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

Section Ⅱ

Title of Project： Condensed Conjugation Molecular Physics and Chemistry: Revisiting "Electronic Conjugation" Leading to Innovative Physical Properties of Molecular Materials

SEKI Shu
(Kyoto University, Graduate School of Engineering, Professor)

Number of Research Area: 20A204　Researcher Number: 30273709

【Purpose of the Research Project】

Herein, we will establish a novel concept of intermolecular electronic conjugation, referred to as “X”-conjugation, by revisiting thoroughly the longitude and latitude in the development of “conjugation” in chemistry. Starting from the precise design of organic molecules with well-confined intermolecular spaces, thermal fluctuations in the condensed phases of molecular systems will be controlled perfectly by the wide-range/spatial alignment of intermolecular interactions as well as the leading-edge energy dissipation theory. Such control will result in extraordinarily high density-of-states (DOS) in the molecular substances. A series of unique assessment techniques of opto- and magneto-electronic properties of molecular materials is presently the central complex of the current research project, pioneering the unprecedented properties of molecular systems with “X”-conjugation.

【Content of the Research Project】

We will approach the establishment of “X”-conjugation and its unprecedented physical properties through the following three strategies:

I) “X”-conjugation beyond σ- and/or π-conjugation

Since the beginning of π-electron conjugation in the 1890s, “π” electrons have been always the key player in electronic conjugation where the electronic states are stabilized by electron delocalization within a molecular skeleton. After the long interval of 50 years, electron delocalization over σ-bonding was established as σ-conjugation. These electronic conjugations have been defined in terms of the angular momentum of electrons in the atomic orbitals of elements. Now, our question is: Are there other electronic conjugations? Revisiting the first definition of conjugation as energy gain in electron delocalization, we must have room for establishing a new electronic conjugation in intermolecular spaces. By filling out the space with electrons/electronic states, the new “X”-conjugation must be found. The establishment of this conjugation is the consensus of our research project entitled “Condensed Conjugation of Molecular Physics and Chemistry” To achieve an extraordinarily high DOS in the condensed phases of organic molecules, including systems with “X”-conjugation, we will pave the following steps: (1) shrinking the intermolecular spaces to the limit (0.3 nm), (2) aligning precisely and programmatically the extremely wide-dynamic-ranging intermolecular interactions that control the thermal fluctuations of molecules, and (3) loading electrons/spins onto molecules and realizing new electronic states that contribute to the overall high DOS.

II) Toward unprecedented properties of “X”-conjugation

The electronic properties of organic molecular systems include extremely wide tunability; this property is the nature of organics, as represented by a single carbon-based material exhibiting both insulating and superconducting phases. The effective mass of electrons is controllable from a massless state to a considerably heavy state in strongly correlated systems; such characteristic inspires us to explore the huge potential of “electrons in space with tunable DOS.” The nature of the electrons and their physical properties will be revealed with the unique complex of assessment techniques.

III) Interpretation of “X”-conjugation through simple and sophisticated theories/formulations.

The history of physics and chemistry illustrates that the new “X”-conjugation must be interpreted with simple and sophisticated theories/formulations. A concrete theoretical basis of intermolecular electronic conjugation, including “X”-conjugation, is provided and published as an international standard for future electronic conjugations.

【Expected Research Achievements and Scientific Significance】

In this research project, we aim to 1) explore the ubiquitous nature of massless electrons and 2) search for “heavy” electrons by designing “X”-conjugated molecular systems embedded with strongly correlated electron systems. The electron mobility in condensed-organic-molecular materials has reached 500 $cm^2V^{-1}s^{-1}$, which is competitive with Si-based materials. We will demonstrate the potentials of “X”-conjugated molecular materials as leading alternatives for future electronic materials. Moreover, the extremely wide tunability of DOS leads to the strong localization of electrons in specific sites with high effective mass, resulting in spin/charge frustrated systems, ferro/antiferro magnetism, and ferro/antiferro electricity of molecular materials. We will lead a paradigm shift in the research of organics from flexible/printable materials to prospective platforms to achieve ultimate opto- and magneto-electronic properties.

【Key Words】

“X”-conjugation: New and unexplored concept of electron conjugation over molecular materials. The major target of the present research groups.

【Term of Project】 FY 2020–2024

【Budget Allocation】 1,168,000 Thousand Yen

【Homepage Address and Other Contact Information】

https://x-con.jp
X-conjugation-admin@t.kyoto-u.ac.jp