Study points way toward 'filming' molecule-light interactions

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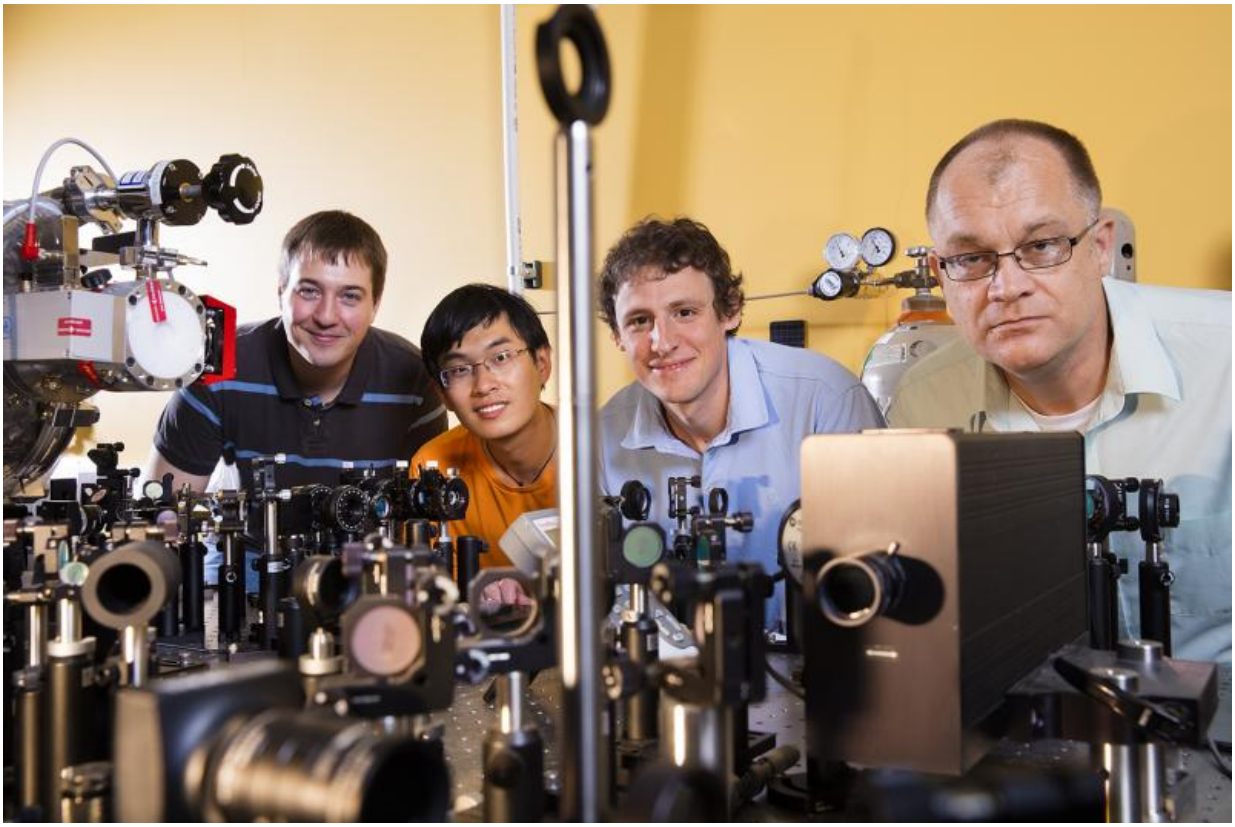

From left, doctoral students Joshua Beck and Jie Yang pose alongside associate professors of physics and astronomy Martin Centurion and Cornelis "Kees" Uiterwaal. Centurion and his team have demonstrated a technique for capturing a "frame" of molecular reactions, a significant step toward creating 3-D movies of them. Credit: Craig Chandler/University Communications

A new study from UNL physicists could inform the future production of 3-D movies starring light-driven molecular reactions that already play leading roles in photosynthesis, vision and many state-of-the-art technologies.

Published in the journal *Nature Communications*, the study examined how gas-suspended molecules of carbon disulfide responded when struck by laser pulses that varied in duration and intensity.

Using a technique they pioneered in 2012, the researchers analyzed these molecular responses by firing electrons at the molecules immediately following a laser pulse impact. The post-collision scattering of these electrons was captured on a luminescent screen and sent to a specialized digital camera.

With the assistance of algorithms, these scattering patterns provided information about which laser pulses managed to rotate the molecules, lengthen or break their atomic bonds, and eject the molecules' own electrons from their atomic orbits.

The researchers determined the minimum laser intensity needed to align randomly oriented molecules in the same direction, which narrows the range of scattering patterns enough to average them into an accurate snapshot of a molecule.

The team further measured the intensity at which a laser begins exciting the molecules—a phenomenon that pushes their electrons to higher energy levels and can begin distorting or even destroying molecular configurations. By comparing molecules subjected to different laser pulses, the team was able to retrieve and illustrate the dynamics produced by this excitation.

"When a molecule absorbs light, what follows is a change in the structure

that then changes the chemical properties and other qualities of the molecule," said lead author Martin Centurion, associate professor of physics and astronomy. "So you want to want to look not only at the structure, but also how that structure changes on fast time-scales. This new experiment—in addition to (offering insights into) the physics—shows that we can image a transient state.

"The end goal is to make movies of these reactions. We're not there yet, but what we've done is capture one frame of that movie."

In reporting the respective thresholds for molecular alignment, excitation and electron ejection, or ionization, the study should also help physicists ascertain whether observed molecular structures reflect natural or light-altered states.

"You might compare it to a case where you have something delicate and want to pick it up so that you can look at it," said co-author Cornelis "Kees" Uiterwaal, associate professor of physics and astronomy. "If you take a pair of pliers and use too much force, by the time you have it in front of you, you've ruined it. But you'd like to have a strong (enough) tool that the molecule won't go all over the place and you won't be able to see it. Martin's expertise is to look at molecules that are held securely with a delicate tool."

As Centurion continues the quest to "film" molecular reactions using this tool, Uiterwaal is examining what happens when the figurative pliers clamp down hard enough to crack a molecule. The team's technique is allowing Uiterwaal and his colleagues to examine these outcomes much more easily than would be possible by relying solely on theoretical principles, he said.

"There are millions of organic molecules that have been reported, which in itself is like collecting stamps," Uiterwaal said. "You wouldn't

necessarily find a pattern among them, so what we do is try to identify certain sequences of molecules that are roughly the same but all differ in one specific respect. We can try this one, then the next one, then the next one … and hope to discover a pattern that we then ascribe to just that little difference."

More information: "Imaging of alignment and structural changes of carbon disulfide molecules using ultrafast electron diffraction." *Nature Communications* 6, Article number: 8172 DOI: 10.1038/ncomms9172

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