15th International Conference on Electroluminescence and Optoelectronic Devices

Book of abstracts and scientific program

UNIVERSITÉ
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15th International Conference on Electroluminescence and Optoelectronic Devices

May 10 – May 14, 2026
Namur – Belgium

Book of abstracts and scientific program

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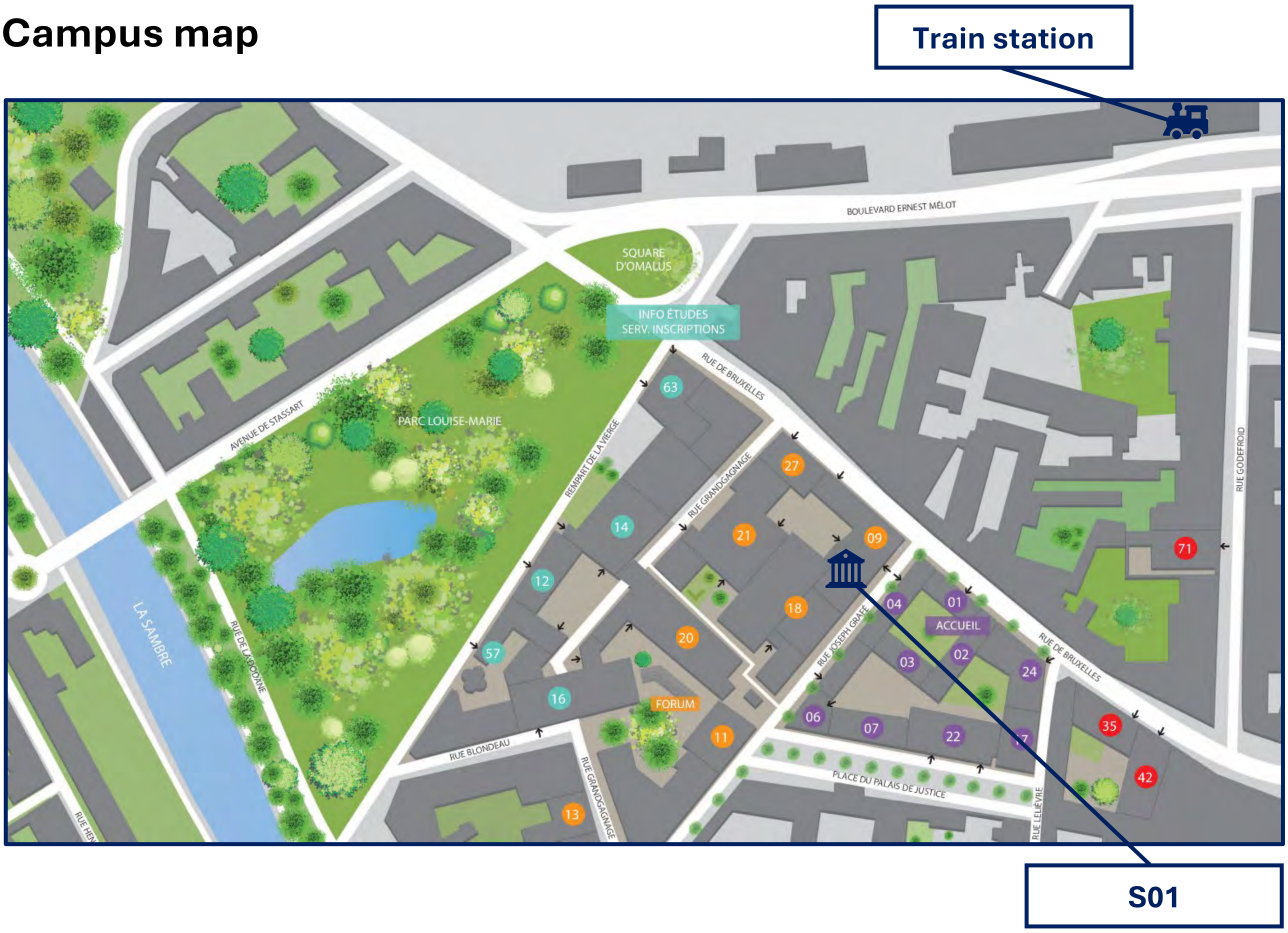
Location

The ICEL2026 conference will take place at the Science (S01 auditorium) building of the University of Namur (Faculty of Sciences, rue Joseph Grafé, 2 - 5000 Namur - Belgium).

The registration will take place at the main entrance of the Science building.

Campus map



Wi-Fi

There are two possibilities to access to the Wi-Fi during the conference:

1. Eduroam is available in the conference room and hall using your credentials from your University.
2. The unamur_events wifi is also accessible in the conference room and hall. The password for the wifi network is **g57uuoxz4w**. You can also connect to this network by scanning the following QR code.

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Organizing Committee

Conference Chairs

Prof. Benoît Champagne – University of Namur
Prof. Yoann Olivier – University of Namur

Local organizing committee

Prof. Benoît Champagne – University of Namur
Matteo Fornasarig – University of Namur
Dr. Danillo Pires Valverde – University of Namur
William Soulié – University of Namur
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Prof. Andy Monkman – Durham University
Prof. Koen Vandewal – University of Hasselt
Dr. Melissa Van Landeghem - University of Hasselt
Prof. Eli Zysman-Colman - University of St Andrews

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11:15 - 11:30	**CONTRIBUTED 3 – Rishabh Saxena** **Max Planck Institute for Polymer Research (Germany)** *“The many roles of host materials in single-layer blue OLEDs: Enabling ohmic charge injection, balanced transport, and enhanced stability”*
11:30 - 11:45	**CONTRIBUTED 4 – Christopher Wallerius** **University of Cologne (Germany)** *“Charge-transfer topology and kinetic modulation as complementary design strategies for high-efficiency TADF OLEDs”*
11:45 - 12:15	**INVITED 3 – Alexander Gillett** **Linköping University (Sweden)** *“A complete picture of rISC in MR-TADF emitters”*
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14:30 - 14:45	**CONTRIBUTED 7 – Riccardo Alessandri** **KU Leuven (Belgium)** *"Molecular simulations uncover the role of soft segments and host-guest design in stretchable TADF emitting polymers"*
14:45 - 15:15	**INVITED 5 – Cyril Poriel** **University of Rennes (France)** *"Pure hydrocarbon hosts for high performance phosphorescent OLEDs: A molecular concept for organic electronics"*
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KEYNOTE SPEAKERS

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Photokineticism: Comprehensive understanding and quantitative prediction of phenomena based on rate constants

Hironori Kaji[1]

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We are currently conducting research on OLEDs from the following aspects: 1) high-throughput development of TADF materials toward highly efficient OLEDs, 2) quantitative prediction and fundamental understanding of emission processes in OLEDs based on precise quantum chemical calculations, 3) quantitative prediction and mechanistic understanding of charge transport processes in OLEDs through multiscale simulations, and 4) NMR analysis of OLEDs.

In the course of these studies, we have recently developed a new quantum chemical calculation method based on rate constants that enables comprehensive and quantitative understanding and prediction of emission phenomena in organic molecules, consisting of multiple elementary processes. [1,2] This method allows us to understand the emission mechanisms of OLED molecules fundamentally, and also to quantitatively predict the photophysical behavior entirely without any experimental input.

We are now further extending this method, which we believe will make a significant contribution to establishing the fundamental science of exciton dynamics. Inspired by the concept of "*Kineticism"* in art, an approach that decomposes a whole process into rhythmic elements for pictorial construction, we have named this new framework "*Photokineticism*," aiming to construct an "-ism" of "kinetics" centered on "photo." In this presentation, we will introduce the concept of Photokineticism and highlight our recent progress, including the works described above.

Our method is not limited to emissive molecules in OLEDs but can be applied to a wide variety of systems. Recently, we have successfully applied it to photocatalytic systems that suppresses the aggregation of amyloid-β peptides, known to be associated with Alzheimer's disease and related disorders, while dramatically reducing side effects. [3]

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Spin management in organic molecules: From TADF to radical emitters

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We will first review recent computational advances on thermally activated delayed fluorescence (TADF) emitters, focusing on how molecular structure governs singlet–triplet energy alignment and enables efficient harvesting of triplet excitons through reverse intersystem crossing. Particular attention will be paid to the respective roles of spin–orbit coupling and hyperfine interactions in mediating spin conversion in both molecular and supramolecular architectures. We will also discuss recent evidence for antisymmetric exchange interactions in triplet exciton pairs in molecular crystals.

We will then turn to stable organic radicals as an emerging class of luminescent materials, highlighting how open-shell electronic structures enable efficient doublet emission while circumventing conventional triplet-loss mechanisms. Finally, we will discuss the broader potential of these open-shell emitters in areas such as quantum information science and photoinduced charge separation.

Spin Radical Molecular Semiconductors

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We have been working with spin-radical molecules that show high luminescence yield within the spin doublet manifold. These can be designed so that this ‘bright’ doublet exciton lies lower in energy than ‘dark’ higher spin states. These enable efficient OLED operation in the red and near-IR [1], and can be engineered to show high luminescence yield [2].

