Integrated approach towards elucidating exciton quenching in OLEDs

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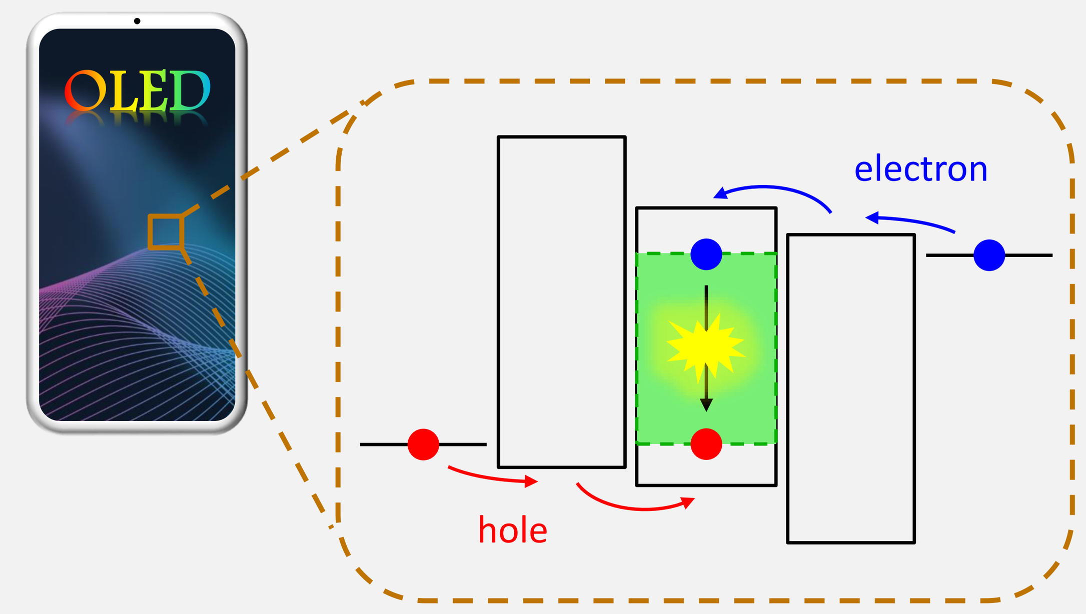
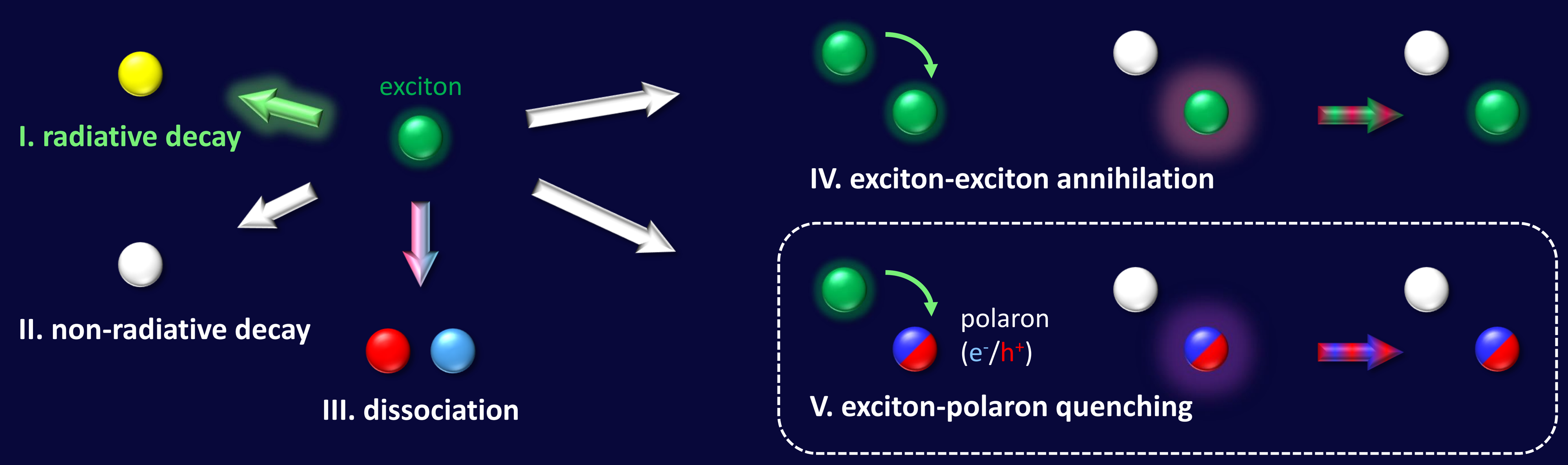
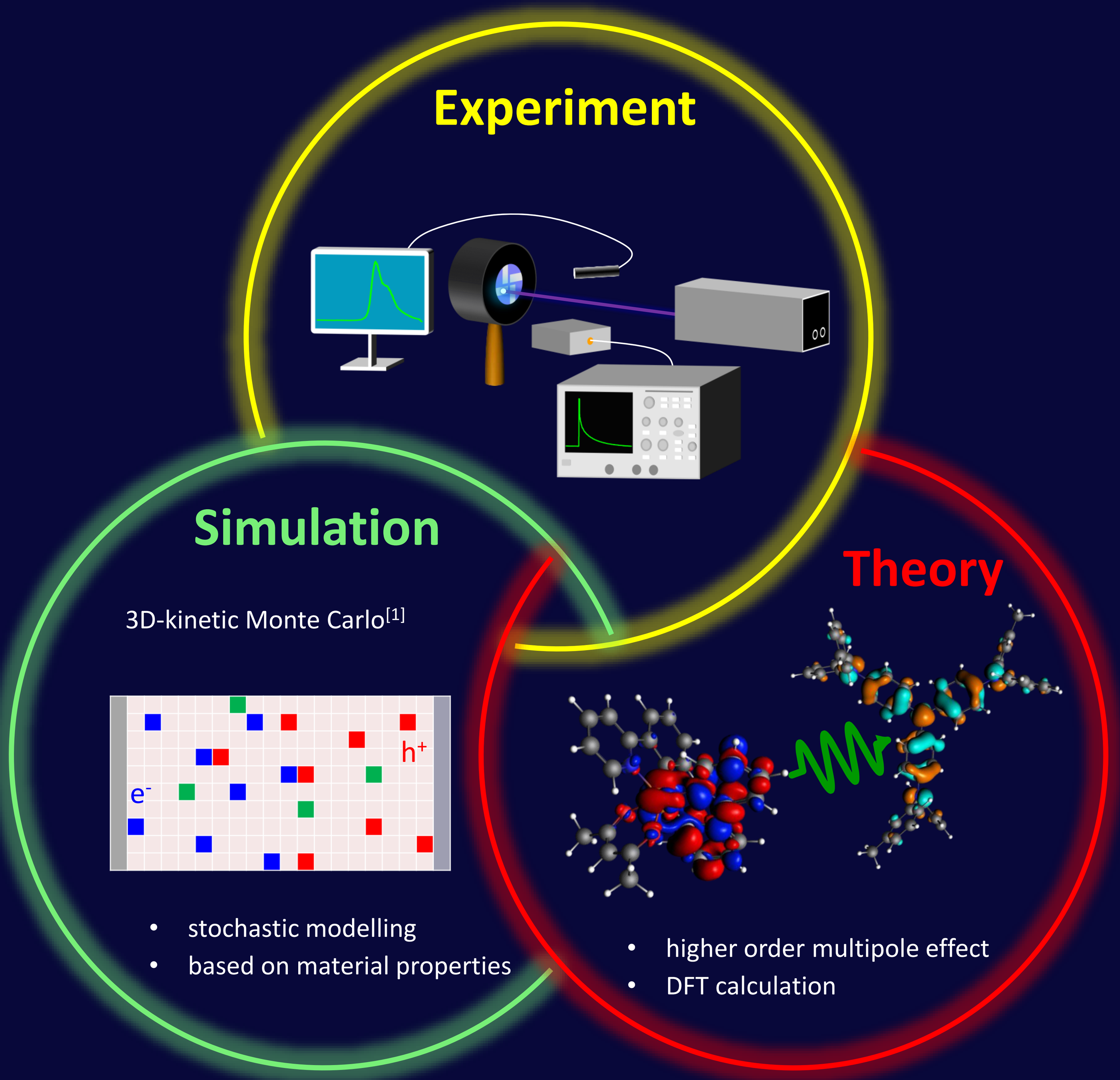
OLED structure



