Physicists Discover New Way To Visualize Shape Changes In Molecules

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Using ultrafast lasers, a team of University of Colorado at Boulder and JILA scientists has developed a novel method to observe the motion of atoms during chemical reactions, opening up new possibilities for detailed understanding of how chemical bonds are made and broken.

The team, which includes CU-Boulder MacArthur fellow Margaret Murnane and her husband, physicist Henry Kapteyn, published their findings this week on the Web site of the *Proceedings of the National Academy of Sciences*. JILA is a joint institute of the National Institute of Standards and Technology and CU-Boulder.

Kapteyn explained that the new technique could someday lead to advances in pharmaceuticals, chemicals and other industries.

"This is an important step in the exploration of the molecular world," said Kapteyn. "If we can understand exactly what's going on in a chemical reaction, our chances of manipulating it in a desired way are greatly improved."

Molecules are generally viewed as the smallest particle of a chemical substance that still retains the chemical composition of the substance. Molecules are comprised of many atoms, which are the smallest particles that retain the characteristics of chemical elements. When molecules combine to form chemical compounds, their shape must change.

"Understanding how atoms move within a molecule to change that molecule's shape is therefore crucial in learning, for example, what makes chemical reactions efficient in the human body or in a chemical catalyst," Murnane said.

Previously, scientists could only gather data that inferred how atoms or molecules move during a chemical reaction. Visible lasers, X-rays or electrons were used to scatter atoms from a molecule. However, visible light cannot see individual atoms in molecules, and it is difficult to produce very short bursts of X-rays or electrons, according to Murnane.

The CU-Boulder team used the electric field from an intense laser pulse to pluck electrons away from a molecule and then slam them back into the same molecule. The highly energetic electrons scatter from the molecule and emit bright bursts of X-rays that are detected and measured.

"The brightness of the X-ray bursts is highly sensitive to the microscopic position of the atoms within a molecule," Murnane said. "This is because, although electrons are particles, they also have wave-like properties and their wavelength is comparable to distances between atoms in a molecule."

The new method shows great promise as a way of imaging energetic molecules undergoing ultrafast structural transformations, including the fundamental action of chemistry, the making and breaking of chemical bonds, according to the CU-Boulder team.

Kapteyn explained that scientists will need years of experimentation with this new technique to determine just how much can be learned about chemical reactions at the molecular level.

Funding for the research was provided by the U.S. Department of Energy and by the National Science Foundation.

Kapteyn and Murnane are known as world leaders in the field of experimental, ultrafast optical science. Their work on short light pulses from lasers has applications for optical technology, faster computer chips, micro-machining, biological imaging and other fields.

Researchers all over the world use the short pulse oscillator developed by Kapteyn. His honors include a National Science Foundation Young Investigator Award, the Adolph Lomb Medal of the Optical Society of America and a Sloan Research Fellowship.

Murnane was named a fellow of the American Academy of Arts and Sciences in 2006. She also is a member of the elite National Academy of Sciences and one of seven CU-Boulder faculty members to win a prestigious $500,000 MacArthur Fellowship, widely known as the "genius grant."

Source: University of Colorado at Boulder