Simulations help explain fast water transport in nanotubes

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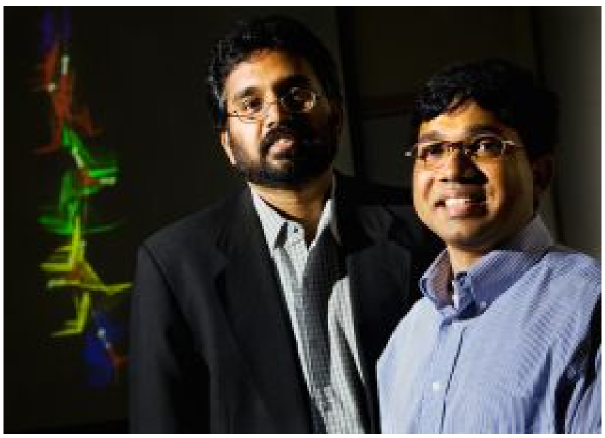

Narayana R. Aluru, professor of mechanical science and engineering, left, and doctoral student Sony Joseph have discovered the physical mechanism behind the rapid transport of water in carbon nanotubes. Image in background shows the trajectory of water molecules in a carbon nanotube moving in the direction of their orientations due to rotation-translation coupling. Photo by L. Brian Stauffer

(PhysOrg.com) -- By discovering the physical mechanism behind the rapid transport of water in carbon nanotubes, scientists at the University of Illinois have moved a step closer to ultra-efficient, next-generation nanofluidic devices for drug delivery, water purification and nano-manufacturing.

“Extraordinarily fast transport of water in carbon nanotubes has generally been attributed to the smoothness of the nanotube walls and their hydrophobic, or water-hating surfaces," said Narayana R. Aluru, a Willett Faculty Scholar and a professor of mechanical science and engineering at the U. of I.

"We can now show that the fast transport can be enhanced by orienting water molecules in a nanotube," Aluru said. "Orientation can give rise to a coupling between the water molecules' rotational and translational motions, resulting in a helical, screw-type motion through the nanotube," Aluru said.

Using molecular dynamics simulations, Aluru and graduate student Sony Joseph examined the physical mechanism behind orientation-driven rapid transport. For the simulations, the system consisted of water molecules in a 9.83 nanometer long nanotube, connected to a bath at each end. Nanotubes of two diameters (0.78 nanometers and 1.25 nanometers) were used. Aluru and Joseph reported their findings in the journal *Physical Review Letters.*

For very small nanotubes, water molecules fill the nanotube in single-file fashion, and orient in one direction as a result of confinement effects. This orientation produces water transport in one direction. However, the water molecules can flip their orientations collectively at intervals, reversing the flow and resulting in no net transport.

In bigger nanotubes, water molecules are not oriented in any particular direction, again resulting in no transport.

Water is a polar molecule consisting of two hydrogen atoms and one oxygen atom. Although its net charge is zero, the molecule has a positive side (hydrogen) and a negative side (oxygen). This polarity causes the molecule to orient in a particular direction when in the presence of an electric field.

Creating and maintaining that orientation, either by directly applying an electric field or by attaching chemical functional groups at the ends of the nanotubes, produces rapid transport, the researchers report.

"The molecular mechanism governing the relationship between orientation and flow had not been known," Aluru said. "The coupling occurs between the rotation of one molecule and the translation of its neighboring molecules. This coupling moves water through the nanotube in a helical, screw-like fashion."

In addition to explaining recent experimental results obtained by other groups, the researchers' findings also describe a physical mechanism that could be used to pump water through nanotube membranes in next-generation nanofluidic devices.

Provided by University of Illinois at Urbana-Champaign

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