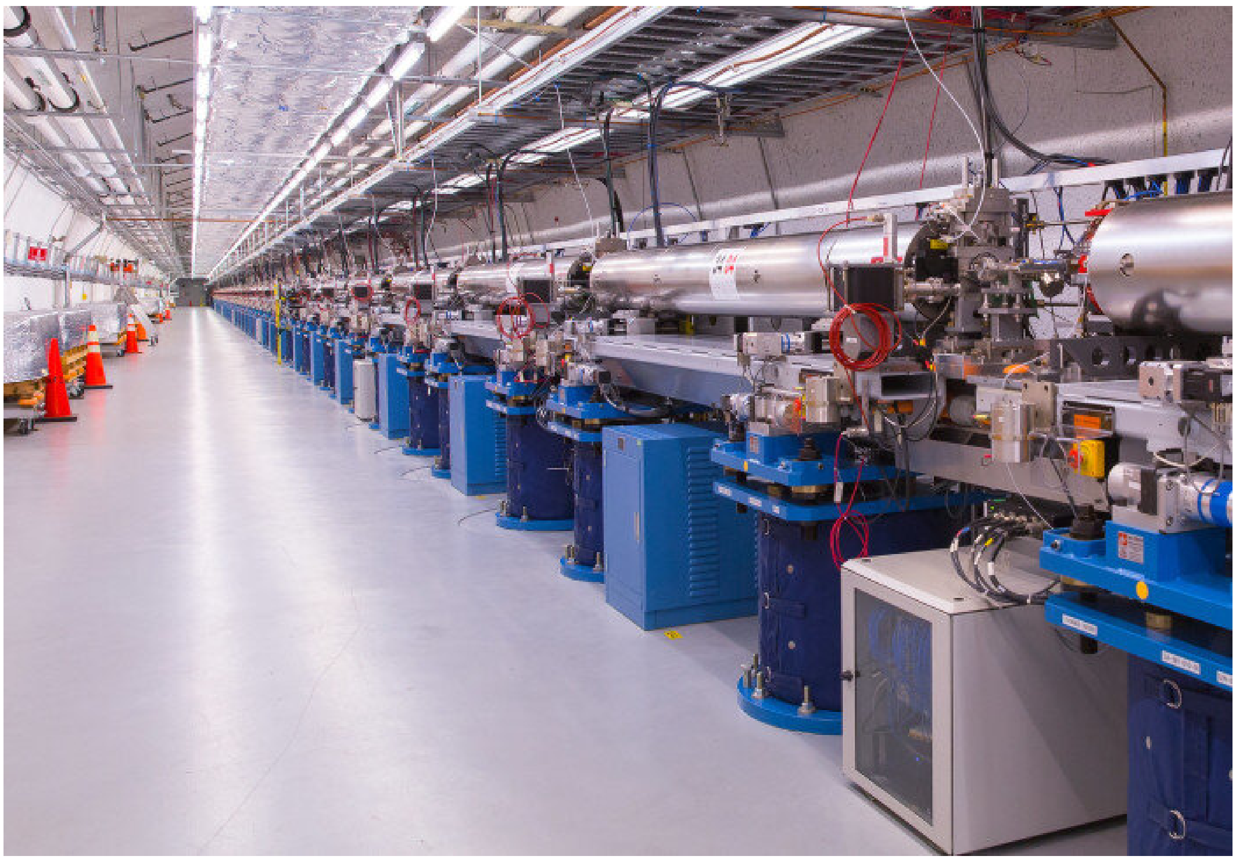
# Understanding how electrons drive chemical reactions

September 1 2021, by Andrew Czyzewski



Credit: Imperial College London

An Imperial-led team of international researchers has used a special X-ray probe to gain new insights into how electrons behave at the quantum level.

Since electrons drive many chemical reactions, the method could lead to a deeper understanding of physics, chemistry and life sciences and could ultimately help design advanced materials and more efficient solar cells.

The team includes researchers from across Europe, the US and Japanled by Imperial's Professor Jon Marangos, Lockyer Chair in Physics. Their paper is published in the open-source journal *Physical Review X*.