When coupled together, either intermolecularly [3] or intramolecularly [4,5] these spin radical systems show properties of Mott-Hubbard spin systems, where the lowest energy electronic excitation is a charge transfer between antiferromagnetically arranged neighbouring radical sites at the cost of the Hubbard U. This process is radiatively allowed and enables optical write and read of spin. We are exploring how these excited states can be used to assist charge photogeneration in the absence of a donor-acceptor heterojunction [3], and to engineer spin-optical interfaces that allow easy magnetic field control of luminescence [4,5].

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Metal-Emitter Interactions in Top-Emitting LEDs: From Interfacial Chemistry to Plasmon-Enabled Upconversion

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Top-emitting organic and perovskite LEDs bring metallic electrodes into intimate proximity with either readily quenched excitons or electrochemically reactive semiconductors, creating intertwined optical and chemical challenges. In this talk, I show how engineering these metal–emitter interactions transform liabilities into opportunities, improving stability, enhancing efficiency, and enabling new functionality.

In perovskite LEDs (PeLEDs), mobile halide byproducts can corrode metal contacts and drive performance loss. I will describe how mixed-polymer hole transport layers suppress triiodide transport to Au anodes, stabilizing emission under repeated operation and revealing degradation mechanisms through a newly developed Au-corrosion-based assay. In parallel, dielectric outcoupling layers reshape the microcavity and far-field emission of top-emitting PeLEDs, enhancing external quantum efficiency through controlled optical mode redistribution [1].

Rather than treating metal-induced plasmonic coupling as parasitic loss, we harness surface plasmon polaritons to drive ultralow-threshold solid-state triplet fusion upconversion [2]. This approach further enables visible-to-UV and near-infrared-to-blue upconversion in organic thin films coupled to 2D monolayer heterostructures, achieving large anti-Stokes shifts, order-of-magnitude threshold reductions, and external quantum efficiencies among the highest reported. We further demonstrate a white OLED that generates blue light from only green and red electroluminescence, offering a potential pathway around longstanding blue-emitter limitations.

Together, these results establish a simple message: metal-semiconductor interactions in top-emitting LEDs are not merely constraints to mitigate, but powerful design parameters to include.

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Strategies for accelerating RISC and their link to high-performance MR-TADF OLEDs

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In this presentation, I will discuss different MR-TADF emitter design strategies that lead to fast reverse intersystem crossing and how these translate into OLEDs showing high maximum external quantum efficiency and low efficiency roll-off.

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Plasmonic PHOLED: Enabling Next-Generation OLED Displays

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Displays incorporating organic light emitting devices (OLEDs) have proliferated due to their superior color saturation, innovative form factors and reduced power consumption compared to conventional display technologies. Plasmonic OLEDs [1] leverage the increased optical density of states of nearby plasmonically-active materials to achieve a reduction in excited state transient that reduces destabilizing excited state interactions and enables a dramatic increase in device stability. Utilizing a nanoparticle-based plasmon outcoupling scheme, plasmon energy can be efficiently converted into light. This fundamentally different operating paradigm for OLEDs enables a higher outcoupling efficiency limit, along with the ability to fine tune the emission profile and color saturation. Leveraging a device-based approach to solving conventional OLED challenges, plasmonic OLED provides a range of tools to enable next-generation OLED displays, including wide color gamut, improved power efficiency, reduced efficiency roll-off and more.

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Fluorescence Efficiency Regulation in Conjugated Organic Materials

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Conjugated organic chromophores have found immense interest in current materials research, and rapid progress has been seen over the past years. In any case, the quest for sustainable research demands pre-synthesis tailor-made targeted design beyond experimental (and computational) trial-and-error strategies. This can only be achieved by a thorough understanding of the underlying photophysical process combined with spectroscopic and computational techniques. [1]

A central figure of merit is the fluorescence quantum yield FF of the compounds, which is decided by the competition of radiative vs. nonradiative processes. [1] This is not only key for obvious applications like OLEDs, OLETs, lasing, sensing, or bio-imaging, but also e.g. for photovoltaics.

In solution, nonradiative decay is mainly driven by internal conversion (IC; and subsequent vibrational relaxation; VR); this is frequently tackled via a 'Fermi's Golden Rule' (FGR) approach.[1] However, in the last years, it has become increasingly evident that FGR may break down both in a quantitative as well as in a qualitative manner, in particular for systems with very effective IC. This was especially shown for compound families which establish an 'inverted energy gap law', contrasting the prediction of FGR in a simple view. Instead, this can be well understood in the framework of conical intersections (CIs), which provides an accurate description of IC. [2,3]

In molecular solids, IC becomes a minor pathway in most cases, as the access to the CI often involves large amplitude motions which are effectively blocked in rigid environments; [2,3] this gives subsequently rise to 'Solid State Luminescence Enhancement' (SLE). [1,2] On the other hand, examples of active CIs in solid state samples have been identified, due to the absence of large amplitude motions on the path to the CI, [3] so that fluorescence quenching may persist across solution and molecular solids.

Nevertheless, the most crucial quenching pathway in molecular solids is trapping (at surfaces/interfaces), which becomes notorious in polycrystalline samples, while single crystals of the same materials are commonly highly luminescent. [1] The central role of trapping is largely underestimated in the community, and strategies how to achieve highly luminescent polycrystalline samples are therefore addressed.

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A complete picture of rISC in MR-TADF emitters

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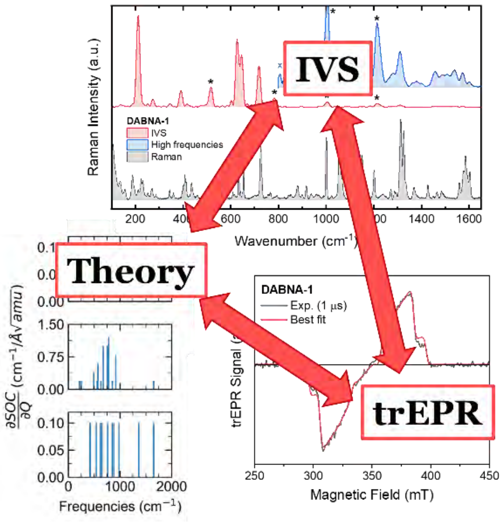
Multiple resonance thermally-activated delayed fluorescence (MR-TADF) materials have the potential to revolutionise OLEDs by combining desirable narrowband deep blue emission with the efficient upconversion of dark spin-triplet excited states into bright singlets via a reverse intersystem crossing (rISC) process. However, current heavy atom-free MR-TADF materials show rISC rates orders of magnitude slower than observed in classic donor-acceptor TADF emitters, leading to extreme efficiency roll-off when used as the primary emitter in OLED devices. Consequently, MR-TADFs are generally limited to use as the terminal emitter in a ‘hyperfluorescence’-type scheme, which does not exploit their TADF properties.

To intelligently design new MR-TADF emitters with faster rISC rates for increased utility in OLED devices, it is necessary to develop a deeper mechanistic understanding of the ISC processes. However, previous theoretical studies provide conflicting views on how rISC proceeds, and experimental validations of the proposed mechanisms are distinctly lacking. In our work, we combine ultrafast optical and magnetic resonance spectroscopies with quantum-chemical calculations to reveal a complete and self-consistent picture of the ISC processes in model MR-TADF materials based on the popular ‘DABNA’ boron-nitrogen molecular motif. We provide unprecedented detail on the role of vibronic coupling in MR-TADFs, including explicitly identifying which vibrational modes are driving the ISC process and how they populate the three distinct triplet sublevels. These insights will enable the chemical design of new MR-TADF materials that directly harness vibrational couplings for faster rISC and better blue OLED performance.



A rigid xanthene–anthracene-based scaffold exhibiting ultra deep blue emission: multifunctional material as emitter and host for blue OLEDs

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Ultra-deep blue fluorescent emitters with Commission Internationale de L'Eclairage (CIE_y) < 0.08 are still in demand for achieving vibrant full-color displays. Herein, we have synthesized xanthene–anthracene-based 14-(4-(10-phenylanthracen-9-yl)phenyl)-14*H*-dibenzo[*a*,*j*]xanthene (PhAn-Xn), in which xanthene and anthracene are linked by an orthogonal phenyl bridge to prevent aggregation-induced quenching. PhAn-Xn exhibits an emission maximum at 430 nm, with a full width at half maximum (FWHM) of 48 nm, and a prompt lifetime of 0.7 ns. Using neat PhAn-Xn as the emitting material, an organic light-emitting diode (OLED) device was fabricated, achieving a maximum external quantum efficiency ($\mathrm{EQE}_{\mathrm{max}}$) of 4.2%, with CIE coordinates of (0.16, 0.06) at 8 V, following European Broadcasting Union standards, and a maximum luminance (L_{max}) of 4110 cd m^{-2} (at 16.5 V). The device maintains an EQE of 4.0% at 1000 cd m^{-2}, retaining 95% of its maximum efficiency. PhAn-Xn, which exhibits superior charge transport properties to those of the widely used blue host bis[2-(diphenylphosphino)phenyl]ether oxide, was used as the host material in OLED devices employing the well-known blue dopant 4,4′-bis(9-ethyl-3-carbazovinylene)-1,1′-biphenyl (BCzVBi). The PhAn-Xn-based device exhibits an electroluminescence maximum at 455 nm, consistent with the photoluminescence maximum of BCzVBi. An $\mathrm{EQE}_{\mathrm{max}}$ of 6.5% was achieved, along with a maximum brightness of 41 557 cd m^{-2} (at 16 V). The device maintains an EQE of 6.4%, retaining 98% of its maximum efficiency at 1000 cd m^{-2}. These results indicate that PhAn-Xn has multifunctionality and can serve as either an emitter or a host for deep blue OLEDs.

