Controlling Electrons in Molecules at Ultrafast Timescales

Scientists have found a way to control electrons in molecules using tailor-made terahertz light pulses, offering new possibilities for advanced technologies.

Scientists at YOKOHAMA National University, in collaboration with RIKEN and other institutions in Japan and Korea, have made an important discovery about how electrons move and behave in molecules. This discovery could potentially lead to advances in electronics, energy transfer, and chemical reactions. Published in the Journal, *Science*, their study reveals a new way to control the distribution of electrons in molecules using very fast phase-controlled pulses of light in the terahertz range.

Atoms and molecules contain negatively charged electrons that usually stay in specific energy levels, like layers, around the positively charged nucleus. The way these electrons are arranged in the molecule is key to how the molecule behaves. This arrangement affects important processes like how light is emitted, how charges move between molecules, and how chemical reactions happen. For example, when light hits an electron and gives it enough energy, the electron moves to a higher energy level, leaving behind a positively charged "hole". This creates an exciton – a tiny energy packet in the molecule that can emit the light. This process is key to technologies like solar cells, where excitons help convert sunlight into electricity, and LEDs, where they release energy as light.

However, there are other important states that molecules can exist in, like charged states and charged excited states. Charged states occur when a molecule gains or loses an electron, while charged excited states involve both a charge change and an electron in a higher energy level. These are important for many processes, but it has been very difficult to control these states, especially on ultrafast timescales, using traditional technology. Normally, light from the visible spectrum doesn't provide enough energy to change the charge of the molecule and therefore cannot change the number of electrons in it.

To overcome this challenge, the researchers used terahertz light pulses, a type of light with a much lower frequency than visible light. These pulses cause electrons to move between a molecule and the metal tip of a specialized microscope that can manipulate individual molecules, allowing the team to either remove or add an electron to the molecule. This new method offers a way to control not only excitons in a controlled manner which is both quick and precise, but also other important molecular states that are essential for chemical reactions, energy transfer and many other processes. The team also demonstrated that terahertz light, which is invisible to the human eye, can be converted into visible light within a molecule, revealing a novel way to transform one type of light into another through molecular energy changes.

"While excitons typically form when light is absorbed by a material, our findings reveal they can also be created through charged states using these specially designed terahertz pulses," says Professor Ikufumi Katayama, the study's corresponding author from the Faculty of Engineering

at YOKOHAMA National University. "This opens new possibilities for controlling how charge moves within molecules, which could lead to better solar cells, smaller light-based devices, and faster electronics."

The team's main achievement was the ability to control exciton formation at the single-molecule level. Professor Jun Takeda, another corresponding author from the Faculty of Engineering at YOKOHAMA National University, explains: "By precisely controlling how electrons move between a single molecule and the metal tip of the specialized microscope, we were able to guide exciton formation and the chemical reactions that follow. These processes usually happen randomly, but with terahertz pulses, we can determine exactly when and how reactions occur at the molecular level. This could lead to breakthroughs in nanotechnology, advanced materials, and more efficient catalysts for energy and industry."

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<u>Summary</u>

Scientists at YOKOHAMA National University, in collaboration with RIKEN and other institutions in Japan and Korea, have made an important discovery about how electrons move and behave in molecules. This discovery could potentially lead to advances in electronics, energy transfer, and chemical reactions. Published in the Journal, Science, their study reveals a new way to control the distribution of electrons in molecules using very fast phase-controlled pulses of light in the terahertz range.

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Using Light Pulses to Control Electrons in a Single Molecule

Image Caption:

A specially designed terahertz pulse moves electrical charge between the metal tip of a specialized microscope and a single molecule, creating an exciton that releases energy as light.