## The importance of photoexcitation

The classic picture of an atom, as taught in schools around the world, envisions a central nucleus of protons and neutrons packed tightly together, around which electrons orbit like planets around the sun. And like planets, the electrons have different orbits, some close to the center, some further away, depending on their energy levels.

While this picture is only an approximation, it can be useful in understanding the behavior of atoms and molecules, for example during photoexcitation. This important process drives photosynthesis and is pivotal to solar energy generation.

Here, light hits a molecule causing an electron to move up to a higher energy orbit, leaving behind an "electron hole" and placing the molecule in an excited state, which can then transfer energy to nearby parts of the extended molecular system, setting off a chain of events that ultimately drive photosynthesis.

Professor Marangos explains, "All solar-driven processes involve photoexcitation and that means initially, that an electron moves, and then the rest of the system responds. But we don't fully understand how exactly that excited electron couples to the nuclear motion in this complex chain of events."

He adds: "We are now realizing how important solar photoexcitation is likely to be to our future, and that is why we do this research, so that we can really get the most detailed understanding and find ways to optimize the coupling between the initial event and the outcome which is technologically most desirable."

## Giving molecules an X-ray

The above picture of electrons as orbiting planets is just an approximation. In fact, quantum physics tells us that electrons are never located in an exact position at any given moment.

We can only say that a particular electron is, on the balance of probabilities, more likely to be located at certain positions, manifested as orbitals. Some people refer to there being a "cloud" or "smear" of electrons, which fluxes and shifts in response to event such as photoexcitation.

The research team set out to understand these electron dynamics, at the quantum level, and track changes moment-by-moment at the level of femtosecond ($10^{-15}$ seconds or a quadrillionth of a second).

This was done using a specially configured X-ray laser at the Linac Coherent Light Source (LCLS) in Stanford, U.S. On every shot the laser delivers two ultrashort X-ray pulses separated by only a few femtoseconds: The first knocks off an electron from a molecule of isopropanol leaving an electron hole and the second, crucially, probes and measures the motion of the hole state.

The team found that these electronic hole states rapidly "relax" into new metastable states of the molecule, through rearrangements of the positions of both the electrons and atoms.

Notably, they observed that the movement of the electrons, driven by interactions with other electrons, can be completed in very short time scales—only a few-femtoseconds ($10^{-15}$ seconds). They also observed the somewhat slower movements of the atoms, around 10 femtoseconds, leading to relaxation of the electron hole state, such that they were no longer detected by the probe.

Collaborator and co-author on the study, Dr. Taran Driver, from Stanford University, commented, "With this work we've been able to demonstrate a new technique for measuring the ultrafast electron motion that happens after photoexcitation—which is relevant for a number of important processes such as solar energy generation or radiation damage in living systems.

"What's particularly exciting about this method is that the X-rays let us see at which atomic site in the molecule the electron hole is sat at a given point in time, with the ability to track it as it moves over only a few femtoseconds or even attoseconds."

## A deeper knowledge of fundamental processes

The method developed by the team to probe electron dynamics could now be used more widely for studying larger molecules and more complex materials.

Ultimately, a deeper knowledge of these fundamental processes could be used to develop advanced materials and steer photochemical reactions —for example in the context of solar cell design.

Professor Marangos explains, "Using this method, you could deduce that in a particular material, you're losing a lot of excitations to some channel, and so the question is how do you engineer that material so that you don't lose excitations though that channel and get a more efficient transfer to the desired outcome. That is a long-term motivation for what we do."

**More information:** T. Barillot et al, Correlation-Driven Transient Hole Dynamics Resolved in Space and Time in the Isopropanol Molecule, *Physical Review X* (2021). DOI: 10.1103/PhysRevX.11.031048

Provided by Imperial College London

Citation: Understanding how electrons drive chemical reactions (2021, September 1) retrieved 27 April 2024 from https://phys.org/news/2021-09-electrons-chemical-reactions.html

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