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Title Pure Hydrocarbon Hosts for High Performance Phosphorescent OLEDs: A molecular concept for Organic Electronics

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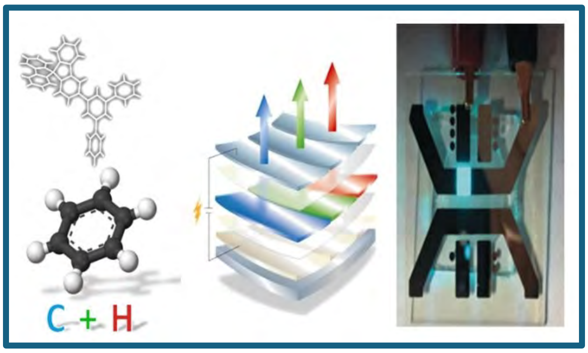
In the Organic Electronic technologies, Phosphorescent Organic Light-Emitting Diodes (PhOLEDs) are the 2nd generation of OLEDs and have encountered a fantastic development. A PhOLED uses a Host-Guest EMitting Layer (EML), which consists in a Triplet Emitter (Guest) disperse into an appropriate organic semi-conductor (Host). During the past two decades, intense research has been focused on developing high-efficiency host materials. Many molecular design strategies have been developed to gather within a single host all the required properties to fit with a phosphor within a device. All these molecular engineering works of host materials have undoubtedly driven the field. The most efficient are the bipolar hosts constructed on a ‘Donor/Acceptor’ design. This design is widely known and consists to judiciously assemble electron-rich and electron-poor fragments to fit with the required properties. The best materials achieved over 35% external quantum efficiency in PhOLEDs. However, the fragile C–N, C–P and C–S bonds of such heteroatoms based hosts are involved in the OLED instability. Thus, as the instability of OLEDs is one of the most important problem to address at the current stage of development, developing new generations of hosts, without heteroatoms (called PHC for Pure HydroCarbons) has appeared as an important challenge. However, reaching high performance PhOLEDs with hosts free of heteroatoms is a real challenge. In this talk, will be presented our advances, which have shown that PHC hosts can now overpassed heteroatoms-based hosts [1-3]. The design strategies developed will be analysed to show their impact on the electronic properties and the final device performance.



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Spectroscopic analysis of inversion of the lowest singlet and triplet energy states in the heptazine HzTFEX2.

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We will present evidence that HzTFEX2 [1] has a long lived phosphorescence emission from the T1 state, with a 0-0 peak at 425 nm and band shape nearly identical to monomer fluorescence, giving an inverted singlet triplet gap of 110±20 meV in frozen toluene at 2µM. It is important that the full conditions of the measurement are given as these energies are sensitivity to environment and dimer/aggregate content. Importantly we observe relatively strong anti-Kasha S2 emission indicating slow internal conversion from S2 to S1. The S2 S1 energy gap is large, 0.85 eV, and as the HzTFEX2 is rigid, there is not crossing of the S2 and S1 energy surfaces and vibronic coupling is weak. Single crystals measurements indicate S2 and S1 orbitals are orthogonal. Phosphorescence is only observed when we excite into the S2 state, and thus propose that ISC/rISC predominantly occurs in the S2 state. Exciting into S1 yields no measurable phosphorescence so endothermic S1¨T1 rISC is suppressed because of weak vibronic coupling.

Dimers dominate most the observed photophysics, including their role in monomer excited state quenching. In dilute frozen 2-MeTHF solution, having a very low dimer content, we estimate that the PLQY reaches near unity because collisional quenching is supressed. This points to negligible excited state loss by internal conversion and non-radiative decay through vibrational channels, supporting the notion that vibronic coupling in HzTFEX2 is highly ineffective, especially in the S1 and T1 manifolds. This does support the idea that inversion requires highly decoupled S1 and T1 states.

We observe hipsochromic solvatochromic effects in HzTFEX2, even though the S1 state is of ππ* character. We resolve this issue through comparison to previous work on molecules containing sp2 hybridised nitrogen atoms within a conjugated structure, where the ground state is strongly localised due to the participation of the localised nitrogen lone pair electrons in the π orbitals, but the excited state is a delocalised π* state. In this situation the transition energy is sensitive to solvent polarizability, thus MCH gives the largest effective red shift of the transition and MeCN the least polarizable solvent the smallest. In this picture we can understand the excited delocalised electron being highly decoupled from its localised hole leading to very weak electron hole interactions, i.e. small or negative electron exchange energies.

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Understanding Efficiency Roll-off in TADF OLEDs

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Thermally activated delayed fluorescence is an attractive way of harvesting triplets to make efficient OLEDs. However, many TADF OLEDs suffer a substantial decrease in efficiency (roll-off) as the brightness is increased. We have developed measurements of photoluminescence of operating OLEDs, and use them to provide new insight into the causes of efficiency roll-off. We find that it arises from the interplay of singlet-triplet annihilation, singlet-polaron annihilation and triplet-polaron annihilation. We measure the bimolecular rate constants for these processes and quantify the contribution of each process to efficiency roll-off. We discuss the implications for molecular design to maintain high efficiency at high brightness.

A cautionary tale on putative negative singlet triplet gap materials

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Materials possessing a negative singlet-triplet gap, so-called INVEST-compounds, seem to offer a route to efficient OLEDs. They are therefore investigated intensively, both by experiment and theory. There are, however, a number of pitfalls,[1] notably for spectroscopic investigations. In this talk I want to address some of the associated issues, exemplified for pentaazaphenalene derivatives.

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Radical light-emitting devices and magnetic field effects

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The spin of ground and excited levels in molecular materials dictates the exciton mechanisms for any photonic, optoelectronic and quantum technology applications. Recent interest in organic radicals containing unpaired electrons has emerged from the design of new materials that undergo efficient light absorption and emission from transitions between doublet spin (S = 1/2) ground and excited levels. I will present our work on radicals in light-emitting devices: showing opportunities for energy upconversion and magnetic field effects that could enable future technology platforms.

Designing Protein Materials for Photon Conversion

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The development of sustainable optoelectronics using photon conversion with fluorescent protein (FP) materials is a new frontier.[1, 2] The major challenge is designing and stabilizing these biogenic materials for integration into energy conversion devices. Herein, we will discuss strategies, challenges, and opportunities for redesigning proteins using the following approaches: i) protein engineering, such as FP-Ferritin cages [3] and sequence ancestral reconstruction [4, 5]; ii) FP-polymer decoration, such as Pegylation [6], and FP-polymer encapsulation in hydrophobic polymers [7,8]. These strategies have enabled us to redesign proteins to be more stable in organic solvents and hydrophobic polymers while maintaining their excellent emission features. We will present myriad proof-of-concept applications for photon manipulation in lighting systems [3–6] and photovoltaic systems [7], as well as for photon-to-heat conversion in photothermoelectrics [8].

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Organic Semiconductor Devices for Light-Based Biomedical Applications: From Optogenetics to Wearables

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Light-based biomedical sensing and therapy offer precise, timely, and contactless approaches to applications ranging from neuronal stimulation via optogenetics to sensing cellular activity through functional fluorescence and monitoring health signals with wearable devices. Organic semiconductors are uniquely suited for these applications due to their tuneable material properties, mechanical flexibility, and ability to be patterned at microscopic scales.

In this work, I will present the development of organic light-emitting diodes (OLEDs) and organic photodiodes (OPDs) as light sources and sensors for biomedical applications. The OLEDs are specifically designed to achieve high power output, with angular and spectral emission properties optimized for application needs. These devices are fabricated on flexible substrates, patterned at sub-millimetre scales, and demonstrated in optogenetics and fluorescence imaging. Additionally, I will showcase flexible OPDs for photoplethysmography under ambient light conditions and underwater, highlighting their versatility and robustness.

Half light, half exciton: Putting polaritons to work in OLEDs, filters and lasers

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Strong exciton-photon coupling in organic microcavities gives rise to exciton-polaritons — hybrid quasiparticles that inherit properties from both light and matter and open new design space for organic photonic devices. This talk gives an overview of how my group is putting polaritons to practical use across three device families.In OLEDs, microcavity designs offer a route to narrowband, colour-pure emission but conventionally come at the cost of strong angular colour shifts — a fundamental obstacle to meeting the BT.2020 display standard. The flat dispersion of the lower polariton branch in the strong coupling regime can largely overcome this trade-off. We will show how this concept, recently extended to high-efficiency TADF emitters via an assistant strong coupling layer, yields green polariton OLEDs combining a spectral width of 24 nm, minimal angular colour shift, and EQE exceeding 20% (Fig. 1) [1]. We will also discuss what currently limits efficiency in these devices and what the path forward looks like, including to access the entire visible and parts of the NIR spectrum.The same physics that stabilises colour across angles in OLEDs can be used to engineer thin-film optical filters with angle-independent pass and stop bands — a capability conventional interference filters cannot offer. We will illustrate how this opens new opportunities in biosensing and imaging [2]. Finally, in organic lasers, we find that engineering the confinement of polaritons yields record-low lasing thresholds and brings the prospect of metallic-mirror and ultimately electrically driven laser diodes within reach. Controlled morphology in liquid-crystalline polymer cavities provides one route to polariton confinement [3]; a more deterministic approach uses evaporation through ultra-thin shadow masks to define isolated organic gain regions down to 5 µm in diameter, reducing lasing threshold fluence by more than an order of magnitude and revealing discrete transverse modes characteristic of strong lateral confinement.

