Nanometer-sized tubes made from simple benzene molecules

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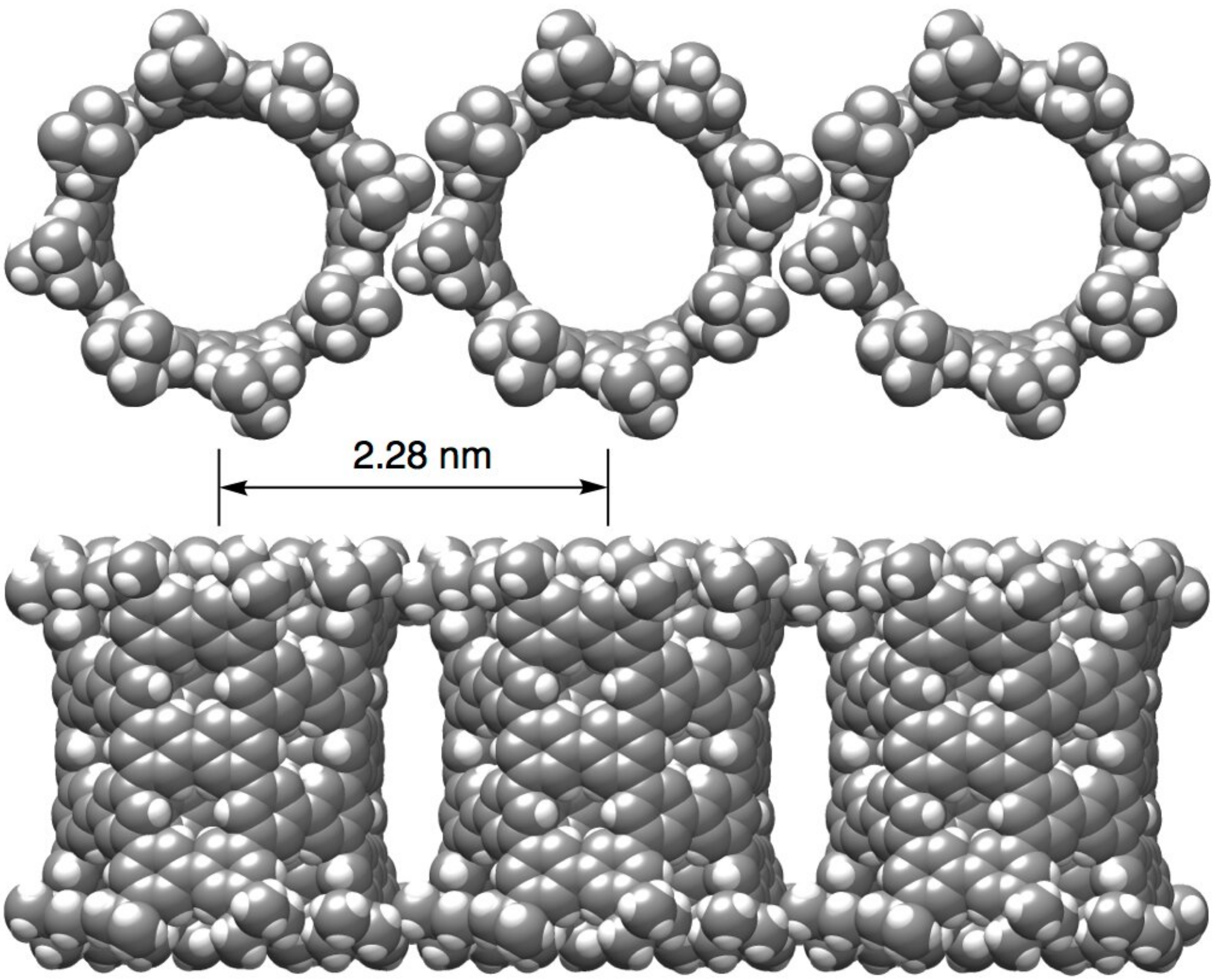


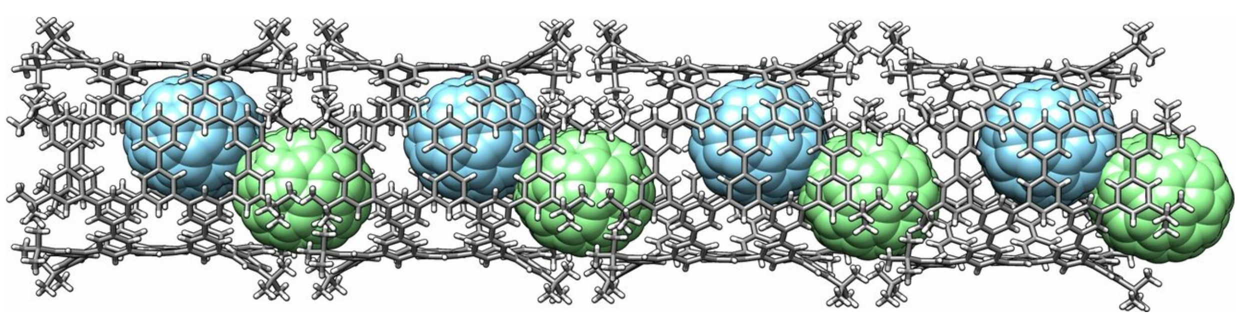
In crystals, pNT molecules are aligned in parallel. Credit: (c)2018 Hiroyuki Isobe

For the first time, researchers used benzene, a common hydrocarbon, to create a novel kind of molecular nanotube, which could lead to new nanocarbon-based semiconductor applications.

