Researchers reveal the structure of individual chemical bonds using specialized imaging techniques

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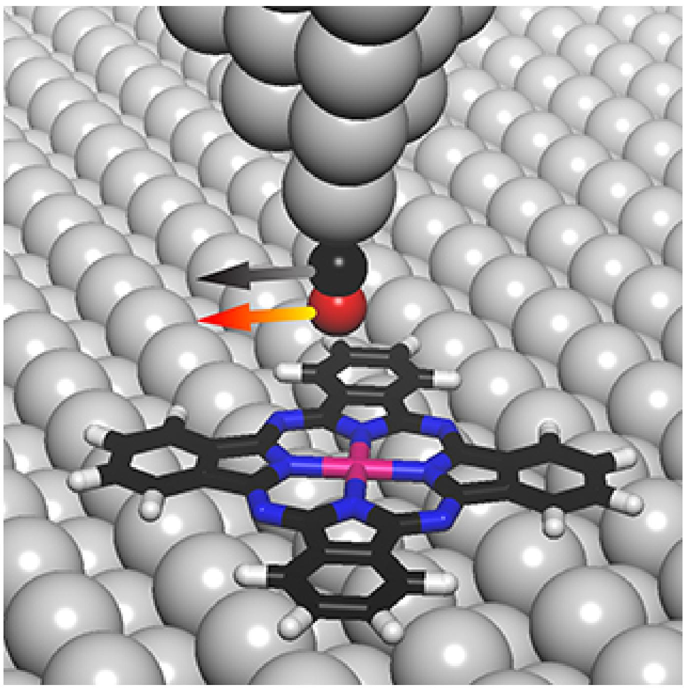

The tip of a scanning tunneling microscope (top center), to which a single carbon monoxide molecule (red and black spheres) has been attached, is scanned in the direction of the arrows over a single cobalt phthalocyanine molecule. Credit: US Department of Energy

Atom and bond arrangements help determine a molecule's identity. Researchers adapted a new technique called "itProbe," based on the scanning tunneling microscope (STM), to produce images of structure and bonding in a single molecule, essentially unmasking the molecules. The STM tip ends with a single carbon monoxide molecule. The tip is scanned over single molecules and changes in the carbon monoxide provide insights about the molecule's internal bonding.

Real-space spectroscopy and imaging using itProbe could lead to a deeper understanding of the nature of different types of chemical bonds and related chemistry. The results may also further clarify the relationship of the structure and function of molecules, opening up vivid new views of molecular chemistry.

The arrangement of atoms and bonds in a molecule influences its physical and chemical properties. With this in mind, a number of techniques have been developed to determine the geometric structure and nature of bonds in individual molecules. Researchers at the University of California, Irvine developed a new technique based on STM called "itProbe," in which a single carbon monoxide (CO) molecule is attached to the tip. As the modified tip passes over the atoms and bonds of a single molecule of cobalt phthalocyanine adsorbed onto a silver surface, changes in the inelastic electron tunneling signal of the CO hindered vibrational mode are monitored and can be used to form an image of the scanned molecule.

The resulting two-dimensional maps provide a skeletal image of the molecule and its surroundings, providing a scientific basis for the "ball-and-stick" model commonly used by chemists to represent the appearance of molecular structures and chemical bonds. This technology has the potential to observe changes in the geometric structure of a molecule as the environment changes due to reacting on surfaces or forming self-assembled nanostructures. The new method should be adaptable to other molecules, possibly providing a better understanding of the nature of different types of chemical bonds and their related chemistry.

More information: C.-l. Chiang et al. Real-space imaging of molecular structure and chemical bonding by single-molecule inelastic tunneling probe, *Science* (2014). DOI: 10.1126/science.1253405

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