Exciton's pathway



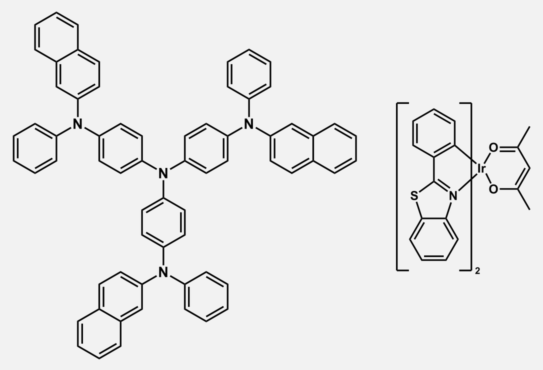
Research goal: Reveal the exciton-polaron quenching mechanisms of OLEDs

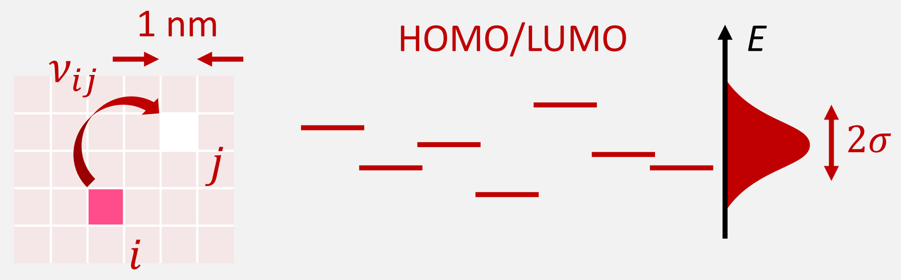


Methods[2]

Charge-transport (*J-V* measurement)

$$\nu_{ij} = \nu_1 \times \exp\left(-\frac{2R_{ij}}{\lambda}\right) \times \exp\left(\frac{-|\Delta E_{ij}| + \Delta E_{ij}}{2k_B T}\right)$$

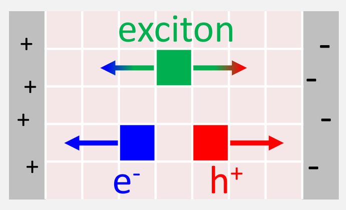




$$\mathrm{DOS} = \frac{N_{\mathrm{total}}}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(E-E_0)^2}{2\sigma^2}\right]$$

Field-induced dissociation (*E*-dependent PL measurement)

$$E_{\mathrm{binding}} = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}} + E_{\mathrm{S/T}}$$



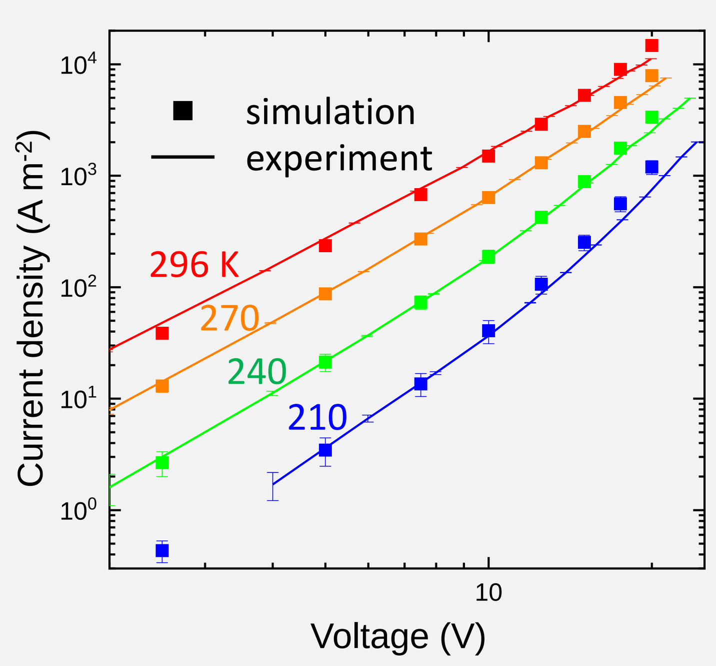
Current-induced quenching (*J*-dependent PL measurement)

$$\Gamma_{\mathrm{TPQ}} = \frac{1}{\tau}\left(\frac{R_{\mathrm{F,TPQ}}}{R}\right)^6$$