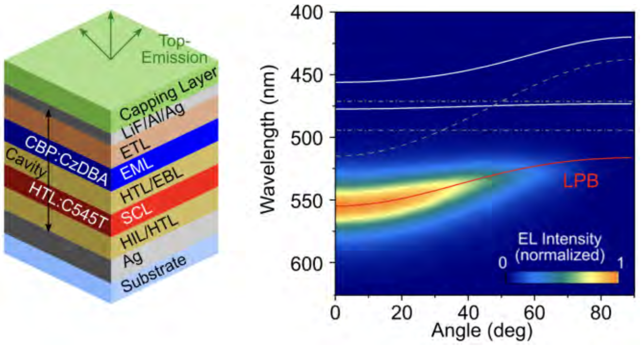

Fig. 1: Architecture of top-emitting TADF polariton OLED with an assistant strong coupling layer (SCL) within the hole transport layer (HTL, left). Angle-resolved electroluminescence showing narrowband, angle-stable emission from lower polariton branch (LPB, right).

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Chiral Conjugated systems for circularly polarised light-emitting diodes

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Conjugated chiral materials can emit circularly-polarised (CP) light within thin films and optoelectronic devices. CP-light is relevant to a range of technologies, including displays, optical communication, and emerging quantum information. Chiral light-emitting polymers have gained increasing attention due to their capability to combine strong chiroptical responses with the optoelectronic characteristics typical of organic conjugated materials, making them attractive for circularly polarised organic light-emitting diodes (CP-OLEDs).

Although circularly polarised electroluminescence can be achieved from intrinsically chiral organic chromophores, chiral polymers and polymer-based thin films can overcome several intrinsic limitations of small molecules: the magnitude of the chiroptical response can be amplified to achieve dissymmetry factors that are unusually large for organic emitters. Blending chiral additives, such as aza[6]-helicene, into conjugated polymer thin films has proven to be an effective route to high-performance CP-OLEDs, enabling high efficiencies alongside strong CP-light emission. Notably, device studies revealed behaviours that could not be explained by treating the emissive layer as a conventional chiral emitter [1].

This talk will give an overview of how charge mobility and charge carrier flow direction have a crucial role in controlling the magnitude and sign of CP-light, together with the role of the chiral additive. We will demonstrate how manipulating and managing the flow of charge carriers allows for the electrical control of CP-Light emission properties in a chiral light-emitting polymer, achieved without changing the intrinsic chirality of the film or the employed device architecture. This approach offers a route toward CP-OLEDs where polarisation characteristics can be tuned and optimised through device-relevant parameters and not solely relying on the chemical design of the emitters [2]. Moreover, we will also showcase the potential of amplifying the dissymmetry of conventional chiral emitters through energy transfer when combined with a chiral polymer host, and the application of these concepts to CP-OLEDs [3].

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Printing Perovskite Light Emitting Diodes: From Combinatorial Materials Development to Large Area Devices

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Inkjet printing has evolved from a flexible patterning method into a digital manufacturing platform capable of linking combinatorial materials development, device design, and scalable fabrication for emerging optoelectronic technologies. This contribution discusses how programmable inkjet deposition enables accelerated exploration of metal halide perovskite compositions and device architectures, allowing materials optimization and functional realization within a unified workflow.

By exploiting spatially resolved deposition and solvent mediated layer interaction, sequential printing strategies enable localized recrystallization and compositional redistribution in mixed halide systems. Such approaches provide a combinatorial pathway to tune bandgap and emission characteristics directly at the device level, demonstrated through bicolour perovskite LEDs integrating green and red emissive regions with feature sizes down to the sub millimetre scale and active areas extending to 1600 mm². Beyond spectral engineering, process innovations required for scale transition are addressed. Controlled crystallization using gas flow assisted vacuum drying enables homogeneous large area emissive layers suitable for device upscaling.

These developments illustrate how digital printing methodologies bridge high throughput materials exploration with manufacturable device architectures, highlighting a pathway toward spatially programmable light sources and integrated optoelectronic systems based on solution processed semiconductors.

Organic photon energy up-conversion devices

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The conversion of low energy into higher energy photons provides an attractive opportunity to improve solar energy technologies. Several types of thin film materials which can transform two or more low energy excited states into a higher energy one, have been previously developed. Due to the non-linear nature of such optical processes, up-conversion is most efficient at high light intensities, typically well above sunlight intensities (100 mW/cm^2). Here, we propose a stacked diode approach relying on novel, low-cost organic- semiconductor materials. The thin-film stack comprises a series of organic NIR photovoltaic stacks, providing sufficient photovoltage to drive an organic light-emitting layer deposited on top. We combine state-of-the-art, vacuum-processable absorbing and emitting systems with careful, simulation-assisted stack engineering. Converting photons from NIR (≤835 nm) to green (530 nm), the stack achieves an external upconversion efficiency (EUE) of 1.9%. Importantly, the EUE stays constant over more than 3 orders of magnitude in intensity, down to less than 1 mW/cm^2. This presentation will focus on efficiency limiting processes within such layer stacks, efficiency limits as well as the potential of this approach for photovoltaic and photocatalytic conversion.

Understanding the Role of Molecular Conformation and Spin Orbit Coupling in Intersystem Crossing of TADF Emitters

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In my talk I will discuss our research toward developing emitters for organic LEDs (OLEDs) with two-coordinate carbene-metal-amide (cMa, M = Cu(I) and Au(I)) complexes.[1, 2] Our efforts have been aimed at achieving very short lifetimes (and high F_{PL}).[3, 4] The cMa complexes studied here emit via thermally assisted delayed fluorescence (TADF) and the TADF lifetime are tied directly to the S_1 decay rate (k_{S1}) and the equilibrium constant for $T_1 \rightleftarrows S_1$ (K_{eq}) and K_{eq} is tied to the energy difference between S_1 and T_1 (ΔE_{ST}).[5] Achieving fast phosphorescence involved designing cMa complexes with small ΔE_{ST} (20-40 meV) while maintaining a k_{S1} in the 10^8 s^{-1} regime. I will discuss how ligand and metal ion choices impact these parameters and the application to OLEDs.

I will also explore the role of spin–orbit coupling (SOC) in facilitating intersystem crossing (ISC) in cMa complexes. Prior studies have shown that ISC rates in these systems span a wide range (10^9-10^{11} s^{-1}).[1] However, the precise contribution of SOC to ISC, and its interplay with TADF, is not well understood. Using a combination of transient absorption spectroscopy, lifetime measurements, and theoretical modeling, we investigate how structural modifications in cMa influences SOC constants (SOCCs). Through Arrhenius and Marcus–Hush theories, we experimentally determined that substituting Cu with Au increases the SOCC from ~2 cm^{-1} to ~7 cm^{-1}, respectively, in agreement with the enhanced ISC rates. Further modifications to the ligands also lead to notable changes in SOCC values. Initial modeling studies suggest that the SOC is greatest for dihedral angles between the carbene and amide ligands near 45°. I will tie these SOC studies back to the observed photophysical properties of both long and short lived cMa complexes. These studies are expected to impact our understanding of organic TADF materials as well.

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Molecular Vibrations, Intermolecular Interactions, and “Heavy” Atoms: Tools to Explore and Improve Organic Materials for Light-Emission Applications

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The advantages and limitations of organic materials originate largely from structural effects, tunable chemical bonding, and intermolecular interactions, which provide and control flexibility of (supra)molecular fragments. In particular, molecular vibrations emerge as a crucial yet underexplored factor governing the performance of organic materials and their heavy-atom derivatives, especially in condensed media.

This talk will address the role of molecular vibrations and intermolecular contacts as both a challenge and an opportunity in understanding and optimizing light emission in functional organic materials for OLEDs, scintillation, and temperature- and pressure-sensing applications. Specific examples will include organic emitters and photosensitizers showing thermally activated delayed fluorescence (TADF) and their derivatives bearing “heavy” atoms such as Cl, S, Br, I [1,2,3]. We will discuss why vibrations involving these atoms play a decisive role in determining photophysical properties, including light emission, photostability and electronic transitions with the change of spin. Hopefully, establishing correlations between experimental light-emission performance, photophysical behavior, and computational analysis brings us a step closer to vibrational materials engineering.

