Graphene stretches to fast ion filtration

Cordelia Sealy

Graphene has potential as a versatile membrane or filtration material for ion filtration or water purification, as well as sensing and drug delivery. Now researchers at the National Institute of Standards and Technology (NIST) predict that stretching graphene that contains special pores could allow even better control of the flow of material through the membrane [Fang et al., *Nature Materials* (2018), https://10.1038/s41563-018-0220-4].

"There are many ways to control permeation via artificial nanopores," explains Alex Smolyanitsky, who led the study. "But we are predicting an additional one... a type of artificial ion channel with high sensitivity to strain."

The idea is to embed ring-shaped molecules composed of oxygen, carbon, and hydrogen atoms called crown ethers into graphene, where they form nanopores. The chemical nature of the crown ether pores allows them to form complexes with metal ions with high selectivity.

"We are just starting to look at these structures, but from what we have seen so far, some ions can be trapped inside the graphene-embedded crown ether pores, while others do not get trapped," say Smolyanitsky and lead author Alta Fang.

The researchers used molecular dynamics to simulate the movement of potassium and sodium ions, as well as mixtures of the two, through crown ether nanopores in graphene. The pores trap positively charged potassium ions but an applied electric field controls the trapping and release of the ions, driving an ion current through the membrane (Fig. 1).

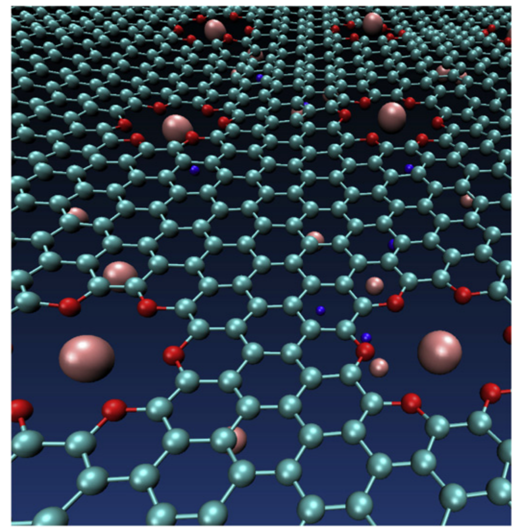

Fig. 1. Aqueous potassium ions (pink) trapped in an array of graphene-embedded crown ether pores.

The next prediction makes graphene membranes even more interesting. When pore-containing graphene is stretched, you might expect the flow to increase in proportion with the larger pore size. But the team's simulations predict that a mere 2% stretch in the graphene leads to a 10-fold increase in ion flow.

"The primary advantage of these graphene-embedded crown ether membranes is that they allow ion permeation to be externally controlled by stretching the membrane," point out Smolyanitsky and Fang.

The sensitivity to strain could be the result of a number of factors, they suggest, including the thinness of graphene, interactions between the ions and the surrounding liquid, and between the pores and the ions.

If membranes with such pores can be fabricated, and if the researchers' theoretical predictions prove correct, there could be many interesting applications. The ability to increase ion flow exponentially under small strains could be useful in fast ion separators or salinity control devices.

"One potentially interesting additional application is pressure sensing in artificial skin," say Smolyanitsky and Fang. "Because the strain is converted directly into changes in ionic flow, in principle, such sensors could form a direct interface with neurons."

It is also conceivable that the approach could work in other membrane materials, opening up a new avenue for the control of permeation. The NIST team is now hoping to work with experimentalists to explore their predictions.

César Moreno of the Institut Català de Nanociència I Nanotecnologia (ICN2) believes the work could be the inspiration for a new type of controllable smart membranes.

"Moving from nanopores as passive elements, allowing or rejecting species to filter, to nanopores as active and dynamic elements, where the pore would be open or closed by an externally actuated mechanism will constitute the next generation of smart membranes," he explains.

Although the idea of creating ion channels in graphene using embedded crown ethers is not new, he points out, the theoretical prediction of non-biological membranes that are very sensitive to mechanical stimuli is novel.

"Mechano-sensitive ion channels are the most ubiquitous elements in living cells and tissues. These theoretical predictions open up an exciting future using solid-state nanopores of atomically thin membranes as an ideal platform to gain fundamental understanding of the complexity of biological membranes and ion transport mechanisms, which is essential in sensing, energy storage, and advanced filtration applications," says Moreno.

It will be challenging, however, to manufacture nanoporous graphene that is robust enough to withstand the required stresses, he cautions.

Cordelia Sealy has many years' experience as a scientific journalist and editor in areas spanning nanotechnology, materials science and engineering, physics and chemistry. She has served as Editor of *Materials Today* and *Nano Today*, and more latterly as Managing Editor of both titles. She has also worked in academic publishing as a books acquisitions editor and in business-to-business publishing as a journalist on *European Semiconductor*. She has a First in Physical Sciences (BSc) from University College London and a DPhil in materials science from the University of Oxford, and is a Member of the Institute of Physics. Cordelia is currently a freelance science writer for her own company, Oxford Science Writing, and News and Opinions Editor for *Nano Today*.

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