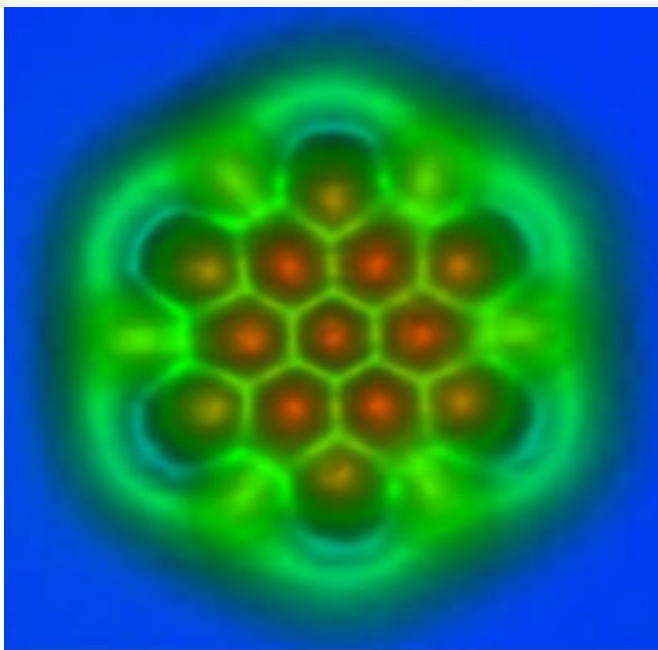


In world's first, atomic force microscope sees chemical bonds in individual molecules (w/ video)

13 September 2012

[electronic displays.](#)

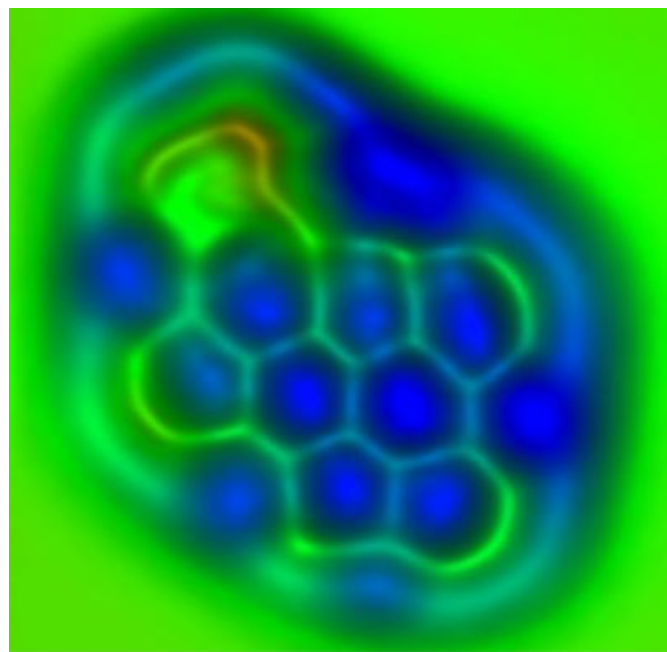


A nanographene molecule exhibiting carbon-carbon bonds of different length and bond order imaged by noncontact atomic force microscopy using a carbon monoxide functionalized tip. This molecule was synthesized at the Centre National de la Recherche Scientifique (CNRS) in Toulouse. Credit: IBM

(Phys.org)—IBM scientists have been able to differentiate the chemical bonds in individual molecules for the first time using a technique known as noncontact atomic force microscopy (AFM).

The results push the exploration of using molecules and atoms at the smallest scale and could be important for studying graphene devices, which are currently being explored by both industry and academia for applications including highbandwidth wireless communication and

"We found two different contrast mechanisms to distinguish bonds. The first one is based on small differences in the force measured above the bonds. We expected this kind of contrast but it was a challenge to resolve," said IBM scientist Leo Gross. "The second contrast mechanism really came as a surprise: Bonds appeared with different lengths in AFM measurements. With the help of ab initio calculations we found that the tilting of the carbon monoxide molecule at the tip apex is the cause of this contrast."



This is a nanographene molecule exhibiting carbon-carbon bonds of different length and bond order imaged by noncontact atomic force microscopy using a carbon monoxide functionalized tip. This molecule was synthesized by Centro de Investigación en Química Biológica e Materiais Moleculares (CIQUS) at the Universidade de Santiago de Compostela. Credit: IBM

As reported in the cover story of the September 14 issue of *Science* magazine, IBM Research scientists imaged the bond order and length of individual carbon-carbon bonds in C₆₀, also known as a [buckyball](#) for its football shape and two planar [polycyclic aromatic hydrocarbons](#) (PAHs), which resemble small flakes of graphene. The PAHs were synthesized by Centro de Investigación en Química Biológica e Materiais Moleculares (CIQUS) at the Universidade de Santiago de Compostela and Centre National de la Recherche Scientifique (CNRS) in Toulouse.

The individual bonds between [carbon atoms](#) in such molecules differ subtly in their length and strength. All the important chemical, electronic, and [optical properties](#) of such molecules are related to the differences of bonds in the polyaromatic systems. Now, for the first time, these differences were detected for both individual molecules and bonds. This can increase basic understanding at the level of individual molecules, important for research on novel electronic devices, organic solar cells, and organic light-emitting diodes (OLEDs). In particular, the relaxation of bonds around defects in graphene as well as the changing of bonds in chemical reactions and in excited states could potentially be studied.

As in their earlier research "[The Chemical Structure of a Molecule Resolved by Atomic Force Microscopy](#)" the IBM scientists used an atomic force microscope (AFM) with a tip that is terminated with a single carbon monoxide (CO) molecule. This tip oscillates with a tiny amplitude above the sample to measure the forces between the tip and the sample, such as a molecule, to create an image. The CO termination of the tip acts as a powerful magnifying glass to reveal the atomic structure of the molecule, including its bonds. This made it possible to distinguish individual bonds that differ only by 3 picometers or 3×10^{-12} m, which is about one-hundredth of an atom's diameter.

In previous research the team succeeded in imaging the chemical structure of a molecule, but not the subtle differences of the bonds. Discriminating bond order is close to the current

resolution limit of the technique and often other effects obscure the contrast related to bond order. Therefore the scientists had to select and synthesize molecules in which perturbing background effects could be ruled out.

To corroborate the experimental findings and gain further insight into the exact nature of the contrast mechanisms, the team performed first-principles density functional theory calculations. Thereby they calculated the tilting of the CO molecule at the tip apex that occurs during imaging. They found how this tilting yields a magnification and the very sharp images of the bonds.

More information: Bond-Order Discrimination by Atomic Force Microscopy, *Science* 14 September 2012: Vol. 337 no. 6100 pp. 1326-1329. [DOI: 10.1126/science.1225621](#)

ABSTRACT

We show that the different bond orders of individual carbon-carbon bonds in polycyclic aromatic hydrocarbons and fullerenes can be distinguished by noncontact atomic force microscopy (AFM) with a carbon monoxide (CO)-functionalized tip. We found two different contrast mechanisms, which were corroborated by density functional theory calculations: The greater electron density in bonds of higher bond order led to a stronger Pauli repulsion, which enhanced the brightness of these bonds in high-resolution AFM images. The apparent bond length in the AFM images decreased with increasing bond order because of tilting of the CO molecule at the tip apex.

Provided by IBM

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