Results

Host-only (2-TNATA 200 nm)

J-V measurement



Best fit for 2-TNATA

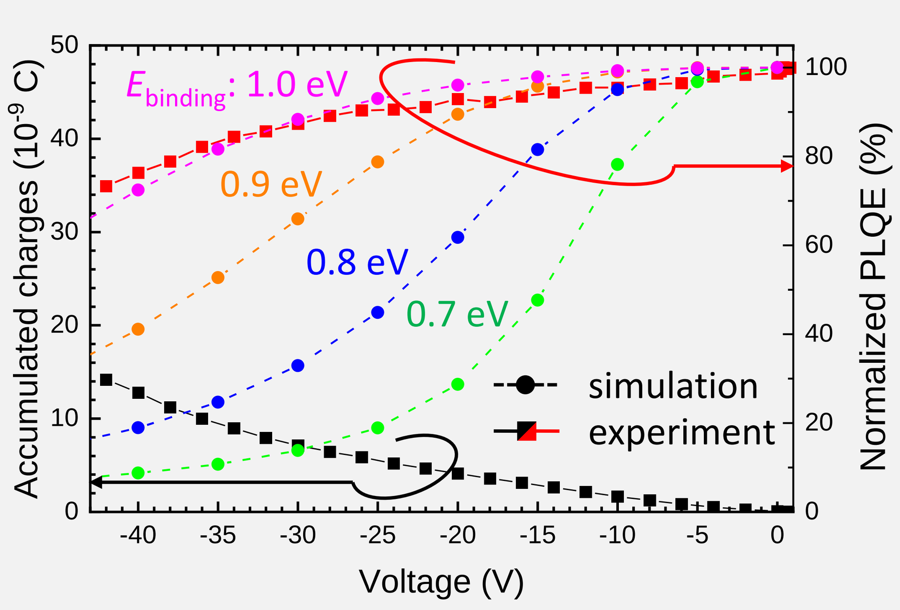
$\nu_{1,\mathrm{h}} = 9.0 \times 10^{10}\ \mathrm{s}^{-1}$

$\lambda_{\mathrm{h}} = 0.2\ \mathrm{nm}$

$\sigma_{\mathrm{HOMO}} = 0.10\ \mathrm{eV}$

Host-only (2-TNATA 200 nm)

PL measurement over electric field



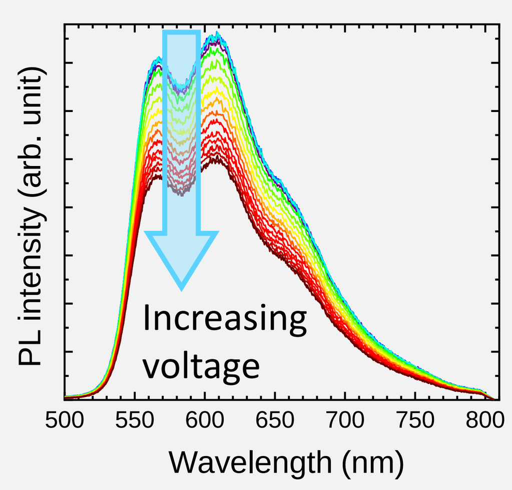
Best fit for 2-TNATA

$E_{\mathrm{binding}} = 1.0\ \mathrm{eV}$

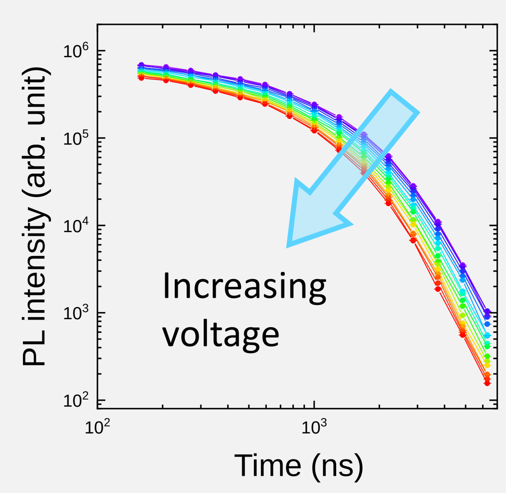
$E_{\mathrm{LUMO}} = -1.3\ \mathrm{eV}$

2-TNATA:Ir(BT)$_2$(acac) (5 wt%)

