhang**, Lijun Liang, Qi Wang, Separation of Hydrogen Gas from Coal Gas by Graphene Nanopore. ***J. Phys. Chem. C***, 2015. 119(45), 25559 – 25565（IF=4.8）
- Yu Kang, Zhisen Zhang, Hui Shi, **Junqiao Zhang**, Lijun Liang, Qi Wang, Hans Ågren and Yaoquan Tu, Na^+ and K^+ ion selectivity by size-controlled biomimetic graphene nanopores ***Nanoscale***, 2014, 6, 10666-10672 (IF=7.4）
- Zhisen Zhang, Jiawei Shen, Hongbo Wang, Qi Wang, **Junqiao Zhang**, Lijun Liang, Hans Ågren, and Yaoquan Tu, Effects of Graphene Nanopore Geometry on DNA Sequencing, ***J. Phys. Chem. Lett.*** 2014, 5, 1602-1607 (IF=7.4）

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发表论文首页：

附后

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Interaction of P-glycoprotein with anti-tumor drugs: the site, gate and pathway

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Understanding the mechanism and pathway of anti-cancer drugs to be pumped out by P-glycoprotein (P-gp) in cancer cell is very important for the successful chemotherapy. P-gp is a member of ATP-binding cassette (ABC) transporters. In this study, random accelerated molecular dynamics (RAMD) simulation was used to explore the potential egress pathway of ligands from the binding pocket. This could be considered as a reverse process of drug binding. The most possible portal of drugs to dissociate is TM4/TM6, which is almost the same for different drugs, such as paclitaxel and doxorubicin. The interactions in the binding site are found to be remarkably stronger than that outside of the binding site. The results were suggested by the free energy calculation between P-gp and different drugs from metadynamics simulation. All the results indicate that the flexibility of inner residues, especially the residue Phe339, is very important for the drugs to access the binding site.

1. Introduction

ATP-binding cassette (ABC) transporters were found to mediate the extrusion of cytotoxic agents.[1] These proteins can pump anti-cancer drugs out of body, thus confer drug resistance on tumor cells.[2] P-glycoprotein (P-gp) is a typical example of this kind of protein.[3,4] It has a molecular weight of ~170 kDa, and its two homologous halves are connected by a flexible linker region. Each one comprises six transmembrane α-helix segments (TM) and a nucleotide-binding domain (NBD).[5]

Understanding the process of multidrug recognition and efflux by P-glycoprotein (ABCB1) is key to revealing the substrate promiscuity (broad drug specificity) of P-gp and the multidrug resistance (MDR) of cell.[6] The phenomenon that tumor cells show resistance to structurally unrelated anti-cancer drugs is called MDR.[7] Generally, MDR is the result of the over-expression of membrane proteins like P-gp, which exhibits power to exclude many kinds of drugs out of cell. It has been reported that up to 40% of human cancers express the MDR phenomenon, which renders multiple anti-cancer drugs ineffective to tumors.[8] Therefore, P-gp has aroused great interest to researchers as one of the main concerns in anticancer therapy.[9,10] In the inward-facing structure obtained from mouse[6] and *Caenorhabditis elegans*,[11] the portals formed by TMs grant substrates the access to the binding site from the inner leaflet and cytoplasm. Although a number of studies have been done, the pathway of drugs to the binding site and the detailed drug–P-gp interaction process are not clear. A previous work suggested that a putative aromatic gating may be present in P-gp,[12] but there is no direct evidence showing which residue plays the role of gating in the way to the binding site. The substrate promiscuity of P-gp, as its enigmatic property, is also not well elucidated.

