

# Division of Environmental Chemistry – Molecular Materials Chemistry –

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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



## Selected Publications

Zhang, D. D.; Suzuki, K.; Song, X. Z.; Wada, Y.; Kubo, S.; Duan, L. A.; Kaji, H., Thermally Activated Delayed Fluorescent Materials Combining Intra- and Intermolecular Charge Transfers, *ACS Appl. Mater. Interfaces*, **11**, 7192-7198 (2019).

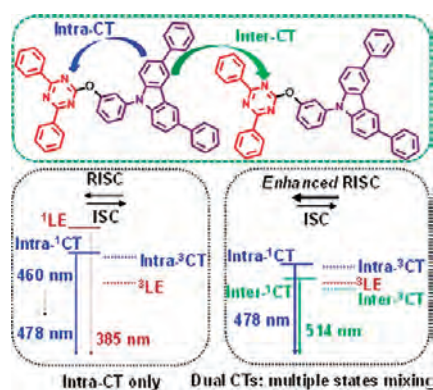
Fukushima, T.; Ishibashi, H.; Suemasa, D.; Nakamura, R.; Yomogida, M.; Isono, T.; Satoh, T.; Kaji, H., Synthesis and Characterization of Cyclic P3HT as a Donor Polymer for Organic Solar Cells, *J. Polym. Sci., Part B: Polym. Phys.*, **57**, 266-271 (2019).

Kusaka, Y.; Hasegawa, T.; Kaji, H., Noise Reduction in Solid-State NMR Spectra Using Principal Component Analysis, *J. Phys. Chem. C*, **123**, 10333-10338 (2019).

## Thermally Activated Delayed Fluorescent Materials Combining Intra- and Intermolecular Charge Transfers

A novel thermally activated delayed fluorescent (TADF) compound, 9-(3-((4,6-diphenyl-1,3,5-triazin-2-yl)oxy)phenyl)-3,6-diphenyl-9H-carbazole (PhCz-o-Trz), with a donor- $\sigma$ -acceptor (D- $\sigma$ -A) motif is developed. A flexible small space  $\sigma$ -junction is adopted to partly suppress the intramolecular charge transfer (intra-CT) while inversely enhancing the intermolecular charge transfer (inter-CT) between D/A moieties, realizing the coexistence of both intra-CT and inter-CT in an amorphous aggregate (Figure 1). The coexistence of dual CTs increases the complexity of the singlet and triplet state mixing, enhancing the triplet-to-singlet spin-flip transition and thereby the TADF emission. Additionally, PhCz-o-Trz is evaluated not only as an emitter but also as a sensitizing host for fluorescent and phosphorescent dopants.

With increasing the PhCz-o-Trz concentration, red-shift of fluorescence spectra was observed. Also, it is observed that both the intra- and inter-CT emissions coexist from 20 wt % to nearly 100 wt %. These results indicate the coexistence of the intra-CT and inter-CT, facilitating the triplet-to-singlet spin-flip transition. The device with DPEPO: 40% PhCz-o-Trz as the EML provided an EQEmax of 8.5%. Furthermore, devices with PhCz-o-Trz as the single host for fluorescence, phosphorescence, and TADF dopants were evaluated, realizing an maximum external quantum efficiency of 11.9, 27.1, and 20.2%, respectively. Our

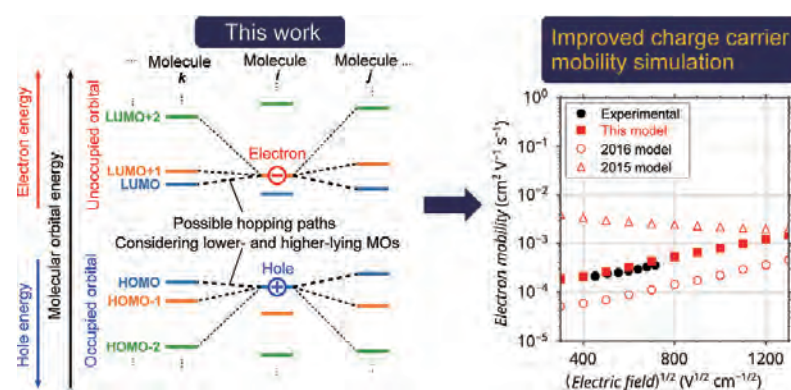


**Figure 1.** Molecular structure and mechanism of intra- and inter molecular charge transfer.

results here will shed new light on developing novel TADF materials with tunable intra- and inter-CT states, enabling not only TADF emitters with dual CT states but also single-molecule exciplex-type hosts with an easy device fabrication procedure, and may also deepen our understanding about TADF mechanisms.

## Parameter-Free Multiscale Simulation Realising Quantitative Prediction of Hole and Electron Mobilities in Organic Amorphous System with Multiple Frontier Orbitals

In amorphous organic semiconducting systems, hole and electron transfer has been considered to occur based on the overlap of highest occupied molecular orbitals (HOMOs) and that of lowest unoccupied molecular orbitals (LUMOs) between two adjacent molecules, respectively. Other molecular orbitals (MOs), HOMO-1, HOMO-2, ... and LUMO+1, LUMO+2, ..., have been neglected in charge transport calculations. However, these MOs could potentially contribute to charge transport. In this study, our multiscale simulations show that carriers are effectively transported not only via HOMOs or LUMOs but also via other MOs when the MOs are close in energy. Because these multiple MOs are active in charge transports, here we call them multiple frontier orbitals. Molecules with multiple frontier orbitals are found to possess high carrier mobility. The findings in this study provide guidelines to aid design of materials with excellent charge transport properties.



**Figure 2.** The charge transport simulation model for this work and electric field dependence of electron mobility.