TOP 10 RESEARCH ACHIEVEMENTS

Tracking the movements of all atoms in a molecule

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Fundamental studies of chemical reactions often consider the molecular dynamics along a reaction coordinate using a calculated or suggested potential energy surface. But fully mapping such dynamics experimentally, by following all nuclear motions is challenging and has not yet been realized even for simple triatomic molecules. In this work, we track the movements of all the gold atoms in the gold trimer complex during photoinduced bond formation using femtosecond x-ray liquidography. Tracking the atomic movements reveals that within the first 35 femtoseconds after photoexcitation, a covalent bond forms and the second covalent bond subsequently forms within 360 femtoseconds. Femtosecond x-ray liquidography offers a means of tracking the atomic motions involved in many chemical reactions.

1. Background

Targeted cancer drugs work by striking a tight bond between cancer cell and specific molecular targets that are involved in the growth and spread of cancer. Detailed images of such chemical bonding sites or pathways can provide key information necessary for maximizing the efficacy of oncogene treatments. In this regard, fundamental studies of chemical reactions often consider the molecular dynamics along a reaction coordinate using a calculated or suggested potential energy surface. However, atomic movements in a molecule have never been captured in the middle of the action, not even for an extremely simple molecule such as a triatomic molecule, made of only three atoms. In this work, we track the movements of all the gold atoms in the gold trimer complex during photoinduced bond formation using femtosecond x-ray liquidography.

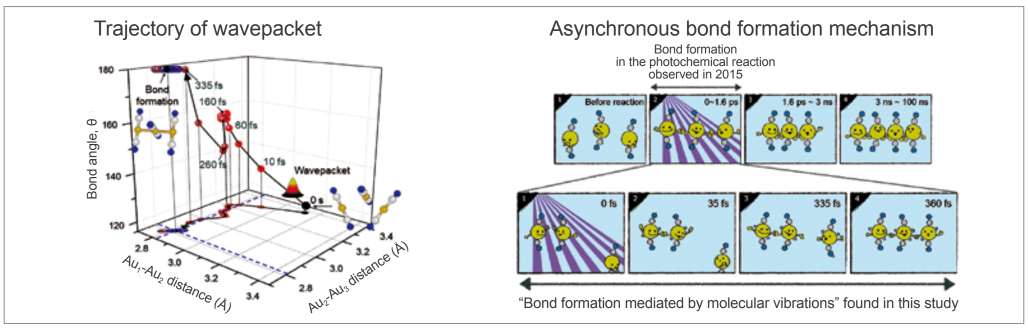
2. Contents

The research team led by Prof. Ihee succeeded in observing the real-time positions of atoms in the molecule that forms chemical bonds and uncovering whether two chemical bonds are formed one by one or simultaneously. They also unveiled how quickly and how far the distance between atoms changes in the process of the chemical bond formation. In 2015, the research team reported in Nature the observation of the formation of two chemical bonds in a gold trimer (Nature, 2015, 518, 385 – 389). After 5 years, based on dramatically improved experimental and analytical methods, they succeeded in observing in real time the movements of the three gold atoms even before the chemical bonds are formed and revealing even the specific reaction mechanism in which two chemical bonds are formed sequentially rather than simultaneously (Nature, 2020, 582, 520-524).

The basic unit that determines the properties of a matter is a molecule, and the basic unit that makes up a molecule is an atom. In other words, a molecule forms when these atoms are bound together through a chemical bond. For example, protein molecules are made up of thousands of atoms, but revealing how these atoms are actually moving has never been observed directly, even for an extremely simple molecule such as a triatomic molecule, made of only three atoms. To find the answer to this basic question, the research team used a gold trimer complex as a model system. In the gold trimer complex, three gold atoms are located in close proximity, and upon laser illumination, they react to form chemical bonds.
It is never easy to capture atomic movements in real time because the atomic movement is extremely fast, that is the femtosecond level in time, and the extent of the movement is minute, that is at the angstrom level in space. To solve this challenging task, the research team used an experimental technique called "femtosecond x-ray liquidography (solution scattering)", which combines laser photolysis and x-ray scattering techniques. A laser pulse was used to irradiate the sample, thereby initiating the chemical bond formation reaction in the gold trimer complex, and "femtosecond x-ray pulses" obtained from a special light source called x-ray free-electron laser were used to interrogate the bond-forming process. By analyzing time-resolved x-ray scattering images, real-time positions of the three gold atoms were tracked.
Tracking the atomic movements reveals that within the first 35 femtoseconds after photoexcitation, a covalent bond forms and the second covalent bond subsequently forms within 360 femtoseconds. In addition, it was observed that the atoms did not stay in the same position after the chemical bonds were formed, but the distance between the atoms increased and decreased periodically, exhibiting the molecular vibration. In this study, how fast and how much the molecule vibrates were observed in real time.

3. Expected effects

The research team plans to apply the method of 'real-time tracking of atomic positions in a molecule and molecular vibration using femtosecond x-ray scattering' realized through this study to reveal mechanisms of organic and inorganic catalytic reactions and reactions involving proteins in the human body. Through the applications, it is expected to maximize the efficiency of various catalytic reactions used industrially, and to provide basic information necessary for controlling protein reactions, treating diseases, and developing new drugs.



Research outcomes

[Paper] J. G. Kim, S. Nozawa, H. Kim, E. H. Choi, T. Sato, T. W. Kim, K. H. Kim, H. Ki, J. Kim, M. Choi, Y. Lee, J. Heo, K. Y. Oang, K. Ichiyanagi, R. Fukaya, J. H. Lee, J. Park, I. Eom, S. H. Chun, S. Kim, M. Kim, T. Katayama, T. Togashi, S. Owada, M. Yabashi, S. J. Lee, S. Lee, C. W. Ahn, D. -S. Ahn, J. Moon, S. Choi, J. Kim, T. Joo, J. Kim, S. Adachi, and H. Ihee*, "Mapping the emergence of molecular vibrations mediating bond formation", Nature, 582, 520-524 (2020) [2019 Impact Factor = 42.778]

Research funding

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