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– Molecular Materials Chemistry –

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

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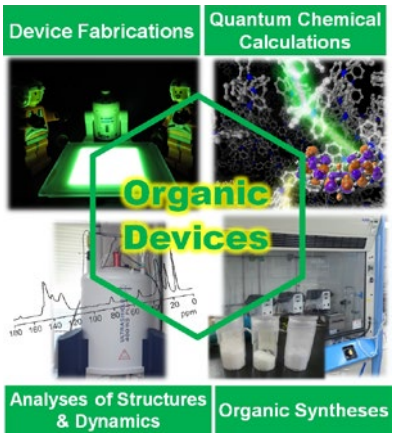
Scope of Research

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
Organic Solar Cells
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials



Selected Publications

Uratani, H.; Kubo, S.; Shizu, K.; Suzuki, F.; Fukushima, T.; Kaji, H., Detailed Analysis of Charge Transport in Amorphous Organic Thin Layer by Multiscale Simulation without Any Adjustable Parameters, *Sci. Rep.*, **6,** 39128 (2016).

Shizu, K.; Kaji, H., Organic Electroluminescent Materials Realizing Efficient Conversion from Electricity to Light, *J. Photopolym. Sci. Technol.*, **29,** 305-310 (2016).

Nishimura, H.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Kaji, H., The Influence of Quasiplanar Structures of Partially Oxygen-Bridged Triphenylamine Dimers on the Properties of Their Bulk Films, *Bull. Chem. Soc. Jpn.*, **89,** 726-732 (2016).

Hayase, G.; Nonomura, K.; Kanamori, K.; Maeno, A.; Kaji, H.; Nakanishi, K., Boehmite Nanofiber-Polymethylsilsesquioxane Core-Shell Porous Monoliths for a Thermal Insulator under Low Vacuum Conditions, *Chem. Mater.*, **28,** 3237-3240 (2016).

Wada, Y.; Shizu, K.; Kubo, S.; Fukushima, T.; Miwa, T.; Tanaka, H.; Adachi, C.; Kaji, H., Highly Efficient Solution-Processed Host-Free Organic Light-Emitting Diodes Showing an External Quantum Efficiency of Nearly 18% with a Thermally Activated Delayed Fluorescence Emitter, *Appl. Phys. Express*, **9,** 032102-1-032102-3 (2016).

Hayase, G.; Kanamori, K.; Maeno, A.; Kaji, H.; Nakanishi, K., Dynamic Spring-Back Behavior in Evaporative Drying of Polymethylsilsesquioxane Monolithic Gels for Low-Density Transparent Thermal Superinsulators, *J. Non-Cryst. Solids*, **434,** 115-119 (2016).

Highly Efficient Solution-processed Host-free Organic Light-emitting Diodes using a Thermally Activated Delayed Fluorescence Emitter

Organic light-emitting diodes (OLEDs) have attracted great interest as a promising technique for developing solid-state lighting source and flexible flat-panel displays. To date, vacuum vapor deposition has been widely used to fabricate OLEDs. However, it has drawbacks, including high production cost and difficulty in fabricating multi-dopant OLEDs. Solution processing is an alternative method to vacuum vapor deposition for fabricating OLEDs. It has an advantage of lowering the production cost and realizing large-area high-resolution displays. An emitting layer of an OLED is generally a doped film composed of an emitting dopant and a host material. To realize a high-performance OLED, the host material is required to have high excited-state energies, ambipolar transport properties, and suitable HOMO and LUMO energy levels. Host-free OLEDs contain a neat film as an emissive layer (that is, the emissive layer consists of an emitting material alone), which can remove the limitations of host materials. In this study, using a spin-coated neat film of a thermally activated delayed fluorescence emitter (DMAC-TRZ) as an emissive layer, we fabricated a solution-processed OLED. The OLED exhibited a maximum external quantum efficiency (EQE) of 17.6% (Figure 1), which is the highest value obtained for solution-processed host-free OLEDs, including phosphorescent systems. By further optimizing the device structure, we achieved an EQE of 16.8% at high luminance.

