

## 【Grant-in-Aid for Specially Promoted Research】

### Science and Engineering

**Title of Project :** Development of novel photo-induced phase conversion materials based on quantum dynamic control of Charge-Structure-Spin-Photon coupled systems



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Research Project Number : 18H05208 Researcher Number : 10192056

Keyword : Optical Properties of Materials, Photoinduced Phase Transition, Ultrafast Structural Dynamics

#### 【Purpose and Background of the Research】

An attractive target for materials science is to achieve control of phase transitions using light (photo-induced phase transitions: PIPTs). To date, PIPT dynamics has been governed by the slow relaxation/dissipation of photo-injected energy leading to decoherence of the multi-electron state in a cooperatively interacting system (classical PIPT). Utilization of the quantum dynamics of a multi-electron state (quantum PIPT) that is coherently and strongly coupled to the electromagnetic field of the excitation photon itself is essential for creating photonic phase-switching materials with ultrahigh speeds and sensitive responses. Combining ultrafast modifications of three main physical degrees of freedom in solids (Charge-Structure-Spin, C-S-S) within the vibrational periods of elementary excitations will enable us to find unique C-S-S-ordered states, which can be obtained only by quantum PIPT (i.e., quantum hidden states: QHS).

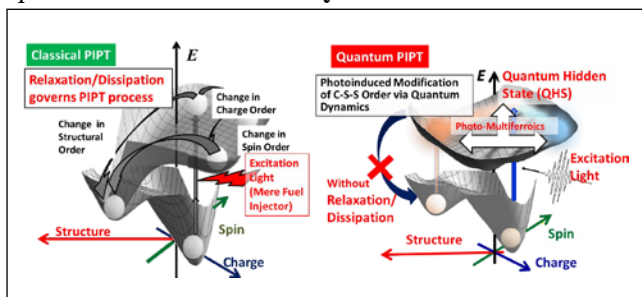


Figure 1 Illustration of classical PIPT dynamics (left-hand side) and quantum PIPT (right-hand side)

#### 【Research Methods】

To clarify the ultrafast C-S-S coupled dynamics in a quantum PIPT system and develop new materials, this project establishes the following three teams and involves deep collaborations among materials scientists, specialists in ultrafast spectroscopy/electron diffraction, and theoreticians:

**Team 1:** Search and develop candidate materials that show QHS *via* ultrafast quantum PIPT based on the strong coupling among C-S-S freedoms.

**Team 2:** Construct an ultrashort (30 fs) pulsed electron-diffraction facility with a spin-polarized /depolarized electron source.

**Team 3:** Construct a theoretical framework for quantum PIPT.

#### 【Expected Research Achievements and Scientific Significance】

In this project, a pulsed electron-diffraction system with a 30-fs width, combined with a spin-polarized electron source will be constructed to enable observations of ultrafast C-S-S dynamics. The combined use of this system and an ultrafast spectroscopic probe will reveal the quantum natures of the microscopic mechanisms driving the initial PIPT process. The accumulated knowledge will unveil a realistic manner for photo-controlling the sensitive and ultrafast changes in magnetic, electronic, optical, dielectric, and structural properties of materials based on C-S-S strong coupling *via* QHS (photo-multiferroics). This research will have a large impact on the general field of photo-functional materials while opening the door for photonic and quantum control of a wide class of materials with ultrahigh speeds.

#### 【Publications Relevant to the Project】

- “Direct Observation of Collective Modes Coupled to Molecular Orbital Driven Charge Transfer”, T.Ishikawa, M.Hada, \*R.J.D. Miller, K.Onda, S.Koshihara, et al. *Science* 350, pp.1501 (2015)
- “Coherent dynamics of photoinduced phase formation in a strongly correlated organic crystal”, T.Ishikawa, S.Koshihara, \*K.Onda et al. *Phys. Rev. B* 89, 161102(R) (2014)

**【Term of Project】** FY2018-2022

**【Budget Allocation】** 484,700 Thousand Yen

#### 【Homepage Address and Other Contact Information】

<http://www.chemistry.titech.ac.jp/~koshihara/english2/index.html>