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Recent Advances in Boron-based MR-TADF Materials

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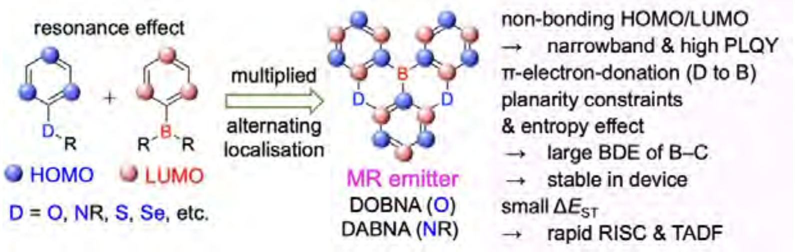
Organic light-emitting diodes (OLEDs) have become a central technology for modern displays, yet further improvements in color purity, efficiency, and operational stability remain critical challenges.[1,2] Thermally activated delayed fluorescence (TADF) materials enable near-unity internal quantum efficiency by harvesting both singlet and triplet excitons without precious metals,[3] but conventional donor–acceptor TADF molecules typically suffer from broad emission spectra due to their charge-transfer character. Such broad spectra limit color purity and necessitate additional optical components, reducing overall efficiency. The introduction of multiple-resonance (MR) TADF materials based on boron and nitrogen doped polycyclic frameworks provided a fundamentally different design paradigm. [4,5] In MR-TADF emitters, alternating electron-donating and electron-accepting atoms localize the HOMO and LUMO on different carbon atoms within the same rigid aromatic framework. This unique electronic structure simultaneously yields a small singlet–triplet energy gap and strongly suppressed vibronic coupling, resulting in intrinsically narrowband TADF. Since the first report of MR emitters, extensive efforts have been devoted to extending their emission color range and improving device performance. Despite this progress, two key issues remain unresolved. First, theoretical studies predict that π-extension of MR frameworks can enhance oscillator strength while maintaining small ΔE_{ST}, but practical realization has been limited by severe synthetic challenges, especially in controlling regioselective multiple borylation. Second, while bathochromic shifts are relatively easy to achieve, general strategies for hypsochromic tuning toward deep blue emission without degrading radiative rates or device stability are scarce. Addressing these challenges requires synthetic methodologies that directly link molecular design to photophysical and device-level requirements. In this contribution, we present recent advances from our group that tackle both issues through boron chemistry. [6-8]



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Design of Coinage Metal Emitters for Stable OLEDs and Nonlinear Photonics

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Two-coordinate coinage metal complexes with linear geometry L–M–X (L = carbene and X = anionic ligand, M = copper, silver or gold) have recently emerged as a new class of strongly photoemissive materials – Carbene Metal Amides [1]. We will discuss the advances in CMA molecular design to cover the full visible spectrum and near-IR region (up to 850 nm). Advanced deep-blue gold CMA emitters will be demonstrated to have radiative rates approaching 10^7 s^{-1} [2 - 4]. CMA OLEDs with significantly improved device lifetimes, for instance, the red CMA OLED with LT95 reaching 195 h @1000 cd m^{-2}, will be presented to demonstrate the promising molecular design concepts and the applied potential of the new CMA materials. A comprehensive comparison across various classes of emitters will be based on the bond dissociation energies of the metal–ligand bond and on intra- and intermolecular contacts in the CMA emitter, to demonstrate molecular designs that lead to the best photophysical and OLED performance. For instance, the role of strong agostic and weak anagostic C–H···M intramolecular interactions will be correlated with non-radiative events, as supported by gas-phase photoluminescence [5] to highlight the impact on the photophysics and future molecular design. CMA molecular design towards bright fluorescence, phosphorescence, TADF, and energy-transfer OLEDs will be covered, including the latest results on host-free CMA OLEDs and proof-of-principle anti-Kasha electroluminescence with narrowband emission (FWHM 26 nm). The first CMA material will be demonstrated to exhibit enhanced two-photon absorption (2PA cross-section up to 105 GM) and bright red 2P-TADF with excellent photostability, encouraging further CMA exploration for future applications that require third-order nonlinear optical properties[6].

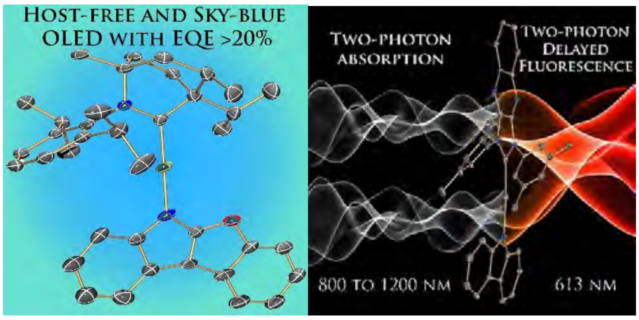

Figure 1. Examples of the CMA for host free (left) and stable red OLED (right) with a two-photon TADF.

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Determination of frontier orbital energies of disordered organic semiconductors for OLED applications

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The functioning of organic light-emitting diodes (OLEDs) depends sensitively on the frontier orbital (HOMO and LUMO) energies of the disordered organic semiconductors that are contained in the layer stack. Sufficiently precise modelling that can guide the design of more efficient OLEDs, for example using kinetic Monte Carlo (KMC) simulations, requires in general that these energies are known with a relative uncertainty that is smaller than 0.1 eV. Here, three recent developments that should help to realize this goal are presented. A first development is the use of quantum-chemical simulations, starting with simulations of the thin film morphology, as a tool to correct the values of HOMO energies that follow from analyses of Ultraviolet Photoelectron Spectroscopy (UPS) or Photoelectron Yield Spectroscopy (PHYS), and the LUMO energies that follow from (Low Energy) Inverse Photoelectron Spectroscopy (IPES/LEIPS) for various material-specific effects. These can introduce significant differences between the results from commonly used analysis methods and the actual bulk-averaged adiabatic HOMO or LUMO energies [1]. In many studies, the LUMO energy of organic semiconductors is estimated by adding the optical gap energy to the HOMO energy that is obtained from (for example) UPS. However, such a approach neglects the sizeable exciton binding energy, which for small-molecule materials can be around 1.0 eV or even larger. In the talk, a recently developed methodology is discussed within which the exciton binding energy is obtained from field-induced dissociation (FID) experiments that are analyzed using KMC simulations. This method has been applied to fluorescent [2], phosphorescent (Ir-based) and TADF emitters. A recently developed third method for obtaining frontier orbital energies is based on a large-data-base analysis of the peak energy of the photoluminescence from exciplexes in 1:1 donor:acceptor films [3]. Use is made of the high level of redundancy that is available from published data, combined with additional original work of our group, which shows that exciplex peak energies can be predicted with accuracies of about ±0.09 eV (±2σ uncertainty interval) when using frontier orbital energies that are obtained from a least-squares fit of the data and assuming a fixed (system independent) effective exciplex binding energy of ~1.0 eV. This effective binding energy can be rationalized by adding to the adiabatic exciplex binding energy of about 0.4-0.5 eV additional contributions due to diffusion-induced relaxation, exciplex-vibron coupling and a Stokes shift. So far, this approach has yielded a database of the HOMO energies of about 150 donor materials and the LUMO energies of about 180 acceptor materials. The talk will be concluded by addressing the question to what extent the view on the frontier orbital energies that is obtained from these various methods is consistent.

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CONTRIBUTED SPEAKERS

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Singlet–triplet gaps for evaluating thermally activated delayed fluorescence: which one is the (b)E_{ST}?

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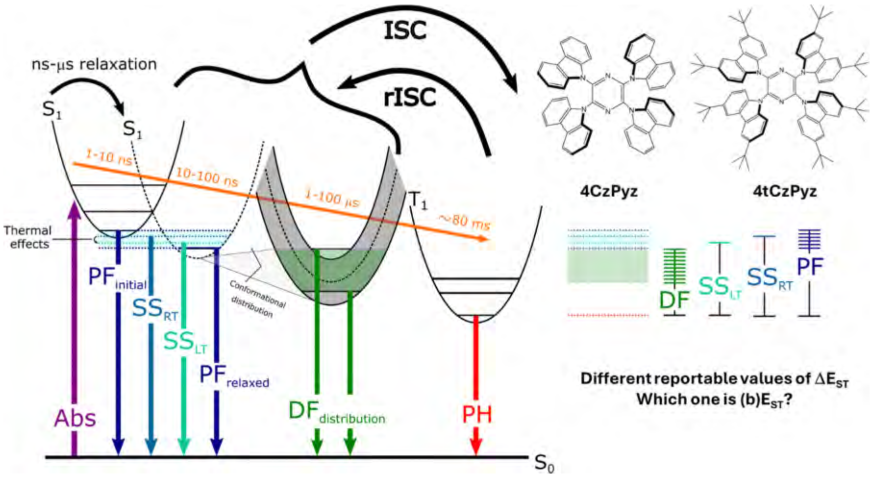

The singlet–triplet energy gap (ΔE_{ST}) serves as a central screening parameter for new thermally activated delayed fluorescence (TADF) materials, and is a valuable indicator of eventual OLED performance.[1] Surprisingly though, various measurement methodologies and reporting standards for ΔE_{ST} persist across the research community. Here we employ **4CzPyz** and **4tCzPyz** as model systems, and correlate their different possible ΔE_{ST} values with their reverse intersystem crossing (rISC) kinetics in films of common and device-relevant hosts. By comparing ΔE_{ST} values with emission decay kinetics and device roll-off performance for these two materials, we propose that the steady-state room-temperature photoluminescence onset should be used to determine E(S_1), although even this should only be taken as an indicator. Instead it becomes clear that device performance is not always reliably predicted by comparing optically derived ΔE_{ST} gaps.

