Division of Environmental Chemistry
– Molecular Materials Chemistry –

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

Prof
KAJI, Hironori
(D Eng)

Assist Prof
FUKUSHIMA, Tatsuya
(D Eng)

Assist Prof
SHIZU, Katsuyuki
(D Eng)

Techn Staff
OHMINE, Kyoko

Techn Staff
MAENO, Ayaka

PD
SUZUKI, Katsuaki
(D Hum Env Sc)

Researchers

ISHIYAMA, Norihiro (D Eng)
NAKAGAWA, Hiromichi (D Eng)

Assist Techn Staff

MIYAKE, Harumi

Lect (pt)

NISHIYAMA, Yusuke (D Sc) JEOL Resonance
YOSHIMURA, Ken (D Eng) Sumitomo Chemical Co., Ltd.

Students

ISHIBASHI, Hirotaka (M2)
KUBO, Shosei (M2)
MIWA, Takuya (M2)
OGATA, Isamu (M1)
MIURA, Tsutomu (M1)
WADA, Yoshimasa (M1)
URATANI, Hiroki (UG)
KIDO, Tsuyoshi (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
Organic Solar Cells
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials

Selected Publications

Suzuki, K.; Kubo, S.; Shizu, K.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Adachi, C.; Kaji, H., Triarylboron-based Fluorescent Organic Light-emitting Diodes with External Quantum Efficiencies Exceeding 20%, *Angew. Chem. Int. Ed.*, **54,** 15231-15235 (2015).

Wada, Y.; Shizu, K.; Kubo, S.; Suzuki, K.; Tanaka, H.; Adachi, C.; Kaji, H., Highly Efficient Electroluminescence from a Solution-processable Thermally Activated Delayed Fluorescence Emitter, *Appl. Phys. Lett.*, **107,** [183303-1]-[183303-4] (2015).

Kaji, H.; Suzuki, H.; Fukushima, T.; Shizu, K.; Suzuki, K.; Kubo, S.; Komino, T.; Oiwa, H.; Suzuki, F.; Wakamiya, A.; Murata, Y.; Adachi, C., Purely Organic Electroluminescent Material Realizing 100% Conversion from Electricity to Light, *Nat. Commun.*, **6,** [8476-1]-[8476-8] (2015).

Shizu, K.; Tanaka, H.; Uejima, M.; Sato, T.; Tanaka, K.; Kaji, H.; Adachi, C., Strategy for Designing Electron Donors for Thermally Activated Delayed Fluorescence Emitters, *J. Phys. Chem. C*, **119,** 1291-1297 (2015).

Fukushima, T.; Yamamoto, J.; Fukuchi, M.; Hirata, S.; Jung, H. H.; Hirata, O.; Shibano, Y.; Adachi, C.; Kaji, H., Material Degradation of Liquid Organic Semiconductors Analyzed by Nuclear Magnetic Resonance Spectroscopy, *AIP Advances*, **5,** [087124-1]-[087124-5] (2015).

Suzuki, F.; Shizu, K.; Kawaguchi, H.; Furukawa, S.; Sato, T.; Tanaka, K.; Kaji, H., Multiscale Simulation of Charge Transport in a Host Material, *N,N'*-dicarbazole-3,5-benzene (mCP), for Organic Light-emitting Diodes, *J. Mater. Chem. C*, **3,** 5549-5555 (2015).

Environmentally Friendly Emitter for Organic Light-emitting Diodes Realizing 100% Conversion from Electricity to Light

Organic light-emitting diodes (OLEDs) are solid-state light-emitting devices applied to display and lighting applications. In OLEDs, singlet and triplet excitons are theoretically generated in a 1:3 ratio by electron–hole recombinations. Triplet excitons are typically deactivated through a non-emissive process. Only singlet excitons are converted into photons, meaning that the conversion from carriers to light is limited to 25%. To overcome this issue, thermally activated delayed fluorescent (TADF) materials are proposed, which have a small energy gap between singlet and triplet excited states (ΔE_{ST}) to convert triplet into singlet excitons at room temperature. In this study, we have developed a new TADF material (DACT-II) with approximately 100% up-conversion of the triplet to singlet excitons as well as approximately 100% photoluminescence quantum efficiency, by fine-tuning the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) distributions. OLEDs containing DACT-II show a maximum external electroluminescence quantum efficiency (EQE) of 29.6%, indicating an internal quantum efficiency (conversion of excitons to photons) of ~100%. An external EQE of 41.5% is obtained by the use of an out-coupling sheet. At a high luminance of 3,000 cd/m^2, the external EQE is 30.7%.

