Researchers measure carbon nanotube interaction

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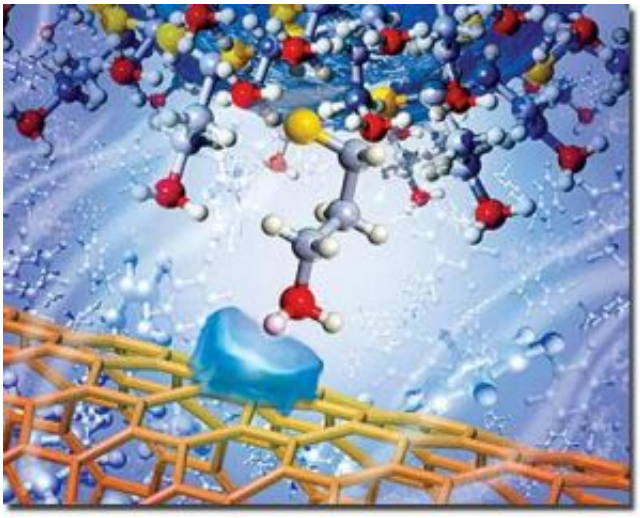

An artist's representation of an amine functional group attached to an AFM tip approaching a carbon nanotube surface in toluene solution. Translucent blue shape on the nanotube represents the polarization charge forming on the nanotube as the result of the interaction with the approaching molecule. Chemical force microscopy measures the tiny forces generated by this single functional group interaction. (Illustration by Scott Dougherty, LLNL)

Carbon nanotubes have been employed for a variety of uses including composite materials, biosensors, nano-electronic circuits and membranes.

While they have proven useful for these purposes, no one really knows much about what's going on at the molecular level. For example, how do

nanotubes and chemical functional groups interact with each other on the atomic scale? Answering this question could lead to improvements in future nano devices.

In a quest to find the answer, researchers for the first time have been able to measure a specific interaction for a single functional group with carbon nanotubes using chemical force microscopy – a nanoscale technique that measures interaction forces using tiny spring-like sensors. Functional groups are the smallest specific group of atoms within a molecule that determine the characteristic chemical reactions of that molecule.

A recent report by a team of Lawrence Livermore National Laboratory researchers and colleagues found that the interaction strength does not follow conventional trends of increasing polarity or repelling water. Instead, it depends on the intricate electronic interactions between the nanotube and the functional group.

“This work pushes chemical force microscopy into a new territory,” said Aleksandr Noy, lead author of the paper that appears in the Oct. 14 online issue of the journal, *Nature Nanotechnology*.

Understanding the interactions between carbon nanotubes (CNTs) and individual chemical functional groups is necessary for the engineering of future generations of sensors and nano devices that will rely on single-molecule coupling between components. Carbon nanotubes are extremely small, which makes it particularly difficult to measure the adhesion force of an individual molecule at the carbon nanotube surface. In the past, researchers had to rely on modeling, indirect measurements and large microscale tests.

But the Livermore team went a step further and smaller to get a more exact measurement. The scientists were able to achieve a true single

function group interaction by reducing the probe-nanotube contact area to about 1.3 nanometers (one million nanometers equals one millimeter).

Adhesion force graphs showed that the interaction forces vary significantly from one functionality to the next. To understand these measurements, researchers collaborated with a team of computational chemists who performed ab initio simulations of the interactions of functional groups with the sidewall of a zig-zag carbon nanotube. Calculations showed that there was a strong dependence of the interaction strength on the electronic structure of the interacting molecule/CNT system. To the researchers delight, the calculated interaction forces provided an exact match to the experimental results.

“This is the first time we were able to make a direct comparison between an experimental measurement of an interaction and an ab initio calculation for a real-world materials system,” Noy said. “In the past, there has always been a gap between what we could measure in an experiment and what the computational methods could do. It is exciting to be able to bridge that gap.”

This research opens up a new capability for nanoscale materials science. The ability to measure interactions on a single functional group level could eliminate much of the guess work that goes into the design of new nanocomposite materials, nanosensors, or molecular assemblies, which in turn could help in building better and stronger materials, and more sensitive devices and sensors in the future.

Source: Lawrence Livermore National Laboratory