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On the role of the host-guest interaction in the spin conversion of Multi-Resonant TADF systems: a vibronic picture

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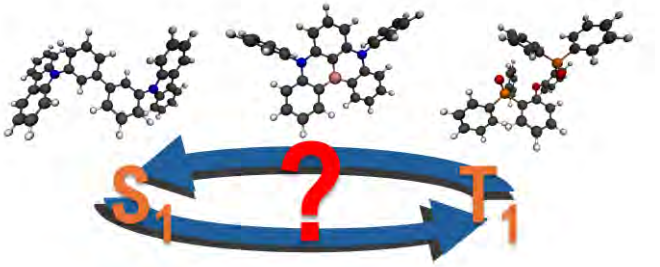
Multi-Resonant Thermally Activated Delayed Fluorescence (MR-TADF) systems are valuable solutions to enhance the performance of light-emitting devices thanks to their narrow emission and small ΔE_{ST}.[1] While TADF is often absent in solutions, it is frequently activated upon introducing the MR emitter in a host matrix. This solid-state enhancement turned out to be sensitive to the host’s chemical nature. Experimental measurements on the MR emitter[2], DABNA-1, suggested that the TADF behavior is active in mCBP but suppressed in DPEPO. This difference was attributed to the mediation of a higher-lying exciplex state in the spin conversion, thermally accessible in mCBP while not in DPEPO. In this work, we employed high-level wavefunction based methods (SCS-CC2) to model the electronic structure and the spin conversion kinetics of mCBP:DABNA-1 and DPEPO:DABNA-1 dimers. Our calculations revealed that, in both host environments, the exciplex state remains nearly 1 eV above S1 and T1, ruling out its direct mediation even when accounting for environmental effects. By including the Herzberg-Teller and the Spin-Vibronic Coupling mechanisms into Fermi’s Golden Rule, the ISC and RISC rates resulted to be of the same order of magnitude (10^6 s^{-1} and 10^3 s^{-1}, respectively) in both mCBP:DABNA-1 and DPEPO:DABNA-1. The identical spin conversion picture predicted in both hosts challenges the current understanding of the host-guest interaction in MR-TADF systems. Further experimental and theoretical studies are necessary to unambiguously rationalize the spin conversion dynamics, also including secondary non-radiative processes.



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The Many Roles of Host Materials in Single-Layer Blue OLEDs: Enabling Ohmic Charge Injection, Balanced Transport, and Enhanced Stability

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Blue organic light-emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) emitters still face major challenges in achieving high operational stability. Single-layer OLEDs, consisting of a single active layer between two electrodes, offer advantages over conventional multilayer devices, including simpler fabrication, lower cost, reduced operating voltage, and improved stability due to a broadened recombination zone. However, achieving efficiencies comparable to multilayer OLEDs requires overcoming two key challenges: barrier-free (Ohmic) charge injection and balanced charge transport. These remain difficult to achieve with blue TADF materials, as their wide bandgaps impede efficient injection from standard electrodes, and their tendency toward electron trapping leads to poor charge balance.

Here, we show that host materials in emitter-host single-layer architectures can simultaneously address both challenges by enabling Ohmic injection and balanced transport. In this design, the host modifies the interface properties, promoting efficient injection of both holes and electrons into the emissive layer. This approach follows a simple design rule: the host ionization energy (electron affinity) should be at least 0.3 eV higher (lower) than that of the emitter. We demonstrate this strategy using the blue TADF emitters DBA-DI and SpiroAc-TRZ with the hosts mCBP-CN and mCBP. The resulting devices consist of just the emissive layer between a polymeric anode and a metal cathode, fabricated in one deposition step, yet achieve external quantum efficiencies (EQEs) exceeding 25%, comparable to state-of-the-art multilayer OLEDs despite the greatly reduced structural complexity.

Charge balance in DBA-DI-based single-layer OLEDs is further improved by incorporating electron-transporting hosts such as mCBP-CN or SiCzTRZ2. Optimal performance is obtained at DBA-DI concentrations of 20-50%, yielding EQEs up to 25%. These hosts also reduce electron density on DBA-DI, suppressing bond dissociation in its anionic state and enhancing operational stability. With mCBP-CN as the host, the LT_{50} lifetime (1000 cd m^{-2}) increases from 120 hours for neat DBA-DI to 720 hours at 25% DBA-DI concentration. [1]

Finally, we demonstrate the generality of this strategy using carbene-metal-amide (CMA) complexes, a promising emitter class with efficient triplet harvesting and submicrosecond emission lifetimes but limited stability. An optimized CMA1:mCBP-CN blend exhibits low operating voltage, high power efficiency, and minimal efficiency roll-off while emitting sky-blue electroluminescence. These devices achieve EQEs above 20% and an LT_{50} of 120 hours at 1000 cd m^{-2}, representing more than a 50-fold improvement over previously reported sky-blue CMA OLEDs.

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Charge-Transfer Topology and Kinetic Modulation as Complementary Design Strategies for High-Efficiency TADF OLEDs

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Thermally activated delayed fluorescence (TADF) enables harvesting of triplet excitons in OLEDs through reverse intersystem crossing (rISC). While minimizing the singlet-triplet gap (ΔE_{ST}) is a necessary requirement, device-relevant performance is ultimately governed by excited-state topology and triplet population kinetics under electrical excitation. In particular, long-lived triplet populations promote annihilation-driven efficiency roll-off and accelerate degradation at high luminance. Here, we combine structural modulation of charge-transfer topology within a unified phthalimide-based donor-acceptor (D-A) platform with complementary kinetic control of triplet dynamics.

We varied the donor planarity and donor-acceptor linkage independently within one chemically consistent acceptor framework [1]. This modular design allows independent control of molecular geometry and electronic coupling, enabling systematic tuning of the energetic alignment between ^{1}CT/^{3}CT and ^{3}LE states. Time-resolved spectroscopy reveals a crossover from an effectively three-level CT system with fast rISC to a vibronically coupled ^{3}LE-mediated regime. OLEDs employing the most decoupled emitter achieve $EQE_{max} \approx 36\%$ with pronounced horizontal dipole orientation of > 80% (anisotropy factor $a \approx 0.16$), demonstrating that excited-state topology directly translates into device-level performance.[1] Beyond structural modulation, we introduce a complementary strategy that reshapes triplet population dynamics under high excitation densities. By controlling triplet depopulation pathways, the steady-state triplet density can be reduced, suppressing non-linear loss channels such as triplet-triplet annihilation (TTA) and singlet-triplet annihilation (STA) [2].

These results demonstrate that high-performance TADF OLEDs require simultaneous control over the excited-state topology and at the same time over the triplet depopulation kinetics. Structural charge-transfer modulation defines the energetic landscape, while the kinetics regulates exciton density under practical device operation conditions, providing a general framework for mitigating efficiency roll-off in blue and sky-blue TADF OLEDs.

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Macrocyclic Covalent Encapsulation of a Multi-Resonant Emitter: Understanding and Controlling Interactions in Highly Efficient Deep-Blue OLEDs

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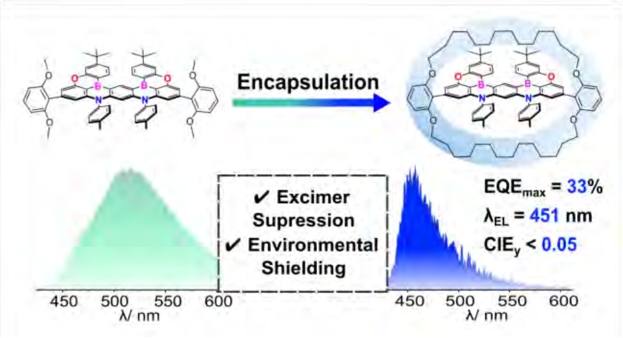
Multi-resonant (MR-TADF) emitters have emerged as popular candidates for organic light-emitting diodes (OLEDs), offering narrowband emission, high photoluminescence quantum yields (PLQYs), and the ability to upconvert triplets to singlets. However, their planar polycyclic structures promote detrimental intermolecular interactions in the solid-state which diminish the color purity and introduce nonradiative loss pathways. Here, we synthetically address these issues by covalently encapsulating a blue-shifted MR-TADF emitter within a protective macrocyclic ring. We identify a previously undiscovered utility of macrocyclic encapsulation, whereby it can shield the MR core from the surrounding environment to enhance its radiative rate and reverse intersystem crossing (RISC) efficiency. Only with spectrally resolved transient photoluminescence measurements were we able to identify the weakly emissive aggregate and excimer species, and definitively confirm that the macrocycle suppresses their formation in the solid-state. When integrated into an OLED device based on the "hyperfluorescent" strategy, this emitter delivers an exceptional combined maximum external quantum efficiency (EQE) of 33% and (0.146, 0.046) CIE$_{x,y}$ coordinates with peak emission at 451 nm, satisfying BT.2020 blue color requirement, and significantly outperforming its nonencapsulated analogue. This work establishes macrocyclic encapsulation as a powerful synthetic strategy for unlocking the full potential of MR-TADF materials for next-generation OLEDs.