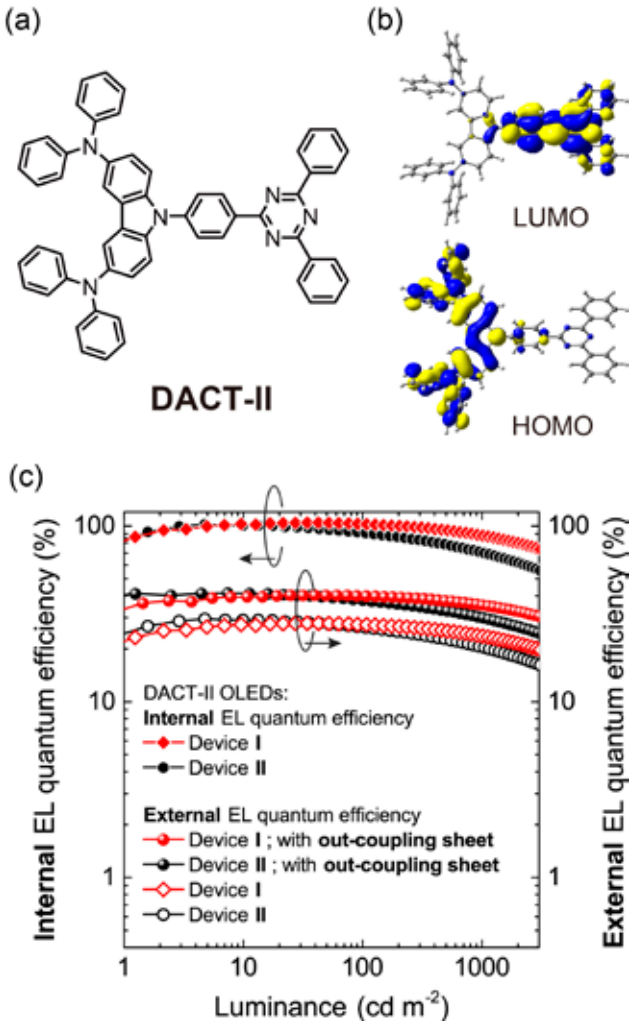

Figure 1. (a) Chemical structure of DACT-II. (b) HOMO and LUMO distributions in DACT-II. (c) Internal EQE–luminance–external EQE characteristics for the DACT-II OLEDs.

Carrier Transport Simulation in an Amorphous mCP Thin Film for Organic Light-emitting Diodes

Carrier injection and carrier blocking at each interface, as well as carrier transport in each layer need to be optimized to improve the performance of OLEDs. Among these processes, the energy levels of the HOMO and the LUMO of organic molecules for injection and blocking of carriers are important and can be well-estimated using quantum chemical calculations for isolated molecules. However, carrier transport in organic films depends strongly on both the intramolecular and intermolecular structures. In this study, multiscale carrier transport simulations were performed for the amorphous structure *N*,*N'*-dicarbazole-3,5-benzene (mCP), which has been used as a host material for OLEDs. We investigated the contribution of respective molecular pairs to carrier transport in an amorphous structure constructed by molecular dynamics. Molecular-level analysis of the carrier transport simulations demonstrates that molecular pairs with large electronic couplings are not the most important factor in carrier transport processes. Carriers are transported effectively in the forward direction via other molecular pairs that do not have substantially large electronic couplings.

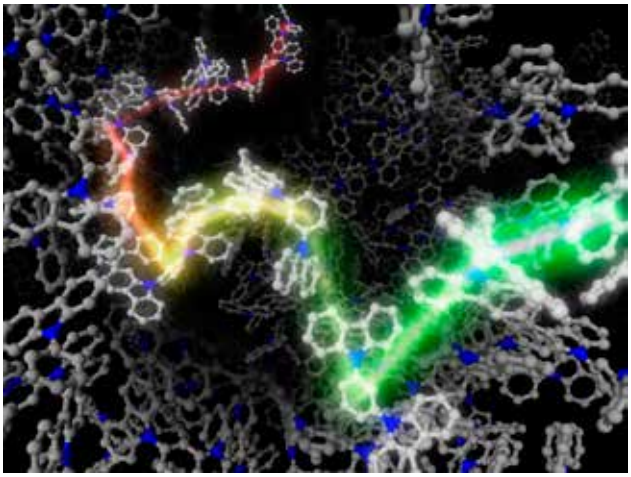

Figure 2. Carrier transport in amorphous mCP films.