Nanopores could take the salt out of seawater

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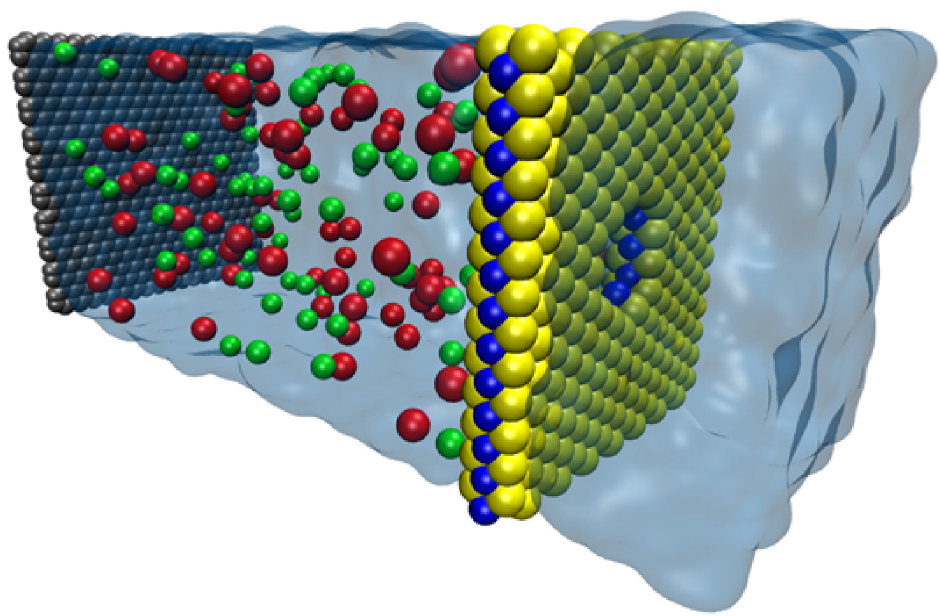

A computer model of a nanopore in a single-layer sheet of MoS_2 shows that high volumes of water can pass through the pore using less pressure than standard plastic membranes. Salt water is shown on the left, fresh water on the right. Credit: Mohammad Heiranian

University of Illinois engineers have found an energy-efficient material for removing salt from seawater that could provide a rebuttal to poet

Samuel Taylor Coleridge's lament, "Water, water, every where, nor any drop to drink."

The material, a nanometer-thick sheet of molybdenum disulfide (MoS2) riddled with tiny holes called nanopores, is specially designed to let high volumes of water through but keep salt and other contaminates out, a process called desalination. In a study published in the journal *Nature Communications*, the Illinois team modeled various thin-film membranes and found that MoS2 showed the greatest efficiency, filtering through up to 70 percent more water than graphene membranes.

"Even though we have a lot of water on this planet, there is very little that is drinkable," said study leader Narayana Aluru, a U. of I. professor of mechanical science and engineering. "If we could find a low-cost, efficient way to purify sea water, we would be making good strides in solving the water crisis.

"Finding materials for efficient desalination has been a big issue, and I think this work lays the foundation for next-generation materials. These materials are efficient in terms of energy usage and fouling, which are issues that have plagued desalination technology for a long time," said Aluru, who also is affiliated with the Beckman Institute for Advanced Science and Technology at the U. of I.

Most available desalination technologies rely on a process called reverse osmosis to push seawater through a thin plastic membrane to make fresh water. The membrane has holes in it small enough to not let salt or dirt through, but large enough to let water through. They are very good at filtering out salt, but yield only a trickle of fresh water. Although thin to the eye, these membranes are still relatively thick for filtering on the molecular level, so a lot of pressure has to be applied to push the water through.

"Reverse osmosis is a very expensive process," Aluru said. "It's very energy intensive. A lot of power is required to do this process, and it's not very efficient. In addition, the membranes fail because of clogging. So we'd like to make it cheaper and make the membranes more efficient so they don't fail as often. We also don't want to have to use a lot of pressure to get a high flow rate of water."

One way to dramatically increase the water flow is to make the membrane thinner, since the required force is proportional to the membrane thickness. Researchers have been looking at nanometer-thin membranes such as graphene. However, graphene presents its own challenges in the way it interacts with water.

Aluru's group has previously studied MoS2 nanopores as a platform for DNA sequencing and decided to explore its properties for water desalination. Using the Blue Waters supercomputer at the National Center for Supercomputing Applications at the U. of I., they found that a single-layer sheet of MoS2 outperformed its competitors thanks to a combination of thinness, pore geometry and chemical properties.

A MoS2 molecule has one molybdenum atom sandwiched between two sulfur atoms. A sheet of MoS2, then, has sulfur coating either side with the molybdenum in the center. The researchers found that creating a pore in the sheet that left an exposed ring of molybdenum around the center of the pore created a nozzle-like shape that drew water through the pore.

"MoS2 has inherent advantages in that the molybdenum in the center attracts water, then the sulfur on the other side pushes it away, so we have much higher rate of water going through the pore," said graduate student Mohammad Heiranian, the first author of the study. "It's inherent in the chemistry of MoS2 and the geometry of the pore, so we don't have to functionalize the pore, which is a very complex process with graphene."

In addition to the chemical properties, the single-layer sheets of MoS2 have the advantages of thinness, requiring much less energy, which in turn dramatically reduces operating costs. MoS2 also is a robust material, so even such a thin sheet is able to withstand the necessary pressures and water volumes.

The Illinois researchers are establishing collaborations to experimentally test MoS2 for water desalination and to test its rate of fouling, or clogging of the pores, a major problem for plastic membranes. MoS2 is a relatively new material, but the researchers believe that manufacturing techniques will improve as its high performance becomes more sought-after for various applications.

"Nanotechnology could play a great role in reducing the cost of desalination plants and making them energy efficient," said Amir Barati Farimani, who worked on the study as a graduate student at Illinois and is now a postdoctoral fellow at Stanford University. "I'm in California now, and there's a lot of talk about the drought and how to tackle it. I'm very hopeful that this work can help the designers of desalination plants. This type of thin membrane can increase return on investment because they are much more energy efficient."

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