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Narrowband Sky-blue Solution-processed Hyperfluorescent OLEDs using MR-TADF dendrimers

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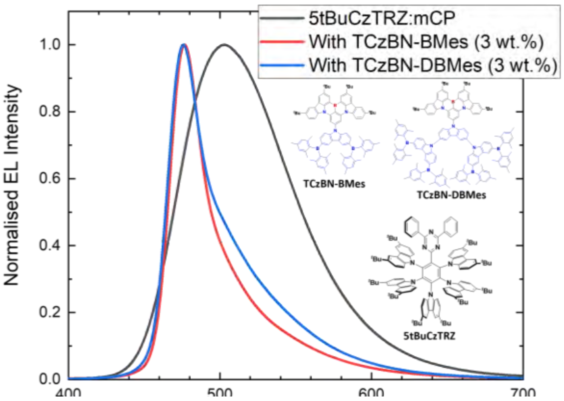

Figure 1. EL spectra of the devices, inset - molecular structures.

One of the key challenges in the current OLED research is achieving a saturated colour point, due to the broad emission of TADF emitters. Moreover, blue colour devices require high photon energy and are prone to rapid degradation [1-2]. A promising way to overcome this issue is to use a hyperfluorescence (HF) approach, where a small amount of a terminal emitter (TE) is introduced to the TADF-sensitiser and the host system. This way, fluorescence resonance energy transfer (FRET) from the sensitiser or the host to the TE enables the narrow emission. As a TE, multiresonant (MR-TADF) compounds are primarily used, because their rigid molecular structure restricts vibrational and geometrical changes, resulting in minimal spectral broadening. In this study, solution-processed (SP) OLEDs were fabricated using a highly efficient green sensitizer 5tBuCzTRZ (516 nm) [3] and novel boron-dimesityl functionalised MR-TADF dendrimers TCzBN-BMes and TCzBN-DBMes (Figure 1). However, HF is not yet well established for SP-OLEDs as the focus seems to be on vacuum-deposited devices. As desired, incorporating MR emitters into the emitter:host system significantly narrowed the electroluminescence (EL) spectrum (from 85 nm to 29 nm with TCzBN-BMes) and blue-shifted the CIE coordinates (from (0.23, 0.48) to (0.16, 0.30)). The HF devices of both MR emitters (3 wt.%) exhibit very similar maximum EQE values - 14.5% and 15.1%, for TCzBN-BMes and TCzBN-DBMes respectively — representing only a slight reduction in efficiency compared to the reference 5tBuCzTRZ:mCP (17.2% EQE_{max}). HF devices also demonstrate an improved efficiency roll-off, with 12.0% for TCzBN-BMes and 13.3% for TCzBN-DBMes (3 wt.%) at 500 cd/m^2. To conclude, MR-TADF allows to maintain a narrower FWHM in EL without sacrificing the device performance. Moreover, when combined with a TADF sensitizer the resulting HF OLEDs achieve enhanced efficiency and reduced roll-off.

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Molecular Simulations Uncover the Role of Soft Segments and Host-Guest Design in Stretchable TADF Emitting Polymers

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Intrinsically stretchable organic light-emitting diodes based on thermally activated delayed fluorescence (TADF) have recently emerged as a promising platform for skin-integrated photonics. Yet the molecular mechanisms governing their simultaneous mechanical and optoelectronic performance remain poorly understood. Here we present atomistic molecular dynamics simulations that elucidate the design principles of two stretchable TADF emitter designs. In the first system [1], non-affine displacement analysis reveals that long backbone alkyl segments act as compliant domains, absorbing disproportionate strain energy while leaving donor–acceptor packing and dihedral distributions essentially unchanged. In the second system [2], a stretchable host–guest architecture, simulations reveal uniform guest dispersion and demonstrate that energy transfer distances between host and guest moieties remain stable under mechanical deformation. Simulations further show that the host matrix increases inter-guest triplet exciton distances, providing a molecular basis for the suppression of triplet–triplet annihilation and the resulting doubling of device efficiency to over 20%. These results offer a molecular-level rationale for the decoupling of mechanical and optoelectronic performance in stretchable TADF emitters.

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Visualising Ir(ppy)$_2$acac distribution in OLED emissive layer blends with single atom resolution HAADF-STEM

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The degree of isolated, aggregated and clustered emitter molecules within the emissive layer of an OLED has been frequently linked to luminescence quenching processes and poor device performance. However, aggregation and clustering is seldom shown explicitly due to the experimental challenges in resolving individual molecules. Nearly two decades ago Reineke *et. al.* showed that the distribution of iridium-based phosphorescent emitters could be visualised by exploiting the sub-atomic resolution of aberration corrected scanning transmission electron microscopy (STEM), paired with the atom number contrast of the high angle annular dark field (HAADF) imaging mode. This allowed for the individual iridium atoms at the center of every organo-metallic emitter complex to be resolved and imaged. The results showed a higher degree of clustering than expected within a single blend produced by evaporative co-deposition, however, investigations beyond this finding have remained unexplored.

In this talk I will describe the results from high-resolution HAADF-STEM studies of a series of OLED emissive layer blends incorporating the archetypal Ir(ppy)$_2$acac emitter, where both the concentration of the emitter and the host were varied. For blends incorporating a tris(4-carbazoyl-9-ylphenyl)amine (TCTA) host, in the lowest concentration blend (3 wt%) most emitter molecules were aggregated with at least one other emitter, whereas in the highest concentration blend (22 wt%) the emitters formed a percolating network of emitters. To calculate the degree of clustering the 3D coordinate of the centre of each emitter molecule was reconstructed with sub-nanometer precision using HAADF-STEM depth sectioning. In contrast, blends incorporating a 4,4'-Bis(N-carbozolyl)-1,1'-biphenyl (CBP) host, the emitter was observed to phase separate during fabrication into emitter rich and emitter depleted regions homogenously throughout the entire film.

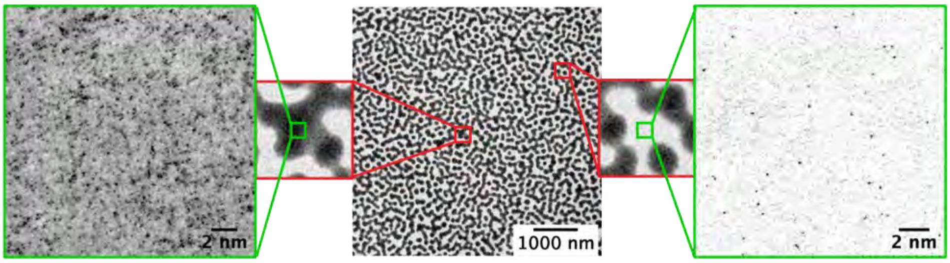

Figure 1. (Central) Moderate magnification, contrast inverted HAADF-STEM image showing submicron phase separation into emitter rich (black) and emitter depleted domains (white). Red insets show higher magnification images of each domain. Higher magnification images of the guest rich (left) and guest depleted (right) domains are shown containing single iridium atoms,

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DCM-PL analysis of charge-exciton interactions in OLED emission layers

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Understanding the correlations between charge carrier and exciton quenching behaviors is essential for optimizing OLED efficiency and operational stability. In this study, we employed a displacement current measurement combined with photoluminescence intensity measurement (DCM-PL)[1] to investigate charge carrier and exciton dynamics in Ir-complex- and TADF-based emission layers (EMLs). The DCM-PL technique effectively captures exciton-polaron quenching (EPQ) and exciton dissociation, providing valuable insights into their behaviors in practical device operation.

Figure 1a shows the structure of a 4CzIPN-based metal-insulator-semiconductor (MIS)-type device and the experimental setup for DCM-PL measurements. The DCM characteristics (top panel of Fig. 1b) clearly detect the hole injection and extraction behaviors during forward and backward sweeps (a and b). Simultaneously, the normalized PL intensity (bottom panel) exhibits changes consistent with hole accumulation, reflecting EPQ. Notably, a pronounced PL increase appears during the forward sweep prior to hole injection (d in Fig. 1b). This originates from radiative recombination of separated charges generated during the preceding backward sweep toward negative bias, where field-assisted exciton dissociation becomes prominent (c in Fig. 1b). Compared with Ir-complex-based EMLs,[1,2] 4CzIPN exhibits much stronger field-induced exciton dissociation, likely due to its smaller exciton binding energy characteristic of donor-acceptor-type TADF molecules.

These results demonstrate that DCM-PL provides a powerful approach for analyzing EPQ as well as exciton dissociation, contributing to improved understanding and design of advanced OLED architectures.

