環境物質化学研究系

分子材料化学

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有機材料の機能を電子、分子レベルから理解することを目的とした基礎研究を進めています。有機合成により得た材料を用いてデバイスを創製し、優れた光・電子特性を発現させるとともに、固体核磁気共鳴法（固体NMR法）・量子化学計算による精密構造解析を行い、機能と構造の相関解明を行っています。

Development of highly efficient emitter based on quantum chemical calculations

Thermally activated delayed fluorescen ce (TADF)

Quantum chemical calculation & Synthesis & Device fabrication

Conflicting factors

Energy difference between S_1 and T_1(ΔE_{ST})

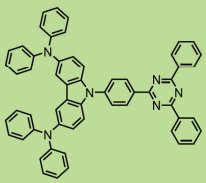
$$\Delta E_{ST} = 2\left\langle \phi_{HOMO}(x_1)\phi_{LUMO}(x_2)\left|\frac{1}{|x_2 - x_1|}\right|\phi_{HOMO}(x_2)\phi_{LUMO}(x_1)\right\rangle$$

Oscillator strength (f)

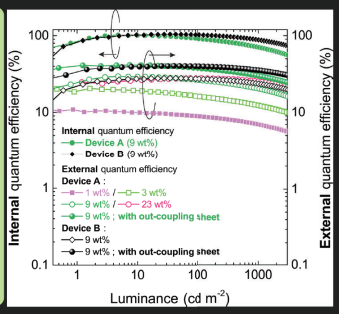
$$f \propto |\mu|^2 \qquad \mu = \langle \phi_{HOMO}(x)\,|\,-ex\,|\,\phi_{LUMO}(x)\rangle$$

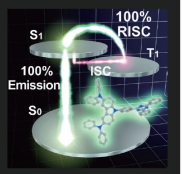
New TADF emitter

(Purely organic material)



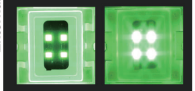
DACT-II





Without out-coupling sheet

Max. EQE: 29.6% (@ 98.8 cd A^{-1})



With out-coupling sheet

Max. EQE: 41.5%

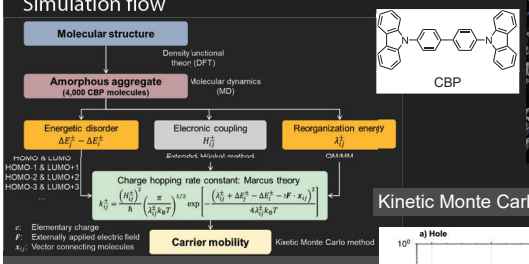
Nat. Commun., 2015, 6, 847

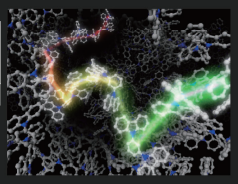
Revealing charge transport mechanism in organic amorphous solids

Charge transport in organic amorphous solids

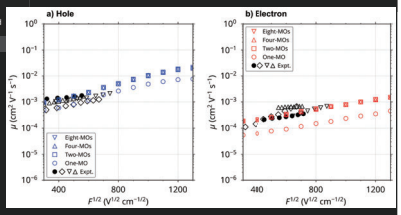
Quantum chemical calculation & Device fabrication

Simulation flow





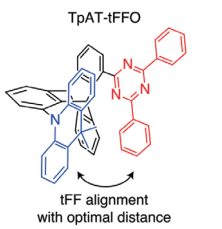
Kinetic Monte Carlo Simulations



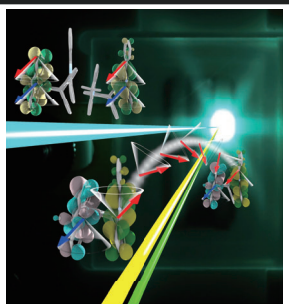
Hopping-type charge transport was simulated by explicitly considering the molecular structure.

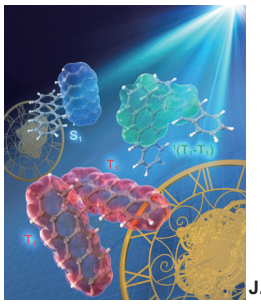
Incorporation of both $\Delta E_i^{+/-}$ & $\lambda_{aggr}^{+/-}$ Reasonably reproduce the experimental μ and ln μ ∝ $F^{1/2}$ relationship (Poole–Frenkel behavior)

Sci. Rep., 2018, 8, 13462



Nat. Photon. 2020, 14, 643





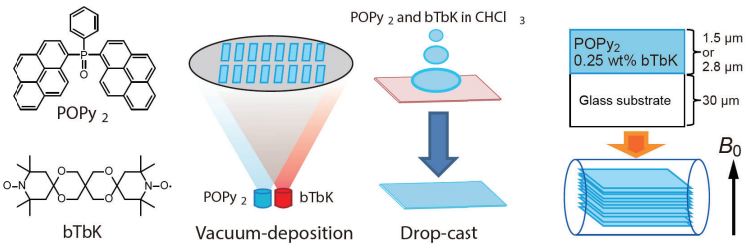
Development of singlet fission materials based on quantum chemical calculation

Decay mechanism of multi-excitonic states was revealed by considering geometry relaxation and vibronic coupling in excited states.

J. Phys. Chem. A, 2020, 124, 3641

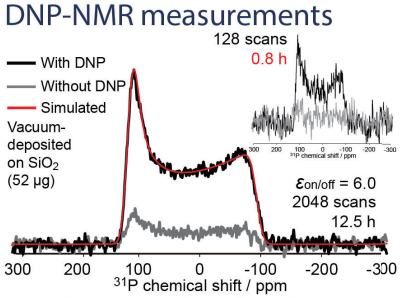
DNP-Enhanced Solid-State NMR Analysis of Molecular Orientation in Organic Thin Films

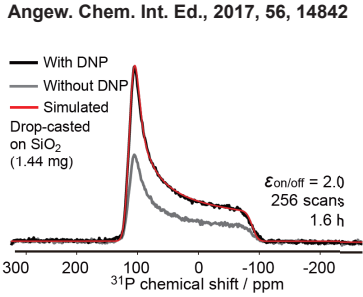
Sample preparations



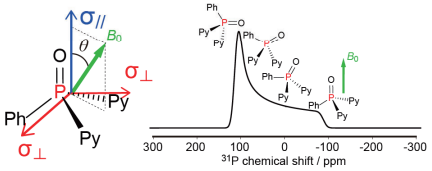
DNP-NMR measurements

Angew. Chem. Int. Ed., 2017, 56, 14842





Legendre moment expansion approach



$$p(\theta) = \sum_{n=0}^{N} \frac{2n+1}{2}\langle P_n\rangle P_n(cos\theta) \quad N = 0, 2, 4, 6, \cdots$$

$$2\langle P_0\rangle = \int_0^{\pi} p(\ell) sin\theta d\theta = 1$$

$$\langle P_n\rangle = \frac{\int_0^{\pi} p(\theta) Pn(cos\theta) sin\theta d\theta}{\int_0^{\pi} p(\theta) sin\theta d\theta}$$

Fitting results for least squares minimization

Sample	σ // (ppm)	σ⊥ (ppm)	BF (ppm)	$\langle P_0\rangle$	$\langle P_2\rangle$	$\langle P_4\rangle$	$\langle P_6\rangle$
Sublimed	114.3	-93.4	8.4	0.5	0.15	0.031	-0.0010
Drop-casted	110.1	-88.4	7.2	0.5	-0.019	0.0059	-0.0014

Distribution of molecular orientations