TADF Emitter Studied by Time Resolved Near-Infrared Spectroscopy

Wiebke Haselbach[1], Matthias Jantz[1], Laura N. Kloeters[2], Thomas J.J. Müller[2], Oliver Weingart[3], Peter Gilch[1], Bárbara E.N. de Faria[1]

[1]*Institut für Physikalische Chemie II, HHU Düsseldorf, 40225 Düsseldorf, Germany;* [2] *Institut für Organische Chemie und Makromolekulare Chemie, HHU Düsseldorf, 40225 Düsseldorf, Germany;* [3] *Institut für Theoretische Chemie und Computerchemie, HHU Düsseldorf, 40225 Düsseldorf, Germany,* E-mail: nogueira@hhu.de

Fluorophores featuring thermally activated delayed fluorescence (TADF) show great potential as emitters in organic light-emitting diodes (OLEDs). These emitters convert triplet into emissive singlet excitons via reverse intersystem crossing reaching internal quantum efficiency close to 100%. Efficient TADF molecules need to exhibit singlet-triplet energy gaps of the order of the thermal energy k_BT (~ 25 meV), and high rate constants for intersystem crossing (ISC) and reverse intersystem crossing (rISC) between these states. As small gaps are encountered in charge transfer (CT) excitations, TADF emitters are commonly composed of donor and acceptor moieties. Yet, for "pure" CT states spin-orbit coupling is negligible and no ISC or rISC transitions ought to occur. As shown theoretically, spin-vibronic coupling can mediate these transitions[1]. The respective expressions contain $S_1 \rightarrow S_n$ (n=2,3,4,…) and $T_1 \rightarrow T_n$ (n=2,3,4,…) transition energies as energy denominators. The respective transition energies ought to be found in near-infrared (NIR) spectral region.

Here, we report on ongoing developments regarding NIR spectroscopy as well as first measurements of $S_1 \rightarrow S_n$ and $T_1 \rightarrow T_n$ transition energies. Experiments were carried out on a TADF emitter containing a triarylamine donor and 1,4-dicyanobenzene acceptor moiety[2]. Upon pulsed excitation the emitter exhibit NIR transitions on the nanosecond ($S_1 \rightarrow S_n$) and microsecond ($T_1 \rightarrow T_n$) timescale. Theoretical calculations predicting the transition energies and strengths are provided and compared to our experimental results.

Financial support from the Deutsche Forschungsgemeinschaft (DFG, grant 396890929/GRK 2482, "ModISC") and DFG (INST 208/704-1 FUGG) to purchase the hybrid computer cluster are gratefully acknowledged.

1. Penfold, T.J.; Gindensperger, E.; Daniel, C.; Marian, C.M.. Spin-vibronic mechanism for intersystem crossing. Chem. Rev., 118(15), 6975-7025, **2018**.

2. Sommer, G.A.; Mataranga-Popa, L.N.; Czerwieniec, R.; Hofbeck, T.; Homeier, H.H.; Müller, T.J.; Yersin, H.. Design of conformationally distorted donor–acceptor dyads showing efficient thermally activated delayed fluorescence. J. Phys. Chem. Lett., 9(13), 3692-3697, **2018**.