Molecular simulation may be an alternative to discover the pathway of drugs to the binding site and the detailed drug–P-gp interaction process. The conventional molecular dynamics has been used to explore the binding energy of P-gp and ligands.[13–15] However, due to the limitation of computational resources, all-atom molecular dynamics are not computationally feasible to sample the timescales which are long enough to observe the detailed drug entry process. There are a few methods used to compute free energy profiles, like umbrella sampling and adaptive biasing force MD.[16] Especially, the metadynamics method was regarded as a successful method to calculate the free energy surface (FES) in recent years.[17,18] By effectively escaping local minima, this method could accelerate simulation of rare events and calculate the free energy surface by summing up potential hills.[19] The metadynamics could well estimate the free energy surface; however, metadynamics is not designed to find the best reaction coordinate.[16] Here, random accelerated molecular dynamics (RAMD) could be an appropriate pathway to explore the buried active site.[20,21] Substrate-exit channels from the buried site of interest could be found by imposing an artificial force. The force was exerted on the substrate, with a randomly chosen direction and a constant value.[22] These two methods could well compensate each other. Therefore, in this study, RAMD and metadynamics

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Drug promiscuity of P-glycoprotein and its mechanism of interaction with paclitaxel and doxorubicin†

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P-glycoprotein (P-gp) pumps a broad range of structurally diverse anti-cancer drugs out of cancer cells. Therefore, multi-drug resistance (MDR) in chemotherapy closely correlates with P-gp. However, how this single transport system recognizes different substrates remains unclear. In this study, we attempt to uncover the mechanism of substrate promiscuity of P-gp by atomistic molecular dynamics simulations. Results indicate that different drugs like paclitaxel and doxorubicin approach the putative binding site of P-gp, and the inner residues are found to be important in this process. An obstacle-overcoming process was observed, illustrating that the inner residues are flexible. Interaction energy calculations suggest that the inner residues possess high affinity toward substrates. The cavity of adaptability to accommodate different drugs would help explain why P-gp has so many different substrates.

1. Introduction

Multidrug resistance (MDR) is largely responsible for the failure of chemotherapy.[1] The most accepted mechanism of MDR is that some membrane proteins overexpress in cancer cells. These proteins expel a broad range of substrates out of the cell and result in lower intracellular anticancer drug accumulation.[2,3] P-glycoprotein (P-gp) is an energy-dependent multidrug efflux membrane protein.[4] Most anti-cancer drugs diffuse through a concentration gradient into the cells without specific drug carriers.[5] P-gp maintains relatively low concentrations in cells by transporting drugs out of the cells. Thus, P-gp confers resistance against a wide spectrum of compounds and allows cancer cells to survive in the presence of different anti-cancer drugs.

The P-gp (ABCB1, MDR1) gene encodes 1280 amino acids and is composed of two homologous halves connected by a flexible linker region. Each half contains a transmembrane domain (TMD) and a nucleotide-binding domain (NBD). Each TMD comprises six transmembrane (TM) segments.[5–7] The high-resolution crystal structure of P-gp from mice was first solved in 2009.[8] In 2012, another P-gp structure was obtained from *Caenorhabditis elegans*.[9] These results allow the study of the mechanism of P-gp through structural information. Unfortunately, the published structures of P-gp are incomplete and lack information corresponding to the structure of the linker region. Therefore, a mechanistic study through structural information necessitates the development of homology models of P-gp. Many studies have developed several homology models of human P-gp.[4,9–11]

A number of models for the mechanism of P-gp binding substrates have been proposed, including the hydrophobic vacuum-cleaner model[12] and the induced-fit model.[13] These models are closely related to the cavity, often called the "drug-binding pocket." The cavity is formed by funnel-shaped TMDs and contains the putative substrate-binding site. Inner residues were found to be important in recent years, most of them are hydrophobic and aromatic.[8] The inward-facing conformation of P-gp results in a large internal cavity open to both the cytosol and the membrane. P-gp has been proposed to be able to recruit hydrophobic substrates from the lipid bilayer[1,7,14] and/or cytoplasm.[15] Regardless of the pathway, substrates are believed to enter the internal drug-binding pocket through opening portals formed by TM 4 and 6 as well as TM 10 and 12.[8,11,16] In that case, the substrate would first get to the vicinity of the cavity (or the "cavity entrance"), and then bind to the binding site in the upper half of the cavity.[8,11] Given this process, the cavity entrance is a reasonable starting point for a mechanistic study of how P-gp interacts with substrates as a multidrug pump. How a single transport system, in this case the protein, can recognize so many different kinds of substrates has long challenged researchers.[1,9] Uncovering the properties of the non-specific drug-binding sites of P-gp is essential for understanding drug–protein interactions and helpful in designing inhibitors. P-gp has a broad range of substrates, including anticancer drugs, HIV protease inhibitors, analgesics, antihistamines, and some fluorescent compounds.[1,5,14]

