Division of Environmental Chemistry
– Molecular Materials Chemistry –

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

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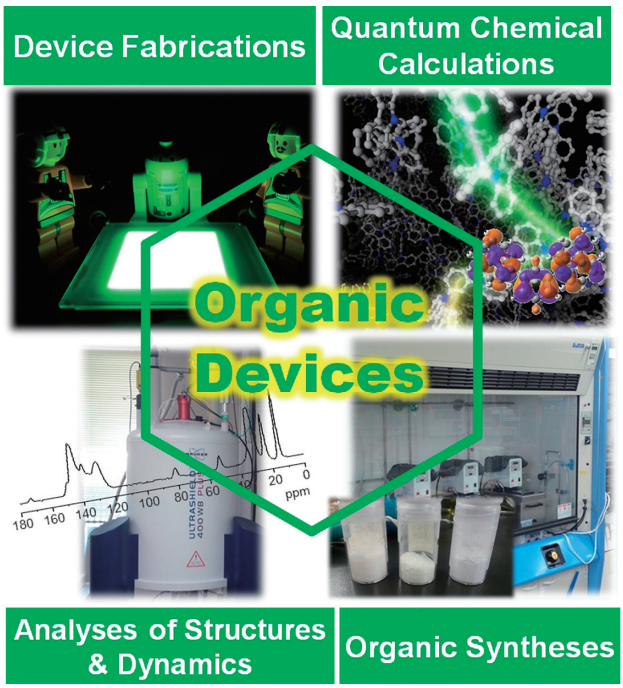
Scope of Research

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

Recent Selected Publications

Kusakabe, Y.; Wada, Y.; Misono, T.; Suzuki, K.; Shizu, K.; Kaji, H., Imidazole Acceptor for Both Vacuum-Processable and Solution-Processable Efficient Blue Thermally Activated Delayed Fluorescence, *ACS Omega*, **7,** 16740-16745 (2022).

Shizu, K.; and Kaji, H., Comprehensive Understanding of Multiple Resonance Thermally Activated Delayed Fluorescence via Quantum Chemistry Calculations, *Commun. Chem.*, **5**, 53(1-6), (2022).

Ren, Y.; Nakagawa, H.; Suzuki, K.; Kaji, H., Near-Infrared-Red-Orange Thermally Activated Delayed Fluorescence Emitters Using a Strong Tetracoordinated Difluoroboronated Acceptor, *Jpn. J. Appl. Phys.*, **61**, [081001-1]-[081001-5] (2022).

Theoretical Determination of Rate Constants for Materials Screening

Theoretical prediction of rate constants has attracted great attention because of its relevance to materials chemistry. We report a cost-effective method of theoretically predicting electronic transition rate constants from the excited states of molecules. Our method is based on quantum chemical calculations of electronic states and the Fermi golden rule. We apply the method to the excited-state decay mechanism of photoexcited benzophenone and show that calculated rate constants, including radiative (fluorescence) and nonradiative decays from S_1 to S_0, radiative decay (phosphorescence) from T_1 to S_0, and intersystem crossing from S_1 to T_2, are quantitatively in good agreement with the experimental ones. From the calculated population kinetics, a stepwise $S_1 \rightarrow T_2 \rightarrow T_1 \rightarrow S_0$ transition is found to be the predominant decay pathway. The direct $S_1 \rightarrow T_1$ transition is suppressed owing to a fast $S_1 \rightarrow T_2$ intersystem crossing. Our method of predicting rate constants is useful for accelerating materials screening.

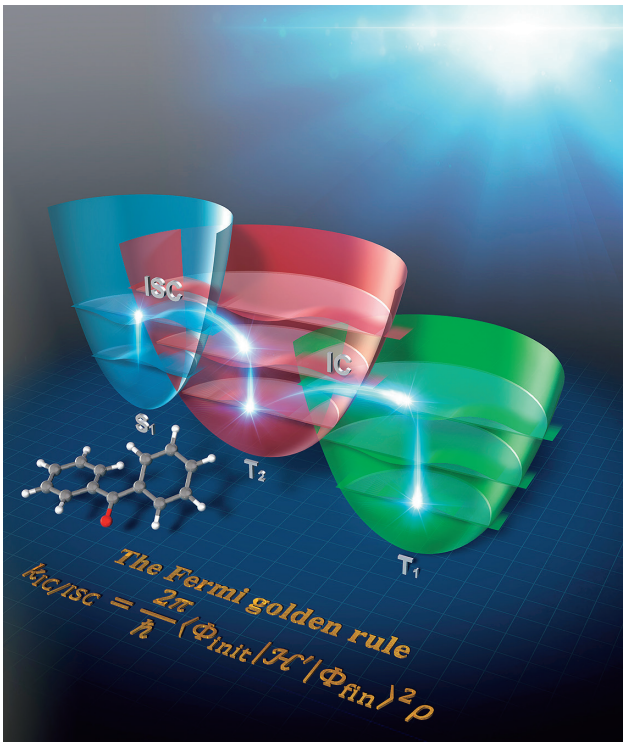


Figure 1. A stepwise $S_1 \rightarrow T_2 \rightarrow T_1$ decay mechanism of photoexcited benzophenone.

Imidazole Acceptor for Both Vacuum-Processable and Solution-Processable Efficient Blue Thermally Activated Delayed Fluorescence

The members of the imidazole family have been widely used for electron transporting, host, conventional fluorescent, and phosphorescent materials. Although the imidazole core also has great potential as an acceptor segment of deep-blue thermally activated delayed fluorescence (TADF) owing to its high triplet energy, the emission color of imidazole-based TADF organic light-emitting diodes (OLEDs) has so far been limited to blue to green. In this work, four acridan-imidazole systems are theoretically designed aiming for deep- or pure-blue emitters. All four emitters exhibit deep-blue to blue emission owing to the high energy levels of the lowest excited singlet states, exhibiting y coordinates of Commission Internationale de l'Eclairage coordinates between 0.06 and 0.26. The molecule composed of a trifluoromethyl-substituted benzimidazole acceptor in combination with a tetramethyl-9,10-dihydroacridine donor (named MAc-FBI) achieves a high maximum external quantum efficiency (EQEMAX) of 13.7% in its application to vacuum-processed OLEDs. The emitter has high solubility even in ecofriendly nonhalogenated solvents, which motivates us to fabricate solution-processed MAc-FBI-based OLEDs, resulting in an even higher EQEMAX of 16.1%.

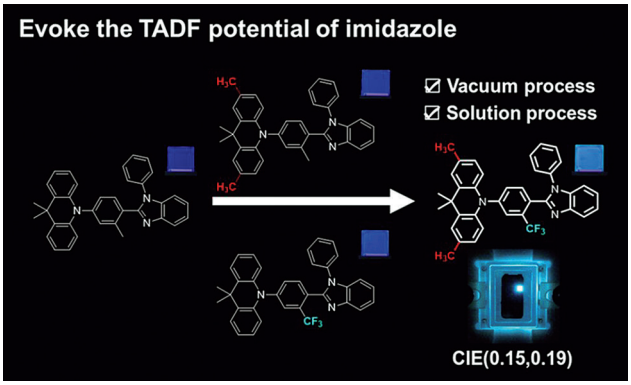


Figure2. Imidazole Acceptor for Both Vacuum-Processable and Solution-Processable Efficient Blue TADF emitters.