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Professor Bongjin Simon Mun's joint research team succeeds in capturing real-time decomposition process of greenhouse gas molecules

☐ GIST (Gwangju Institute of Science and Technology, President Kiseon Kim) Department of Physics and Photon Science Professor Bongjin Simon Mun's (SRC Ultrafine Ultrafast X-ray Science Research Center, C-AXS) joint research team with Institute for Basic Science (IBS, Director Do-Young Noh) Assistant Director of Research for Center for Nanomaterials and Chemical Reactions Jeong Young Park (KAIST Department of Chemistry professor), and Chungnam National University Department of Materials Science and Engineering Professor Hyun You Kim succeeded in directly observing the moment when carbon dioxide molecules decompose on the surface of the rhodium (Rh) catalyst.

- The results of this study presented direct evidence of a chemical reaction capable of removing carbon dioxide, which is the main cause of global warming, and converting it into useful substances.

☐ As the damage caused by climate change increases year by year, technologies that can convert carbon dioxide, a greenhouse gas that accelerate global warming, into useful substances are being actively researched in recent years. If collected carbon dioxide is converted into clean fuels such as methane or methanol, it can solve environmental and oil energy dependence problems.

- The problem is that carbon dioxide (CO_2) is chemically very stable, so high energy is consumed for conversion. The initial process of decomposing carbon dioxide into carbon monoxide (CO) and oxygen (O) requires a high-pressure reaction of several tens of atmospheres. For this reason, it is important to carefully understand the mechanism of decomposition of carbon dioxide in order to design an optimal reaction route and improve conversion efficiency. However, until now, only limited evidence such as spectroscopic analysis has been presented, and there has been no study that accurately presented the chemical mechanism of the carbon dioxide decomposition process at the atomic level.

☐ The research team started a study to observe the decomposition process of carbon dioxide in real time in the reaction environment. The idea was derived from the theoretical prediction that carbon dioxide molecules with a size of only a few angstroms (Å·10 billionths of a meter) can cause structural changes on the surface of the catalyst if the pressure inside the chemical reactor* is sufficiently increased.

* chemical reactor: where the supply and temperature and pressure of the reactant are controlled in order to proceed with an optimal chemical reaction

☐ Chungnam National University Professor Hyun You Kim said, "The atmospheric pressure environment in which we live is a high pressure environment in which considerable energy is supplied from the perspective of these small carbon oxide molecules. It was confirmed that the number of collisions between molecules per unit area rapidly increased due to the ambient pressure, and the molecules became unstable and finally decomposed."

- Afterwards, the researchers measured the microscopic changes in chemical bond energy on the surface of the rhodium catalyst using a radiation accelerator called a 'giant light microscope,' confirming that the carbon monoxide gradually increased after the reaction started in the atmospheric environment. In addition, it was found that the difference in density of the electron cloud** of carbon dioxide that caused the structural change was maximized on the surface of the rhodium catalyst. The evidence suggests that the decomposition of carbon dioxide begins on the surface of the rhodium catalyst.

** electron cloud: probabilistic distribution of electron locations that may exist in certain locations within an atom

☐ Professor Bongjin Simon Mun said, "To effectively remove and utilize carbon dioxide, which is pointed out as a cause of global warming, the mechanism of decomposition of carbon dioxide must be thoroughly explored. This study is meaningful in that through joint research in the fields of experimental and computational science, the change of surface carbon dioxide was observed at the atomic level, and a standard research methodology was proposed for subsequent research."

☐ IBS Assistant Director of Research Jeong Young Park said, "The theory that carbon dioxide decomposes on its own on the surface of the catalyst has been proposed a long time ago, but no direct experimental evidence has been provided, which has been considered a challenge for over 40 years. In the future, we plan to conduct research to identify key links that affect the conversion rate of carbon dioxide."

☐ The results of this research were published on November 6, 2020, in the online edition of *Nature Communications* (IF 12.121), an international academic journal.

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