【Grant-in-Aid for Transformative Research Areas（A）】

Section Ⅱ

Title of Project： Dynamic Exciton: Emerging Science and Innovation

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Number of Research Area：20A201　Researcher Number：90243261

【Purpose of the Research Project】

Photochemistry is expected to play a versatile role in electronics, energy, medicine/heath care, and functional materials in modern society. In molecular donor-acceptor (D-A) systems, charge-transfer (CT) has been regarded as "static exciton" governed by Coulombic interaction (left bottom of Figure 1). However, in addition to Coulombic interaction, dynamic effects including movement of atomic nucleus and lattice as well as spin-orbit interaction influence behavior of electron and spin with the passage of time ranging from femtoseconds to seconds (defined as "dynamic exciton", right middle of Figure 1). For instance, recently power conversion efficiencies of organic photovoltaics (OPV) have been improved remarkably, but there is a limit to understanding the underlying mechanism solely from a framework of "static exciton", as things stand at the moment, becoming a bottleneck of high-performance OPV. Moreover, to get more deep insight into the dynamic effects occurring at primary stages of photophysical and photochemical events, it is needed to exploit precise spectroscopic measurements and theoretical treatments. In this project, we aim to solve the above issues by merging rational molecular design based on the dynamic effects with world-leading high-resolution spectroscopies and unique theoretical analyses. In particular, we focus on manipulating CT states for energy conversion such as organic light-emitting diodes (OLED) and OPV in term of electron-vibration and spin-orbit couplings (Figure 1).

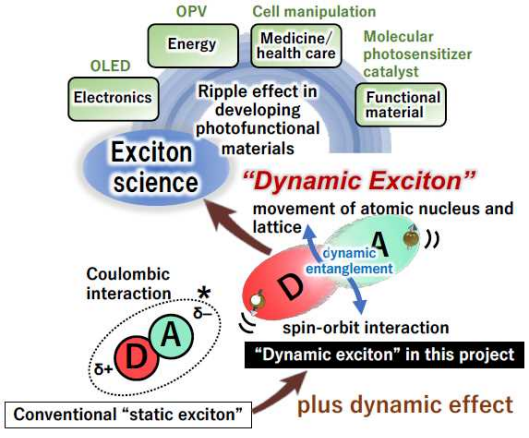

Figure 1. Purpose of the research project.

【Content of the Research Project】

In this project, we concentrate on four major topics: (1) creation of new D-A molecules and D-A model systems; science and technology of (2) OLED, and (3) OPV; (4) exploration of synthetic and biological features. Meanwhile, "Dynamic Exciton Creation (A01)", is a group of experts on well-tailored design and synthesis, "Dynamic Exciton Evaluation (A02)", that on the advanced measurements and precise analysis, and "Dynamic Exciton Function (A03)", that on the exploration of novel features. By integrating three complimentary groups synergically, we commit ourself to finding solutions to the above challenges.

【Expected Research Achievements and Scientific Significance】

In this project, we work towards not only interdisciplinary fusion of various academic fields including physics, chemistry, and biology by focusing on "dynamic exciton", creating a new comprehensive, photoinduced CT science, but also exploring versatile practical features such as OPV, OLED, molecular photosensitizer catalyst, and optical cell manipulation, which would be beneficial for modern society.

【Key Words】

Exciton: In physics exciton is defined as a state where electron and hole are bound tightly by Coulombic interaction. In chemistry exciton is considered as a locally excited (LE) state of donor (D*) or acceptor (A*) molecule. If a system composed of D and A segments is excited, partial charge-transfer (CT) may take place from D* to A or from D to A* to yield a CT state $(D^{\delta+}\text{-}A^{\delta-})^*$ possessing character of the LE states. In an extreme case complete ET occurs from D* to A or from D to A*, generating a charge-separated (CS) state $(D^{+\bullet}\text{-}A^{-\bullet})$ losing character of the LE states. Since all three cases highlight electron-hole pairs, we propose to extend the terminology exciton into an integrated class of LE, CT, and CS states.
Organic photovoltaics: OPV is a molecular D-A-based device for solar energy-electricity energy conversion. In this research project, we strive to manipulate CT states for achieving high photovoltaic performance.

【Term of Project】

FY2020-2024

【Budget Allocation】

1,140,800 Thousand Yen

【Homepage Address and Other Contact Information】

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