GIST discovered the secret to 'maximizing' hydrogen production efficiency... Implementing continuous electron transfer without energy loss by imitating the principle of natural enzymes

- Professor Junhyeok Seo's team in the Department of Chemistry elucidates the hydrogen production reaction mechanism through precise control of electron spin interaction

- 100% hydrogen production compared to the amount of electricity, 220,000 hydrogen molecules generated per second... High-efficiency iron-based catalyst presented

- Biomimetic energy conversion technology and sustainable fuel production are also possible, and it is expected to have a ripple effect throughout the energy industry, such as fuel cells... Published in the international academic journal 《Journal of the American Chemical Society (JACS)》

▲ (From left) Professor Junhyeok Seo of the Department of Chemistry, Jueun Lee, a student in the integrated master's and doctoral program, and , a student in the integrated bachelor's, master's, and doctoral program at GIFT

As the importance of hydrogen (H_2) as an eco-friendly energy storage medium to replace fossil fuels for carbon neutrality is increasing, interest in the development of technologies and catalysts that can efficiently produce it is increasing.

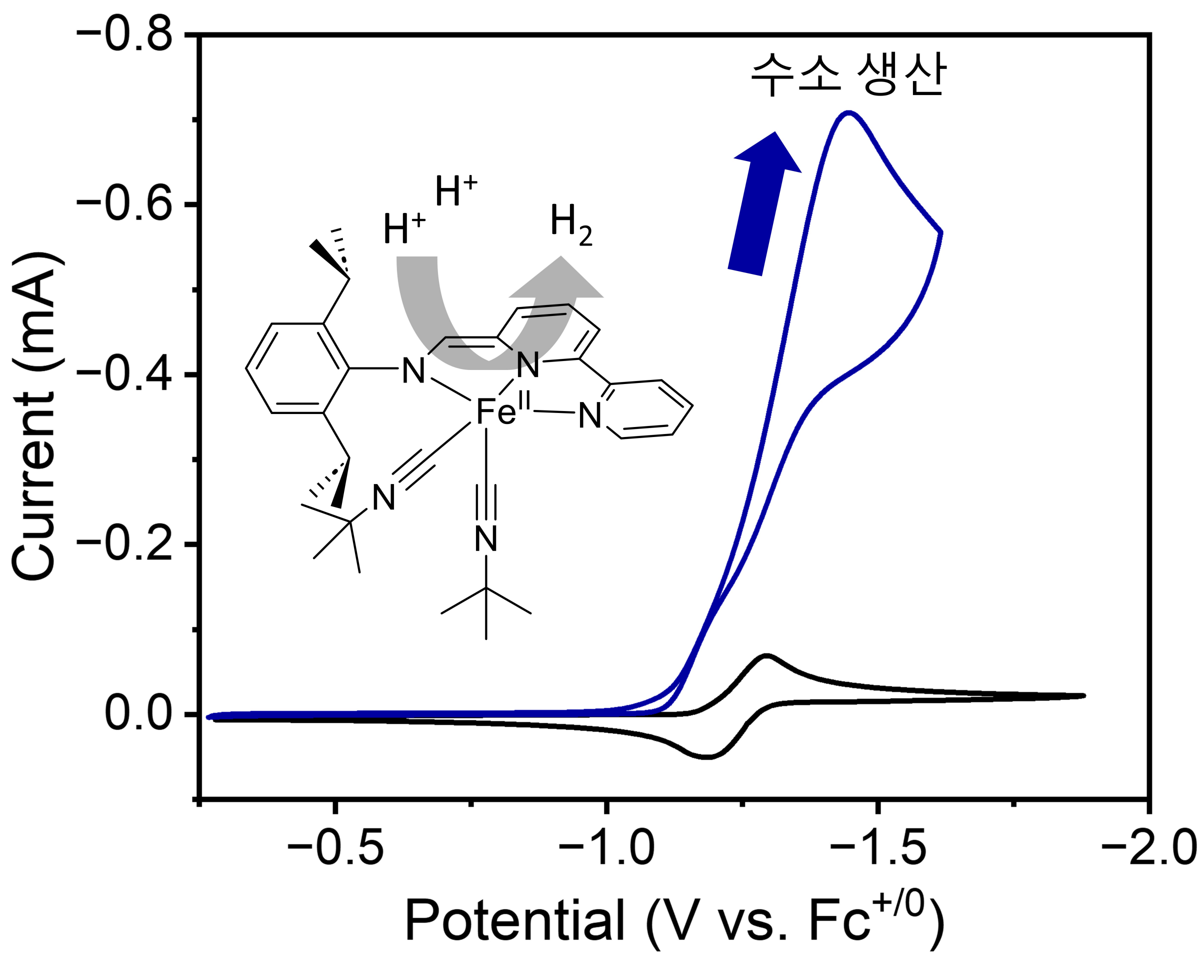
The Gwangju Institute of Science and Technology (GIST, President Lim Ki-chul) announced that Professor Junhyeok Seo's research team in the Department of Chemistry has identified a hydrogen production reaction mechanism in which electron transfer occurs more quickly and efficiently by precisely controlling the interaction between electron spins in iron (Fe)-based compound catalysts.