Researchers from the Department of Chemistry have been hard at work in their recently renovated lab in the University of Tokyo's Graduate School of Science. The pristine environment and smart layout affords them ample opportunities for exciting experiments. Professor Hiroyuki Isobe and colleagues share an appreciation for "beautiful" molecular structures and created something that is not only beautiful but is also a first for chemistry.

Their phenine nanotube (pNT) is noted for its pleasing symmetry and simplicity, which is a stark contrast to its complex means of development. Chemical synthesis of nanotubes is notoriously difficult and challenging, and controlling the structures in question to provide unique properties and functions is even more complex.

Carbon nanotubes are famous for their defect-free graphite structure, but they vary widely in length and diameter. Isobe and his team wanted a single type of nanotube, a novel form with controlled defects within its nanometer-sized cylindrical structure allowing for additional molecules to add properties and functions.

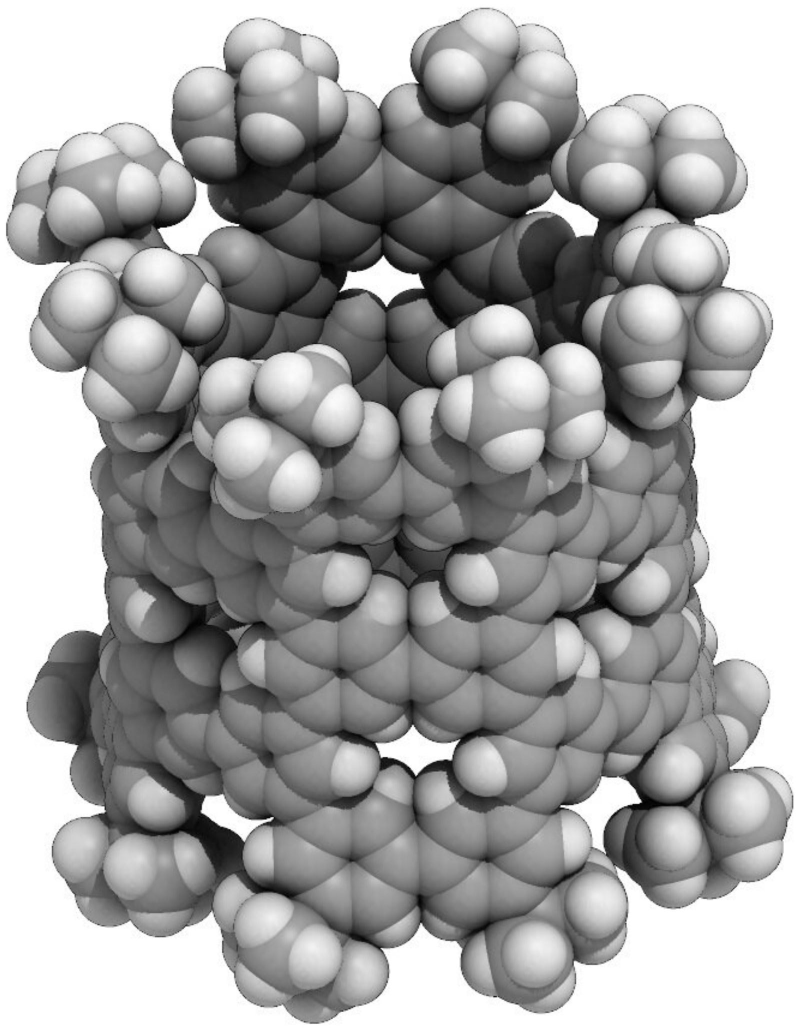


One pNT molecule encapsulates two C70 molecules in its interior. pNT molecules are aligned in a crystal, which results in a linear array of C70 molecules. Credit: (c)2018 Hiroyuki Isobe

The researchers' novel process of synthesis starts with benzene, a hexagonal ring of six carbon atoms. They used reactions to combine six of these benzenes to make a larger hexagonal ring called a cyclo-meta-phenylene (CMP). Platinum atoms allowed four CMPs to form an open-ended cube. When the platinum is removed, the cube springs into a thick circle and this is furnished with bridging molecules on both ends, enabling the tube shape.

It sounds complicated, but amazingly, this complex process successfully bonds the benzenes in the right way over 90 percent of the time. The key also lies in the symmetry of the molecule, which simplifies the process of assembling as many as 40 benzenes. These benzenes, also called phenines, are used as panels to form the nanometer-sized cylinder. The result is a novel nanotube structure with intentional periodic defects. Theoretical investigations show these defects imbue the nanotube with semiconductor characters.

"A crystal of pNT is also interesting: The pNT molecules are aligned and packed in a lattice rich with pores and voids," Isobe explains. "These nanopores can encapsulate various substances which imbue the pNT crystal with properties useful in electronic applications. One molecule we successfully embedded into pNT was a large carbon molecule called fullerene (C70)."



A nanometer-sized pNT cylinder made of 40 benzenes.The cylinder is tens of thousands of times thinner than a human hair. Credit: (c)2018 Hiroyuki Isobe

"A team lead by Kroto/Curl/Smalley discovered fullerenes in 1985. It is said that Sir Harold Kroto fell in love with the beautiful molecule," continues Isobe. "We feel the same way about pNT. We were shocked to see the molecular structure from crystallographic analysis. A perfect cylindrical structure with fourfold symmetry emerges from our chemical synthesis."

"After a few decades since the discovery, this beautiful molecule, fullerene, has found various utilities and applications," adds Isobe. "We hope that the beauty of our molecule is also pointing to unique properties and useful functions waiting to be discovered."

The study is published in the journal *Science*.

More information: Finite phenine nanotubes with periodic vacancy defects *Science* (2019). science.sciencemag.org/cgi/doi … 1126/science.aau5441

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