

Division of Environmental Chemistry – Molecular Materials Chemistry –

<http://molmat.kuicr.kyoto-u.ac.jp/index-e.html>



Prof
KAJI, Hironori
(D Eng)



Assist Prof
SHIZU, Katsuyuki
(D Eng)



Assist Prof
SUZUKI, Katsuaki
(D Human & Environmtl. Studies)



Techn Staff *
OHMINE, Kyoko



Techn Staff
MAENO, Ayaka

*Re-employed Staff

PD

GELDSTZER, Jan (Ph D)
WADA, Yoshimasa (D Eng)

Researcher

NAKAGAWA, Hiromichi (D Eng)

Students

REN, Yongxia (D2)
MORIWAKI, Kazuki (M2)

HU, Weizhe (M2)
KUSAKABE, Yu (M2)

MURAMATSU, Tomomi (M1)
ISHIHARA, Kuraudo (UG)

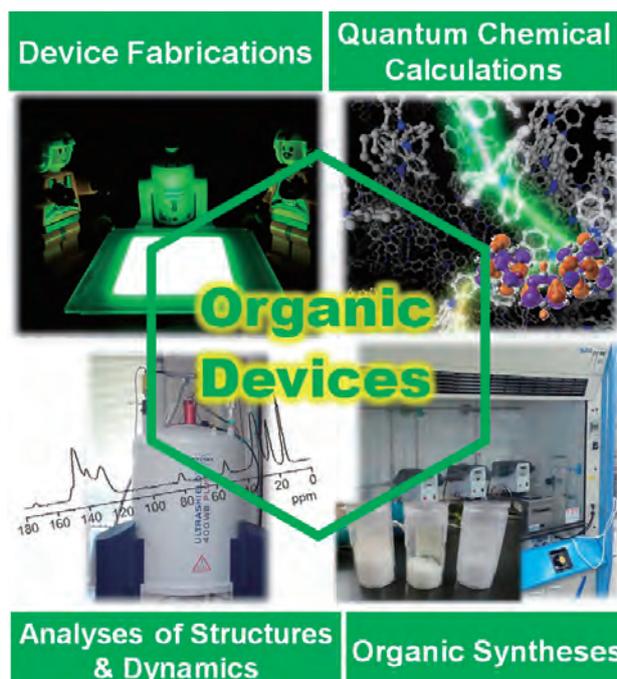
KANDA, Syun (UG)
SATO, Hiroki (UG)

Scope of Research

Our research goal is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. Toward this, we carry out syntheses, device fabrications, precise structure characterizations, and quantum chemical calculations for high functional organic materials. Along with exploring novel synthetic routes and novel devices, we perform detailed analyses of structures and dynamics, mainly by sophisticated solid-state NMR spectroscopy, in order to obtain structure–dynamics–property relationships.

KEYWORDS

Organic Light-Emitting Diodes
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials
Dynamic Nuclear Polarization Enhanced NMR



Selected Publications

- Kusakabe, Y.; Wada, Y.; Nakagawa, H.; Shizu, K.; Kaji, H., Conformation Control of Iminodibenzyl-Based Thermally Activated Delayed Fluorescence Material by Tilted Face-to-Face Alignment with Optimal Distance (tFFO) Design, *Front. Chem.*, **8**, [530-1]-[530-9] (2020).
- Wada, Y.; Nakagawa, H.; Matsumoto, S.; Wakisaka, Y.; Kaji, H., Organic Light Emitters Exhibiting Very Fast Reverse Intersystem Crossing, *Nat. Photon.*, **14**, 643-649 (2020).
- Shizu, K.; Adachi, C.; Kaji, H., Visual Understanding of Vibronic Coupling and Quantitative Rate Expression for Singlet Fission in Molecular Aggregates, *Bull. Chem. Soc. Jpn.*, **93**, 1305-1313 (2020).
- Shizu, K.; Adachi, C.; Kaji, H., Effect of Vibronic Coupling on Correlated Triplet Pair Formation in the Singlet Fission Process of Linked Tetracene Dimers, *J. Phys. Chem. A*, **124**, 3641-3651 (2020).
- Shizu, K.; Adachi, C.; Kaji, H., Correlated Triplet Pair Formation Activated by Geometry Relaxation in Directly Linked Tetracene Dimer (5,5-Bitetracene), *ACS omega*, **6**, 2638-2643 (2021).

