【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Chemistry)

Title of Project : Novel Energy and Information Conversions, Created by Solid-State Electrochemical Processes

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Research Project Number : 16H06353 Researcher Number : 20202772
Research Area : Materials Chemistry
Keyword : Electronic Functions, Surface and Interface, Solid State Electrochemistry

【Purpose and Background of the Research】

Development of novel information and energy conversions using ubiquitous materials and methods has attracted much attention. From this perspective, solid-state electrochemistry, which has innovated various rechargeable batteries and dye-sensitized solar cells, is receiving a new spotlight. In this project, we will develop novel energy and information conversions, by using the methodology of solid-state electrochemistry in organic electronics.

【Research Methods】

This project consists of three research themes.

Plan A. Bidirectional research between organic electronics and solid-state electrochemistry. We synthesize the porous compounds, such as metal-organic frameworks (MOFs) and covalent-bond frameworks (COFs), which possess structural robustness for ion doping/dedoping in electro-chemical processes. These materials are examined as cathode active materials for rechargeable Li batteries (Fig. 1). On the other hand, we try to establish novel molecular magnetism. Through the continuous valence control of the MOFs and COFs by means of electrochemistry, we realize new functions such as para-ferromagnetic switching.

Plan B. Electrochemical organic electronics. The electric double layers (EDLs) at solid-liquid interfaces can produce a huge electric field reaching to ~10^9 V/m. In this project, we make use of the EDLs in organic electronics and develop organic transistors and effective organic photocells. We develop the [Metal|Semiconductor|Insulator|-Metal] photocells, to effectively covert pulsed light into transient photocurrent, and to realize novel technology for energy and information conversions.

Plan C. Development of operando measurements and theory for solid-state electrochemical processes. To systematically conduct the research plans A and B, we work on various operando measurements under solid-state electrochemical reactions, such XAFS, XRD, solid-state NMR, and magnetic and electric measurements. We also improve the theoretical treatments for these processes, by combing molecular dynamics and molecular orbital calculations.

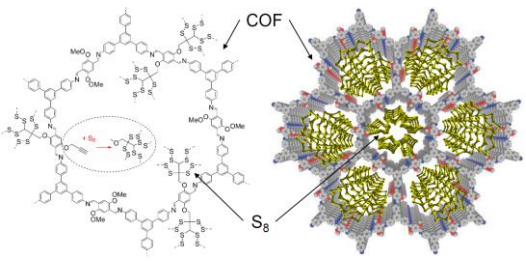

Fig. 1 Hybridization between COF and S_8, and its application to Li-S battery.

【Expected Research Achievements and Scientific Significance】

The expected research achievements are (i) high-energy-density molecule-based rechargeable batteries consisting of ubiquitous materials, (ii) electrochemically-controlled molecular magnets, and (iii) effective optoelectronic conversions using transient photocurrent. By exchanging the materials and methodology between solid-state electrochemistry and organic electronics, we would like establish a win-win relation between the two.

【Publications Relevant to the Project】

・"Discovery of a "Bipolar Charging" Mechanism in the Solid-State Electrochemical Process of a Flexible Metal–Organic Framework," Z. Zhang, H. Yoshikawa and K. Awaga, *Chem. Mater.*, 2016, **28**, 1298.
・"Organic optoelectronic interfaces with anomalous transient photocurrent", L. Hu, X. Liu, S. Dalgleish, M.M. Matsushita, H. Yoshikawa and K. Awaga, *J. Mater. Chem. C*, 2015, **3**, 5122.

【Term of Project】 FY2016-2020

【Budget Allocation】 143,000 Thousand Yen

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