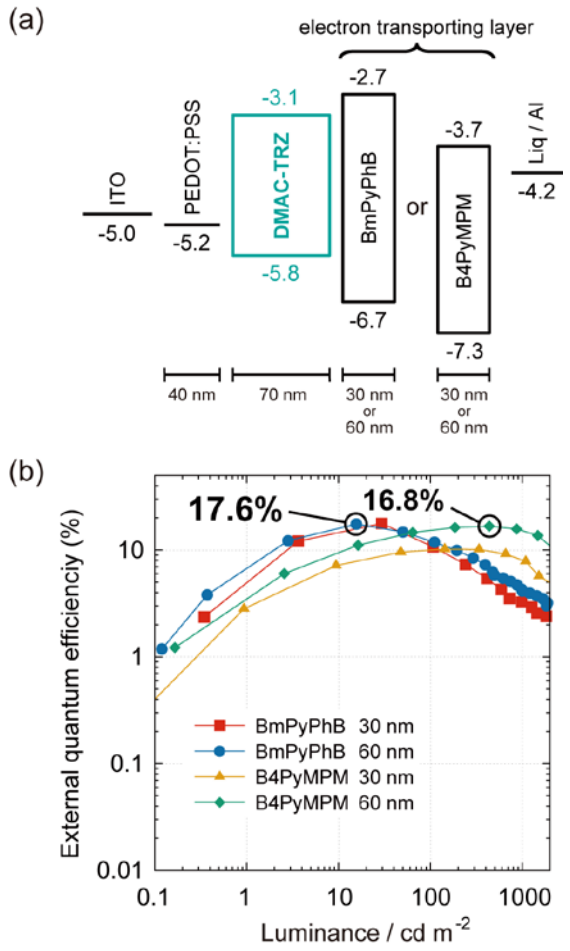


Figure 1. (a) Energy diagram of solution-processed host-free OLEDs containing DMAC-TRZ as an emitter. (b) Luminance–EQE characteristics of the solution-processed host-free OLEDs.

Charge Transport Simulations in Amorphous Thin Films for OLEDs

A fundamental understanding of charge transport properties of organic thin films is essential to improve OLED performance. Charge transport properties of organic molecules have been discussed in terms of their HOMO and LUMO energy levels and electronic couplings between molecules. The HOMO and LUMO can be calculated using quantum chemical calculations for isolated molecules, while the electronic couplings are considered to depend largely on an aggregated structure. We performed multiscale charge transport simulations for amorphous structures of *N,N'*-dicarbazole-3,5-benzene (mCP) and 4,4'-bis(*N*-carbazolyl)-1,1'-biphenyl (CBP), which have been used as a host material for OLEDs. By explicitly considering organic molecules, we investigated the contribution of respective molecular pairs to the charge transport in amorphous thin films. The molecular-level analysis of the charge transport simulations showed that molecular pairs with large electronic couplings are not most important in charge transport processes. Charges were found to be transported effectively in the forward direction via other molecular pairs that do not have substantially large electronic couplings.

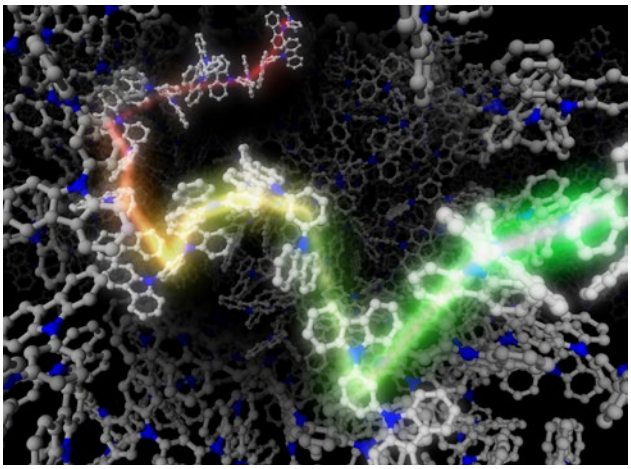


Figure 2. Image of charge transport in amorphous mCP films.