Thermally Activated Delayed Fluorescent Materials Showing Very Fast Reverse Intersystem Crossing

We report a robust molecular design, named “tilted Face-to-Face alignment with Optimal distance (tFFO),” for thermally activated delayed fluorescence materials showing very fast reverse intersystem crossing (RISC). tFFO design simultaneously realizes near-degenerate ^1CT , ^3CT and ^3LE states (where ^1CT and ^3CT denote singlet and triplet charge transfer states, respectively and ^3LE denotes triplet locally excited state) and notable spin-orbit coupling between them by controlling the through-space distance between the donor and acceptor segments in a molecule with tilted intersegment angles. Based on the concept, the first example molecule, TpAT-tFFO, realized very fast RISC with a rate constant of $1.2 \times 10^7 \text{ s}^{-1}$. In its application to organic light-emitting diodes, TpAT-tFFO exhibited high performance even at very high brightness owing to the ultrafast RISC. Our tFFO strategy can be versatilely expanded to various types, numbers, and combinations of segments.

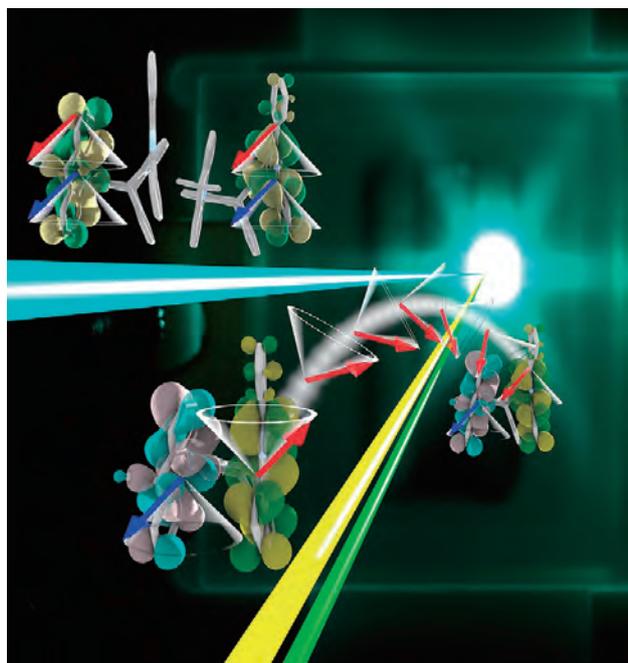


Figure 1. A thermally activated delayed fluorescence molecule showing very fast reverse intersystem crossing.

Singlet Fission Materials for Triplet Sensitizers in Organic Optoelectronics

Singlet fission (SF) or singlet-exciton fission is a multi-excitonic process that splits one singlet exciton into two triplet excitons. SF molecules are potential candidates for triplet sensitizers in organic light-emitting diodes. We develop a simple method for quantitatively predicting the SF efficiency on the basis of quantum chemical calculation and the Fermi golden rule. We apply this method to various SF molecules. Calculated SF rates are quantitatively consistent with experimental results, suggesting the validity of our method. Towards more realistic model, we combine the above approach with quantum mechanics/molecular mechanics (QM/MM) method to consider effects of environment on SF mechanism in molecular aggregates. Using the combined method, we quantitatively reproduce the SF rate in crystalline tetracene.

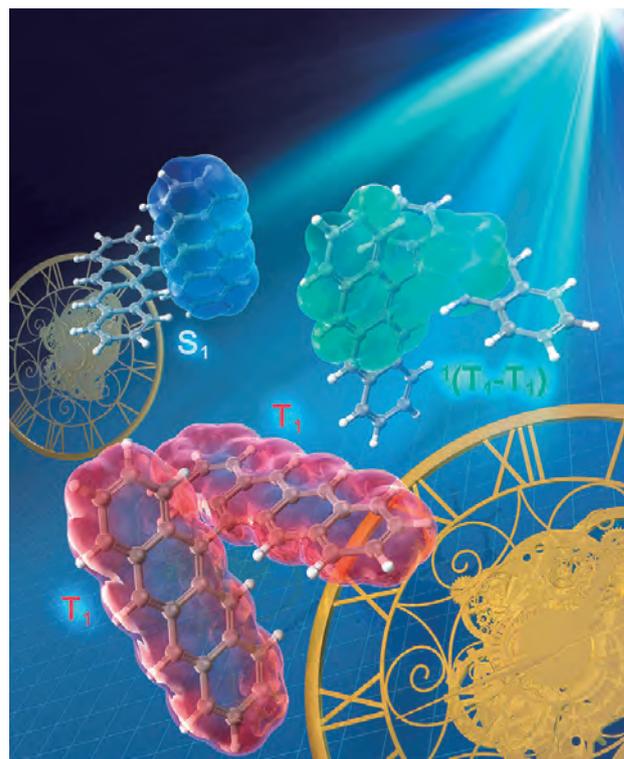


Figure 2. Theoretical design of singlet fission molecules.