Gwangju Institute of Science and Technology

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School of Materials Science and Engineering Professor Jaeyoung Lee's joint research team develops a practical fuel cell catalysts for the hydrogen economy

□ GIST (President Kiseon Kim) Ertl Carbon Emission Research Center Professor Jaeyoung Lee and KAIST Professor Hyungjun Kim have succeeded in developing a practical catalyst for high-efficiency non-precious metal-based fuel cells.

◦ The precise factors that determine the performance of the oxygen reduction reaction as a fuel cell cathode reaction were observed by experimental and computational chemistry, respectively. Based on the results, a high performance, high durability, low cost noble metal-based oxygen reduction catalyst was developed. This study suggests new possibilities for the development of high performance fuel cell for the hydrogen economy.

□ Electrode oxygen reduction reaction is a stumbling block to the improvement of fuel cell efficiency because it requires a slow reaction rate and high voltage. Currently, platinum is regarded as the most suitable catalyst, but it is an expensive and limited resource with unfavorable price competitiveness. As a result, studies on the

production of cheaper catalysts with superior performance and durability have been attracting attention.

- The most important point in the development of noble metal catalysts is to find the parameters that determine the oxygen reduction reaction performance and to design the optimum catalysts based on these parameters. In order to find out the variables, it is necessary to support it based on electrochemical experiments and modern computational theory.

□ The team has fabricated carbon nano-fiber catalysts bearing various noble metals (nickel, cobalt, iron, silver) through electrospinning * and compared the performance of oxygen reduction on aqueous solutions. The structure and work function of the catalyst prepared on the basis of the density function ** theory were calculated and tried to find a parameter correlated with catalyst performance.

> * electrospinning: a fiber production method which uses electric force to draw charged threads of polymer solutions or polymer melts up to fiber diameters in the order of some hundred nanometers
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> ** density function: a function whose value at any given sample in the sample space can be interpreted as providing a relative likelihood that the value of the random variable would equal that sample

- The performance of the catalyst was determined by the work function of the noble metal supported on the carbon nano-fibers. The low work function of the noble metal has been shown to transfer a large amount of electrons to the nearby carbon layer, which allows oxygen to be reduced to a higher frequency on the surface of the carbon layer. As a result, iron-based nano-fibers had the best work function and the highest performance for oxygen reduction reaction.

- In addition, the durability of the catalyst is also an important factor for increasing the lifetime of the fuel cell. That is, it is important to design a noble metal oxygen reduction catalyst that satisfies both high performance and high durability. In order to maximize the durability of iron-based carbon nano-fibers, the team included 10%

cobalt to maximize the durability of the steel-based carbon nano-fiber.

□ GIST Professor Jaeyoung Lee and KAIST Professor Hyungjun Kim said, "This study solves the durability problems of iron-based noble metal catalysts by experiments and calculations. It is expected that the commercialization of alkaline hydrogen-based fuel cell will be accelerated."

□ This study was led by GIST Professor Jaeyoung Lee and KAIST Professor Hyungjun Kim with KAIST Ph.D student Yoonhoo Ha and GIST master's student Sinwoo Kang as co-first authors. The research was supported by Technology Development Program to Solve Climate Changes through the National Research Foundation of Korea funded by the Ministry of Science, ICT and was published on May 22, 2019, in *The Journal of Physical Chemistry Letters*.

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