Development for functional catalysts, Development for functional materials

Elucidation for reaction mechanism of CO_2 immobilization in nanopores of C_{60} polymer via quantum chemical theory and computer simulation

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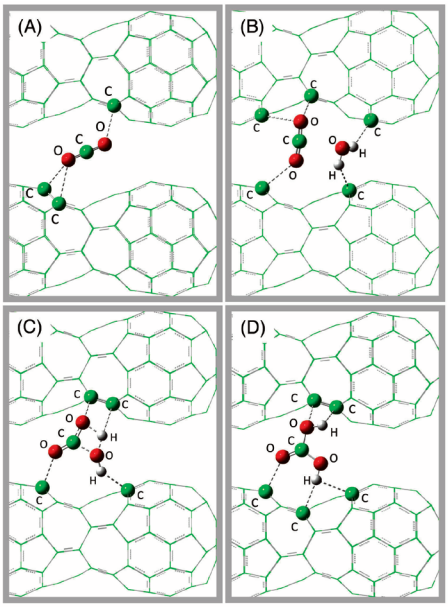
Abstract

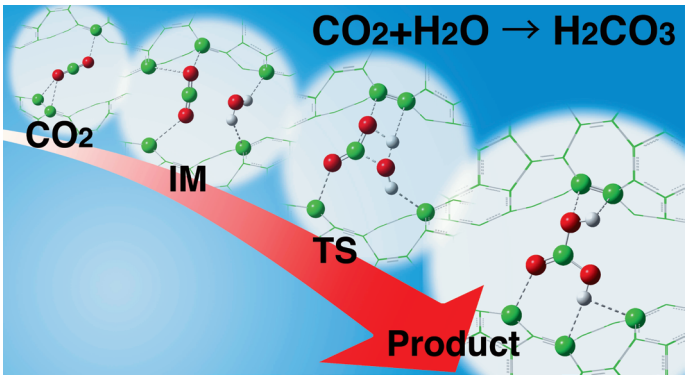
A reaction mechanism that carbon dioxide and water molecules become carbonate in the nanopores of fullerene C_{60} polymers was examined by the computer simulation based on quantum chemical theory (quantum chemical calculation). The quantum chemical calculation suggested the following mechanism: the carbon dioxide, as the first step, is trapped and bridges two C_{60} polymers. By its distorted structure and the charge polarization of the C_{60} polymers, the trapped carbon dioxide is activated. The water molecule approaches to the activated carbon dioxide molecule, and then the reaction is considered to be easily occurred.

Background & Results

Immobilization and reuse of the carbon dioxide are important issues for achieving the SDGs. An effective method that makes the stable carbon dioxide active and that leads it to the reaction, however, has not been established yet. One of the effective approaches for the problem is considered to be the use of nanoporous materials such as zeolites and metal-organic frameworks that have nano-sized spaces (nanopores) inside the compounds. The nanopores are well-known to be used for storage, exchange, and separation of molecules and ions. In addition, they also provide specific reaction fields due to their narrow space, and are known as catalysts.

It has been found that the one-dimensional C_{60} polymer which involves nanopores is synthesized via the irradiation of the electron beam to the thin layer of fullerene C_{60} by Professor Jun Onoe (Nagoya University) and coworkers. In addition, they also found that the carbon dioxide and water molecules become the carbonate ion inside the nanopores of the one-dimensional C_{60} polymer. To elucidate the reaction mechanism, the quantum chemical calculation was performed. The simulated result suggested the following mechanism: the carbon dioxide, as the first step, is trapped and bridges two C_{60} polymers. By its distorted structure and the charge polarization of the C_{60} polymers, the trapped carbon dioxide is activated. The water molecule approaches to the activated carbon dioxide molecule, and then the reaction is considered to be easily occurred.





Significance of the research and Future perspective

The computer simulation based of the quantum chemical theory can elucidate the reaction mechanism that is hard to be clarified by experiments. In addition, it is also a powerful tool for a design of the new functional materials. For the reason, the quantum chemical calculation can accelerate the studies towards the achievement of SDGs.

Patent	
Treatise	Nakaya, Masato; Kitagawa, Yasutaka; Onoe, Jun et al. Immobilization of CO_2 at Room Temperature Using the Specific Sub-NM Space of 1D Uneven-Structured C_{60} Polymer Film. Advanced Sustainable Systems. 2021; 5(1): 2000156. doi: 10.1002/adsu.202000156
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Keyword	quantum chemical theory, computer simulation, catalytic reaction mechanism, CO_2 immobilization