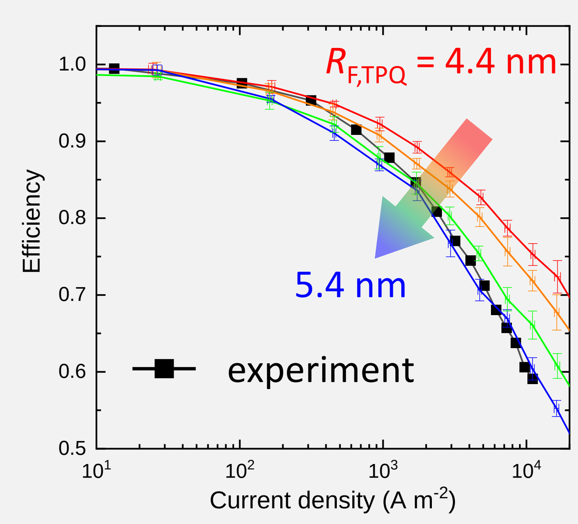
❑ PL measurement



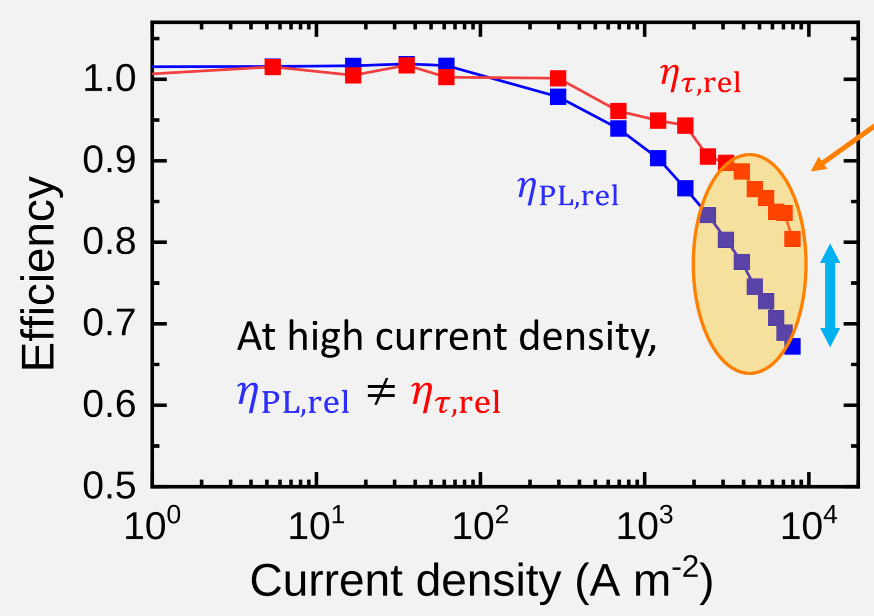
❑ TRPL measurement



❑ $\eta_{\mathrm{PL,rel}}$ simulation fit



$$\eta_{\mathrm{PL,rel}} = \frac{\int_0^\infty I_{\mathrm{total}}(\lambda, J)\mathrm{d}\lambda}{\int_0^\infty I_{\mathrm{total}}(\lambda, 0)\mathrm{d}\lambda}, \quad \eta_{\tau,\mathrm{rel}} = \frac{\tau(J)}{\tau(0)}$$



η roll-off due to TPQ

Best fit for 2-TNATA:Ir(BT)$_2$(acac)

$R_{\mathrm{F,TPQ}} = 4.4 - 5.4\ \mathrm{nm}$

Conclusions

- ➢ Optoelectronic property of 2-TNATA determined from KMC model
- ➢ Förster radius for TPQ (2-TNATA:Ir(BT)$_2$(acac)) determined

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[1] The Bumblebee KMC software is provided by SCM (https://www.scm.com)

[2] A. Ligthart *et al., Organic Electronics*, **91**, (2021) 106058.