Title of Project: Dynamic Exciton: Emerging Science and Innovation

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【Purpose of the Research Project】
Photochemistry is expected to play a versatile role in electronics, energy, medicine/health 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 photovoltaics (OPV). In this project, we concentrate on four major topics: (1) creation of new D-A molecules and D-A model systems; (2) 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*, 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 losing character of the LE states. Since all three cases highlighting 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-utility 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

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