Physicists steer electrons with laser pulses: Method could be used to create custom-made chemical compounds

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Theoretical physicist Uwe Thumm and his colleagues Feng He and Andreas Becker not only work with some of the smallest molecules in the universe, but they now have found a way to control the motion of the molecules' building blocks, electrons and nuclei.

Thumm is a professor of physics at Kansas State University, Feng He is a research associate at the K-State physics department, and Becker is a professor at the University of Colorado in Boulder. The collaborators have found a way to steer the movement of electrons in a hydrogen molecule using ultrafast laser pulses. These pulses are so short that their duration is measured in attoseconds -- that's one billionth of a billionth of a second.

In a recent research paper, the three collaborators explained how attosecond laser pulses can be used to direct the motion of an electron inside a hydrogen molecule, and what the measurable consequences of this control over the electron would be. The paper appears this month in Vol. 101 of The *Physical Review Letters*.

As theoretical physicists, Thumm and his colleagues do not perform experiments, but instead simulate the outcome of present and future experiments by developing mathematical models. These models explain the nature of atoms, molecules, light and their interactions in terms of mathematical equations that are solved with the help of powerful computers.

The researchers' model describes experiments that are currently being performed at various laboratories worldwide, including the J.R. Macdonald Laboratory at K-State.

For the past few years, Thumm and his colleagues studied what happens with the hydrogen molecular ion when it interacts with short laser pulses. They used hydrogen because it's the simplest molecule, although they have now extended their research toward the imaging and control of the much faster moving electrons.

The hydrogen molecular ion has two protons and just one electron that "glues" them together. A few years ago, by performing computer simulations, they found that laser pulses can control the motion of the protons by setting them in motion or slowing them down.

The researchers use a first ultrafast laser to pump the molecule with infrared pulses. The protons vibrate and move apart slowly, but the electron still tries to hang on. The second part of their model uses the laser to probe the particles with a second delayed light pulse to see what happens when the electron fails to keep the protons glued together. The infrared laser pulses create an electric field that puts a force on the electron. Eventually, Thumm said, the electron has to choose which proton it will stick with.

Thumm and his colleagues were surprised to find that for certain laser pulses the electron can move in the opposite direction from what they anticipated.

"Our naive expectation was that the electron would follow the laser electric force," Thumm said. "That's what other simulations predicted, and they agree with classical physics and common intuition."

For instance, if you're pulling on a shopping cart, the cart will move in the direction of the force -- in this case, toward you. But at the quantum level, the rules are different.

The researchers found that sometimes the electron moves in the direction of the force, but sometimes not. Thumm, He and Becker found that the electron picks the proton on the left or the one of the right depending on the intensity of the laser pulse. Knowing which intensity will make the electron move to the left or the right gives physicists the ability to steer the electrons by setting the laser pulse to a specific intensity.

Thumm said this finding is not only a contribution to basic physics research, but it also could help chemists better understand and possibly control chemical reactions.

"We would like to see a 'molecular movie' that shows the redistribution of electrons in time -- within attoseconds -- during a chemical reaction," he said. "It would promote our understanding of basic processes that eventually enable life: electrons bind atoms to simple molecules, such as the hydrogen molecule or water. Through many chemical reactions, these simple molecules react with each other and eventually form huge bio-molecules that make life, as we know it, possible."

One possible commercial application of the finding, Thumm said, could be helping companies become more efficient in producing a desired chemical compound while minimizing unwanted byproducts in the reaction.

Source: Kansas State University