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

Broad Section E

Title of Project： **Innovative energy storage materials based on the peculiar functions realized by isolated molecules/orbitals.**

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Research Project Number: 20H05673 Researcher Number：30359690

Keyword：Isolated molecule, Isolated orbital, Rechargeable battery, Electrochemical reaction, Molecular dynamics

【Purpose and Background of the Research】

For a coming low carbon society, ultimately with energy self-sufficiency, dispersive use and smart controlling of renewable energy would be of critical importance. On-demand energy storage device is necessary to compensate for the time-dependent energy supply inherent to, for example, sunshine, where rechargeable batteries should serve as an important infrastructure providing a temporary buffer not only for transportation but also for a center of electricity management.

Solids and liquids are the self-condensed systems composed of limited types of atoms and molecules, where many of the electronic/chemical properties emerges as a result of orbital interaction induced by their condensation. Based on the new principles we have recently established, we will intentionally introduce high-density "isolated" molecules/orbitals that are free from the self-interactions in solids or liquids.

Approaching from such "isolated chemistry", we will extract and maximize the hitherto unknown but useful electrochemical super-functions related to the energy storage and conversion.

【Research Methods】

"Isolation strategies" will be applied to organic electrolytes, aqueous electrolytes, solid electrodes, and electrode/electrolyte interface. Target properties are (i) extension of the electrolyte window using modified frontier orbitals induced by the isolated solvent molecule, (ii) increasing the operating voltage and reversible capacity of electrode materials by maximum isolation of electron orbitals related to the redox reactions, (iii) maximizing the double layer capacitance at electrode-electrolyte interface utilizing modified dielectric function of confined and isolated molecules.

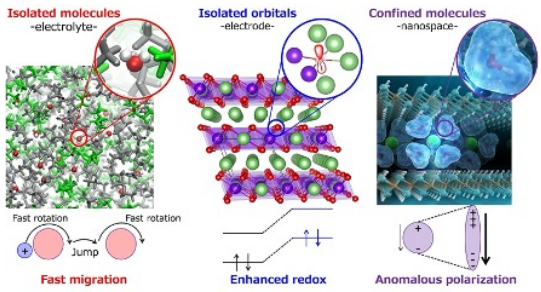

Fig. 1 Isolated molecules and isolated orbital incorporated into condensed solid or liquid systems.

【Expected Research Achievements and Scientific Significance】

The original new concept, "isolation strategies for molecules and orbitals", should be promising toward "realistic" breakthrough, as it still satisfies the essential requirements for highly reversible electrochemical reaction such as, "maintaining original structure and morphology" and "spontaneous formation of electrode/electrolyte interface in a closed system".

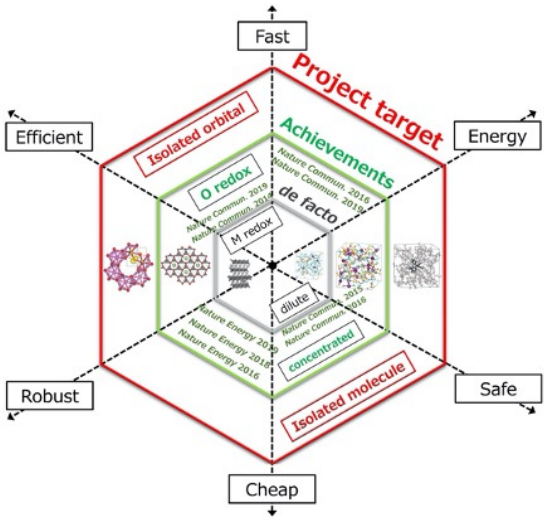

Fig.2 Hirearchy of the originality and its impact. The red line represents the functional frontier we are exploring.

【Publications Relevant to the Project】

- Q. Zheng, Y. Yamada, R. Shang, E. Nakamura, A. Yamada, A cyclic phosphate-based battery electrolyte for high-voltage and safe operation, Nature Energy, 5, 291-298 (2020)
- T. Sudayama, D. Asakura, X. Shi, B. M. Boisse, E. Watanabe, Y. Harada, M. Nakayama, M. Okubo, A. Yamada, Multibond orbital formation for stable oxygen redox reaction in battery electrodes, Energy Environ. Sci., 13, 1492-1500 (2020)

【Term of Project】 FY2020- 2024

【Budget Allocation】 151,100 Thousand Yen

【Homepage Address and Other Contact Information】

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