The molecular mechanism of the substrate promiscuity characteristics of P-gp remains unknown. Thus, determination of the process of transporter interaction with diverse substrates is essential. In this study, two potent anticancer drugs, paclitaxel

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Letter

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Effects of Graphene Nanopore Geometry on DNA Sequencing

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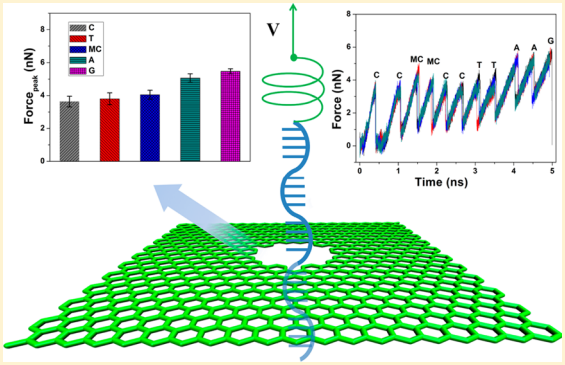
Supporting Information

ABSTRACT: In this Letter we assess the effect of graphene nanopore geometries on DNA sequencing by considering DNA fragments including A, T, C, G, and 5-methylcytosine (MC) pulled out of graphene nanopores of different geometries with diameters down to ∼1 nm. Using steered molecular dynamics simulations it is demonstrated that the bases (A, T, C, G, and MC) can be indentified at single-base resolution through the characteristic peaks on the force profile in a circular graphene nanopore but not in nanopores with other asymmetric geometries. Our study suggests that the graphene nanopore surface should be modified as symmetrically as possible in order to sequence DNA by atomic force microscopy or optical tweezers.



SECTION: Physical Processes in Nanomaterials and Nanostructures

INTRODUCTION

DNA sequencing with nanopores has attracted much attention ever since DNA translocation through the biological nanopore α-hemolysin was first demonstrated.[1] In nanopore DNA sequencing, a negatively charged DNA molecule is electrophoretically driven though the nanopore and its sequence is read off through measuring the reduction of the ion current during the DNA translocation through the pore. Such DNA sequencing with nanopores provides a promising technology for cheap and fast DNA sequencing free of enzyme-dependent amplification and fluorescent labeling steps.[2,3]

While both biological and solid-state nanopores can be used for DNA sequencing, the latter technique[4] offers a number of advantages, such as superior mechanical properties,[5,6] multiplex detection,[7] and high stability to complex environments.[8] Significant progress has been made in DNA sequencing with solid-state nanopores.[9−11] However, conventional nanopores are of several nanometers in thick and, as a result, they are occupied by many DNA bases during the sequencing, making it difficult to detect a single-stranded DNA (ssDNA) molecule at single-base resolution.

It has been demonstrated that nanopores fabricated from graphene sheets can be made extremely thin, even one-atom-thick,[12] and structurally robust,[13] something that has opened a new chapter in DNA sequencing with nanopores with a resolution that allow identification of single nucleotides. DNA translocation through a nanopore can be recognized by measuring the blocked current,[14−19] which has increasingly been used in DNA detection in recent years.[20−22] However, compared with traditional thick solid-state nanopores, graphene nanopores with diameter down to ∼5 nm in experiments (or ∼2 nm in simulations) have not achieved current signals with appropriate resolution for nucleotide identification.[18,21] Up to now, the effect of pore geometries on DNA translocation through graphene nanopores remains unclear.