This study is significant in that it suggests a new reaction path without energy loss by inducing continuous electron transfer through the control of electron spins in iron compounds. This achievement can be widely utilized in the development of high-performance hydrogen catalysts as well as biomimetic energy conversion technologies and sustainable fuel production.

The 'electron transfer' process, which is the core of most chemical reactions, greatly changes the reaction speed and efficiency depending on the interaction of the 'spin', which is the rotational direction of each electron.

By precisely controlling these electron spin interactions, the research team discovered that two consecutive electron transfers are possible with just a single iron atom without additional energy consumption.

This mechanism satisfies the conditions required to produce hydrogen molecules and can act as a key principle for increasing hydrogen production efficiency.



▲ Schematic diagram of a high-efficiency iron complex and catalytic cyclic voltammetry curve. Through the efficient design of a ligand that can control the spin state, two electrons are quickly transferred to carry out a high-efficiency hydrogen production reaction. The rapidly increasing catalytic current indicates high-efficiency catalytic performance.

Hydrogenase, an enzyme that produces hydrogen in nature, continuously transfers electrons through a structure in which two iron atoms are combined. However, this high-efficiency electron transfer has not been well reproduced in structures that have been artificially simulated so far.

This study is noteworthy in that it experimentally proved that continuous electron transfer in a manner similar to natural enzymes is possible with just one iron atom.

The research team induced this reaction using a molecule called ‘ligand*’ that binds to iron ions. Previously, a lot of energy was needed for this reaction to occur, but by precisely adjusting the interaction between iron and ligands, it was confirmed that continuous electron transfer was possible while reducing energy consumption.

* ligand: A molecule that binds to a metal and controls the electronic structure or properties of the metal, and plays an important role in greatly affecting the stability and reactivity of the catalyst. For example, it helps the metal to easily give and receive electrons, and it also functions to lower the energy required for a reaction to occur.

In general, after transferring an electron once, more energy is needed when sending a second electron due to the repulsive force between the electrons.

However, in this study, a reaction path that enables continuous electron transfer without an energy barrier was implemented by precisely controlling the electron spin interaction and stabilizing the energy of the iron compound.

This iron-based catalyst recorded 100% hydrogen production efficiency compared to the amount of electricity and showed high reaction performance of producing more than 220,000 hydrogen molecules per second.

Professor Junhyeok Seo said, “This study is a basic scientific achievement that proves that the efficiency of electron transfer can be increased through electron spin control,” and explained, “This principle will be an important foundation that can be applied not only to hydrogen production but also to various energy conversion technologies such as fuel cells and electrochemical-based carbon dioxide conversion.”

This study, supervised by Professor Junhyeok Seo of the Department of Chemistry at GIST and led by doctoral students Jueun Lee and Donguk Heo, was supported by the National Research Foundation of Korea. The results of the study were published online in the international academic journal 《JACS (Journal of the American Chemical Society)》 on April 23, 2025.

Meanwhile, co-first author Donguk Heo is a first-year student of GIST's integrated undergraduate/graduate/doctoral program GIFT*, and joined Professor Jun-Hyeok Seo's research team early and actively participated in this research.

* GIFT (Graduate Integrated Fast Track): GIST is operating an excellent science and technology talent training program starting in the fall semester of 2024. It is a system designed to select undergraduate students with outstanding research potential and capabilities early and complete their degrees from bachelor's to doctoral in about 7 years. This program provides faster advancement and systematic research participation opportunities than before, creating an environment where students can immerse themselves in research from their undergraduate years and support them to grow early into professional researchers who will lead future science and technology.

Donguk Heo is receiving attention as a successful case of GIFT by entering the GIST integrated graduate/graduate program early through the GIFT program, conducting active research activities, and producing excellent results.

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