Simulated fullerene tubules act as straws

Few children fail to marvel when they first discover that water, unassisted, can sneak part way up a thin straw. Now, computer simulations show that carbon tubules – cylindrical versions of the all-carbon molecules called fullerenes – act as molecular straws.

These nanotubes can suck up all sorts of small molecules, says Jeremy Q. Broughton, a physicist at the Naval Research Laboratory in Washington, D.C.

Broughton and Navy lab colleague Mark R. Pederson created on their computer a tubule with 120 carbon atoms and then calculated how that tubule's electrons shift when a hydrogen fluoride molecule is brought close to each of its ends.

For the simulation, they arranged the tubule's hexagons of carbon to make the open-ended cylinder metallic. They then put hydrogen atoms on the ends of the tubule so the dangling bonds of the carbons there would not latch onto any molecule that came near them.

As the hydrogen fluoride molecules close in on the tubule, the two researchers found, the distribution of positive and negative charges in these dipolar molecules causes the tubule's mobile electrons to bunch up near the hydrogen fluoride. The attraction of the electrons, in turn, sucks the hydrogen fluoride molecules up and holds them, Pederson and Broughton report in the Nov. 2 PHYSICAL REVIEW LETTERS.

In more recent work, the Navy lab theorists have discovered that tubules will also take up molecules that are not dipoles. In these new simulations, the scientists tracked the movements of atoms, not electrons. They brought a 960-carbon tubule close to a 20,000-atom liquid reservoir of neon warmed to about its melting point. As it neared the neon surface, the tubule drew neon atoms from the surface into itself, Broughton told SCIENCE NEWS.

With nonpolar atoms or molecules, weak attractions called van der Waal's forces lead to the capillary action, Broughton says.

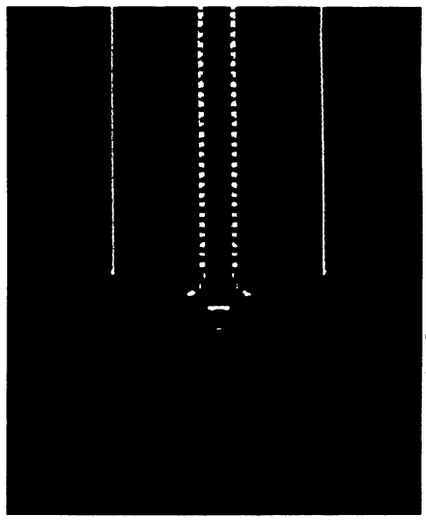
These results demonstrate that tubules will suck up and retain any molecule small enough to fit into them, he adds.

Broughton and Pederson think scientists can tailor the tubule to be selective about the molecules it picks up, in part by changing the way the hexagonal sheets of carbon wind around to form it. They have also determined that they can increase the sucking strength by narrowing the tubule's radius.

"With [these tubules], you can start making nanoscale devices that are mechanical, not electronic," Broughton notes. He envisions molecular-sized solenoids, pistons, and pumps, some of which may become components of nanoscale engines or devices used to restore function to ailing body parts.

Even though scientists know how to mass-produce layered tubules (SN: 7/18/92, p.36) and fullerenes in the shape of layered spheres (SN: 10/24/92, p.277), no one has made single tubes. But, says Broughton, now that he and Pederson have come up with uses for these fullerene cylinders, chemists are more likely to synthesize single tubules.

Meanwhile, Broughton offers a new name for them. "Rather than call them 'bucky tubes,' we can say they are 'sucky tubes,'" he says. *– E. Pennisi*



Pederson & Broughton/Naval Research Lab

Computer graphic shows locations of carbon atoms (red) in a sliced-open tubule and of moving neon atoms (light blue) that eventually settle at spots (yellow) along the inside and outside of the tubule.

Clues to the sex chromosome gender gap

Two separate teams of geneticists have begun untangling the mystery behind one of the most fundamental differences between men and women – the fact that whereas both of a man's two sex chromosomes stay active, only one of a woman's does.

The findings may improve researchers' understanding of so-called sex-linked genetic disorders. These disorders – such as fragile X syndrome, the most common inherited cause of mental retardation (SN: 6/8/91, p.359) – affect men more frequently and severely than women.

Women have two X chromosomes, and men have one X and one Y chromosome. While the X chromosome contains genes that direct a broad range of functions, such as blood clotting and some aspects of color perception, the Y chromosome for the most part bears only those genes responsible for male sexual characteristics.

In the 1960s, geneticists discovered that female mammalian embryos randomly inactivate one of their X chromosomes. Although researchers are still not sure exactly why this occurs, many assert that X inactivation initially arose to prevent the genetic inequity that would result if females had a double dose of active X chromosome genes.

A group led by Huntington F. Willard at Stanford University and another led by Neil Brockdorff of the Medical Research Council Clinical Research Center in Harrow, England, have isolated two forms of a gene that may play a role in X inactivation in females. Both groups report their discoveries in the Oct. 30 CELL. Willard – who is now at Case Western Reserve University in Cleveland – also discussed his team's results at this week's annual meeting of the American Society of Human Genetics in San Francisco.

Willard and his colleagues compared DNA taken from inactive human X chromosomes with that taken from active human X chromosomes. The researchers found a gene – which they named XIST, for X inactive-specific transcript – that functions only in inactive X chromosomes. They concluded that the gene may control the inactivation process.

Brockdorff's team used a similar procedure to isolate a candidate X-inactivation gene from mouse cells. Because the mouse gene's DNA sequence closely resembles that of the human gene, Brockdorff and his colleagues also named their gene xist, but in lower-case letters to differentiate it from the human gene.

Both Willard's and Brockdorff's groups also determined that their newly identified genes have something else in common. While both genes actively produce messenger RNA – the chemical intermediary that genes use to tell a cell to make proteins – these messages never get delivered to the protein-production apparatus outside the cell's nucleus. Instead, the RNA accumulates inside the nucleus, where the researchers suggest it may stick to the X chromosome that produces it, permanently shutting off that chromosome.

The RNA "might literally be caging up one of the X chromosomes," says Willard. But he cautions that neither group has proven that XIST inactivates X chromosomes. "We haven't come up with the answer [to X inactivation] yet," he says, "but it's our best guess that this gene is at least part of the puzzle." *– C. Ezzell*