In this Letter, we report studies on the effect of graphene nanopore geometries on DNA sequencing, using all-atom steered molecular dynamics (SMD) simulations and thereby extending earlier studies of DNA detection with nanopores using this technique.[23,24] As shown in Figure 1A, an ssDNA molecule translocates through a graphene nanopore in a ratchet-like way when it is pulled through the pore. By characterizing the force profile acting on the ssDNA, we are able to distinguish the nucleotides and 5-methylcytosine (MC, a methylated form of cytosine that may be involved in the regulation of gene transcription) passing through a circular nanopore with the diameter of ∼1 nm.

System Setup. A graphene sheet was placed in the $x-y$ plane with the center of mass in the Cartesian coordinate origin (0, 0, 0). A circular nanopore was constructed by

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Na^+ and K^+ ion selectivity by size-controlled biomimetic graphene nanopores†

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Because biological ionic channels play a key role in cellular transport phenomena, they have attracted extensive research interest for the design of biomimetic nanopores with high permeability and selectivity in a variety of technical applications. Inspired by the structure of K^+ channel proteins, we designed a series of oxygen doped graphene nanopores of different sizes by molecular dynamics simulations to discriminate between K^+ and Na^+ channel transport. The results from free energy calculations indicate that the ion selectivity of such biomimetic graphene nanopores can be simply controlled by the size of the nanopore; compared to K^+, the smaller radius of Na^+ leads to a significantly higher free energy barrier in the nanopore of a certain size. Our results suggest that graphene nanopores with a distance of about 3.9 Å between two neighboring oxygen atoms could constitute a promising candidate to obtain excellent ion selectivity for Na^+ and K^+ ions.

1. Introduction

Ionic channels in proteins play a key role in several cellular transport phenomena[1] and provide sources of inspiration for the development of a variety of biomimetic-type nanopores. This notion is based on the fact that biological ionic channels contain precisely arranged charged amino acids to achieve extremely high permeability simultaneously with high selectivity to pass the ions.[2] These superior selectivity features of biological channels have attracted much research interest[3] and inspired many experiments and theoretical studies alike to mimic these properties in technical applications.[4–10] Proteins can always lose their bioactivity outside of the biological setting,[11] and harsh environmental demands and poor mechanical properties of proteins have strictly limited their applications *ex vivo*. Therefore, it would be of great value if the key functionalized core of proteins could be simulated by man-made mechanical nanopores for use in industrial applications. The simulation of functions of proteins is also very important to the development of biomimetic materials in general.

Solid state nanopores fabricated from graphene sheets[12–14] have attracted much attention due to the unique properties of graphene.[15,16] Thanks to the fast development of etching nanotechnology, graphene nanopores with radii as small as 0.3 nm have been synthesized.[17] Many studies have shown that graphene nanopores can be used in functionalized applications.[13,14,18–25] Jiang *et al.* found that graphene nanopores can be used for gas separation.[20] Aksimentiev *et al.* used molecular dynamics (MD) simulations to show that graphene nanopores can be used for DNA sequencing.[23] Sint *et al.* demonstrated the selectivity of ion passage by means of functionalized graphene nanopores,[24] and Zeng *et al.* reported an outstanding graphyne membrane for water desalination at a high rate and potentially low cost.[25] Thus, graphene is a promising biomimetic material for a variety of applications, such as for nanofluidics, biosensors, and for ion selective devices.

To mimic the functions of proteins, it is essential to understand their core structures and functional mechanisms. Herein, the potassium channel from *Streptomyces lividans* (KcsA) (PDB ID: 1BL8) was selected as a model protein.[26] As we know, the properties of Na^+ and K^+ are almost the same, since they are both alkali cations with the same charge. Thus, it is difficult to distinguish them by simple pores like those in zeoiltes[27] and silica.[28] However, biological K^+ channels have the ability to make an up to 1000-fold selection of K^+ from Na^+[29] The functional core in K^+ channel proteins is an ion filter that is lined by four rings of backbone carbonyl groups, which compensate for energy lost during the dehydration process.

In this work, graphene nanopores with different radii were designed for ion selectivity for Na^+ and K^+ by means of MD simulations. We study the sensitivity and the separability of Na^+ and K^+ ions with respect to the variation of pore dimensions in order to determine the optimal conditions, attempting to find a deeper explanation for selectivity in this respect. The work can

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Article

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Separation of Hydrogen Gas from Coal Gas by Graphene Nanopores

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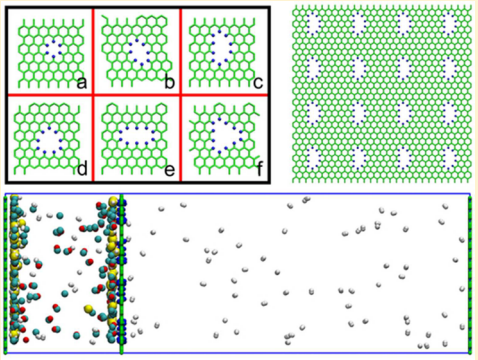
Supporting Information

ABSTRACT: We designed a series of porous graphene as the separation membrane for hydrogen gas in coal gas. The permeation process of different gas molecules (H_2, CO, CH_4, and H_2S) in porous graphene was evaluated under the atmospheric pressure and high pressure conditions. Our results indicate the hydrogen permeability and selectivity could be tuned by the size and the shape of the porous graphene. For graphene with bigger pores, the selectivity for hydrogen gas could decrease. In the porous graphene with same pore area, the hydrogen gas selectivity could be affected by the shape of the pore. The potential of mean force (PMF) of different gases to pass through a good separation candidate was calculated. The order of PMF for different gases to pass through the good separation candidate is $H_2 < CO < CH_4 \approx H_2S$, which is also confirmed by the first-principle density function theory (DFT) calculation.



1. INTRODUCTION

Gas separation is a significantly important issue due to its wide range of applications, such as cleaning air and recycling hydrogen gas.[1,2] Hydrogen separation from coal gas (primarily composed of CO, CH_4, H_2S and H_2) is significant for a new clean technology.[3,4] Compared with traditional gas separation technology, membrane separation technology is considered as low-cost, environment friendly, and highly efficient.[5−7]

Based on its different compositions, the membrane could be mainly divided into organic membrane,[8−10] inorganic membrane,[11,12] and hybrid membrane.[13−15] The organic membrane made from polymer is usually inappropriate for hydrogen gas separation because the gas permeation through the organic membrane is very low.[16] In addition, the polymeric membrane could not be used in such a long time due to the aging and plasticization problems.[17] Inorganic membrane made from carbon molecular sieve is proven to effectively separate different gas molecules, but the membrane is too fragile for industrial applications.[18] Recently, the single layer thick membrane, made from graphene, has attracted many attentions due to its unique electronic and mechanical properties.[19−21] In addition, porous graphene can also be synthesized by creating pores in the pristine graphene sheet using electron beam sculpting,[22] oxidative etching,[23] ion bombardment,[24] or graphene oxide reduction.[25] What is more, the porous graphene with specific geometry has been successfully synthesized by a cross-coupling method.[26,27] More interestingly, graphene nanopores fabricated from graphene sheets are shown to be extremely thin and structurally robust. It has been extensively studied on potential applications over a wide range from ion-selectivity,[10,28] water desalination,[29,30] to DNA sequencing.[31−33] Meanwhile, some experimental and theoretical investigations have suggested that porous graphene membrane is a good option for gas separation.[34−38] Kim et al. pointed out that high CO_2/N_2 selectivity could be achieved by well-interlocked graphene and graphene oxide membrane.[35] High selectivity on the order of 10^8 for H_2/CH_4 was found in a nitrogen-functionalized graphene pore by computational study.[34] The results from Du's work show that hydrogen gas could be separated by a small graphene nanopore.[36] All these results indicate that hydrogen gas could be separated by modified porous graphene. However, the effect of pore shape especially with the same area of porous graphene was not considered in these studies. In addition, the permeation mechanism of hydrogen gas through porous graphene was poorly understood.

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