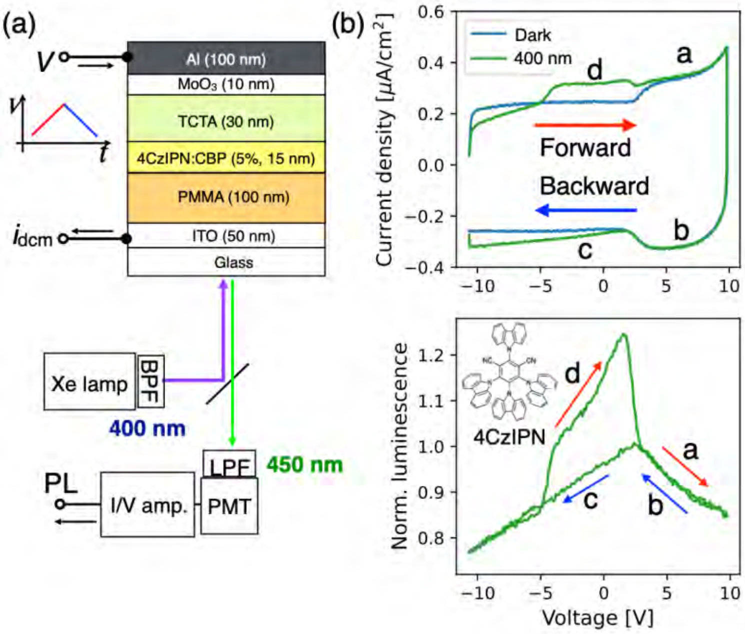

Figure 1. (a)Device structure and experimental setup for DCM-PL. (b) DCM-PL characteristics of 4CzIPN-based MIS-type device.

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Thickness dependence of molecular orientation in organic layers: insights from single-molecule microscopy on ensemble trends

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The orientation of organic molecules is a key parameter that determines both the electrical and optical performance of organic light-emitting diodes (OLEDs). Horizontal orientation of emitter molecules can increase light outcoupling by ~50%.[1] In turn, the orientation of host and transport-layer molecules can further impact light out-coupling, charge injection, and charge transport.[2] Nonetheless, despite significant progress across nearly two decades of research, we still lack comprehensive understanding of the factors that guide molecular orientation in thermally evaporated layers, and conclusions are hard to draw from cross-comparisons across the many existing studies.

In this contribution, we present novel results on the orientation of a range of vacuum-deposited host materials and host-emitter systems as a function of film thickness. Using variable-angle spectroscopic ellipsometry, we show that the average orientation of anisotropic host molecules is more horizontal in thicker films, particularly for materials with measurable birefringence. We further investigate how host orientation guides the alignment of a small-molecule emitter dopant through angle-resolved photoluminescence measurements. Importantly, we show that the measured emitter orientation can depend more strongly on film thickness than on the glass-transition temperature of the host, a parameter that has been established as one of the main drivers of small-molecule emitter orientation. Finally, we present results from single-molecule orientation and position imaging that map the orientation distributions of emitter molecules dispersed in different host materials as a function of their vertical position in the film.[3] These results further back our observations from ensemble-averaged measurements and provide a higher level of detail on the film morphology.

This systematic study on thickness and z-position dependence reveals that molecular orientation can be strongly influenced by the film interfaces. Crucially, molecular orientation in films thinner than 20 nm (a thickness range frequently used in emitter orientation studies) can significantly differ from the “bulk” orientation measured in thicker films. Based on our findings, we propose practical guidelines for sample fabrication and characterization that will support more accurate, reproducible, and cross-comparable molecular orientation studies in OLED materials research.

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Flipping the Rules:
From Inverted Singlet-Triplet Gaps to Diradical Switches

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Molecular platforms for optically addressable spin states are emerging as fascinating alternatives to solid-state spin centers, offering scalable synthesis, structural tunability, and chemical versatility.[1,2] In this talk, we present a molecular design strategy for achieving photoinduced spin polarization in organic diradicals bridged by systems featuring an inverted singlet-triplet (InveST) energy gap (see **Error! Reference source not found.**).[3] These InveST units possess HOMO and LUMO orbitals localized on complementary atomic sites. By covalently linking the non-SOMO-bearing positions of alternant hydrocarbon radicals to the LUMO-localized atoms of the InveST bridge, we construct diradicals in which the radical centers remain electronically decoupled in the ground state, yielding degenerate singlet and triplet configurations. Upon photoexcitation, population of the InveST LUMO activates an excited-state exchange interaction between the radicals, generating a finite singlet-triplet gap and enabling spin-selective intersystem crossing to polarized triplet states. Using a combination of model Hamiltonians and multireference *ab initio* calculations, we establish design principles for tuning exchange interactions and spin-orbit coupling to achieve molecular-level control over optical-spin interfaces. The resulting InveST-bridged diradicals emerge as promising scaffolds for molecular quantum technologies.

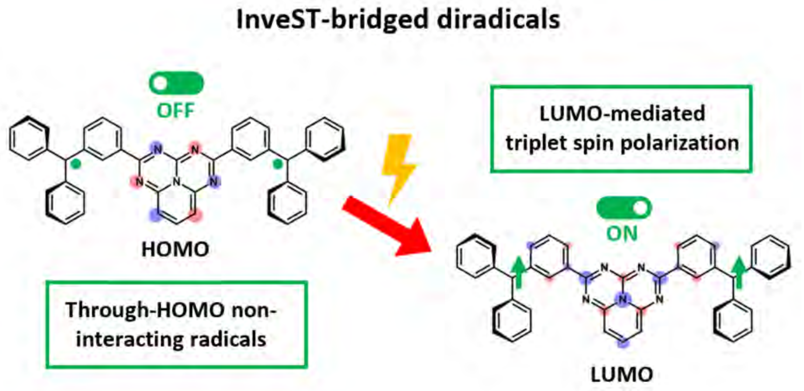

Figure 2 Schematic overview of the InveST-bridged diradical design and of the spin-spin locking as induced by the InveST-localized HOMO→LUMO transition.

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Toward Blue Emission in Radical emitters: TEMPO radical coupled to TADF and INVEST Scaffolds

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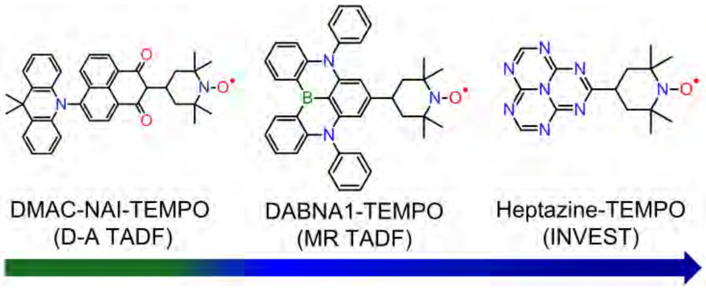
Organic radicals have emerged as promising emitters for organic light-emitting diodes (OLED) because they allow bypassing the unfavorable 1:3 singlet-triplet spin statistics encountered for conventional closed-shell molecules by emitting light from the spin-allowed first doublet excited state (D_1), enabling internal quantum efficiency (IQE) of up to 100% [1]. Yet, the color palette of these OLED radical emitters was limited to the red/near-infrared emission regions, and they also suffered from color purity issues due to the pronounced charge transfer (CT) character of the emissive D_1 state. This limitation was recently overcome by covalently linking a non-emissive stable TEMPO (2,2,6,6-tetramethylpiperidin-1-yl)oxyl) radical to a donor-acceptor (D-A) thermally activated delayed fluorescence (TADF) compound that shifted emission to green [2]. However, blue-emitting radicals remain scarce, and design rules are needed. Motivated by these experimental findings and seeking potential green/blue radical emitters, we performed quantum chemical calculations on TEMPO radicals covalently linked to well-known closed-shell emitters: DMAC-NAI, a D-A TADF compound, DABNA-1, a multi-resonance TADF (MR-TADF) emitter, and Heptazine, an inverted singlet-triplet gap (INVEST) molecule. These compounds exhibit a peculiar electronic structure where the triplet state, localized on the chromophore, couples with the radical spin to form two dark states, namely trip-doublet ($^2[D_0T_1]$) and trip-quartet states ($^4[D_0T_1]$). The energy splitting is typically small (~ k_bT) and the sign of the exchange coupling (J) indicates ferromagnetic ($J > 0$) or antiferromagnetic ($J < 0$) interactions that in turn determine the relative stability of the two states. Across all systems, multireference QD-NEVPT2 suggests an antiferromagnetic coupling, consistent with NEVPT4 prediction, despite NEVPT4 predicting larger J coupling. Relative to their closed-shell counterparts, the singlet-triplet energy gap (ΔE_{ST}) is larger for DMAC-NAI-TEMPO and Heptazine-TEMPO, but smaller for DABNA1-TEMPO. Another interesting feature is that the oscillator strength increases by around one order of magnitude for DMAC-NAI-TEMPO and Heptazine-TEMPO compared to their closed-shell analogues, while it remains strong for DABNA-1-TEMPO. This study opens up new avenues and provides new insights into the design of radical-chromophore compounds with green/blue emission.



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Dual TADF and TTA Emission in D-A-D molecules from Green to Deep Red with Mechanochromic Properties

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Materials which display thermally activated delayed fluorescence (TADF) have been widely employed in organic light emitting diode (OLED) applications. This is because of their ability to harvest light from the triplet state, T_1 allowing devices to have theoretical internal quantum efficiencies (IQEs) of 100%. Donor-acceptor-donor (D-A-D) molecules have been shown to be good candidates for TADF and efficient OLEDs [1,2]. However, obtaining efficient deep-red emitters remains a challenge due to the energy gap law as non-radiative decay is enhanced [3]. Triplet-triplet annihilation (TTA) is another mechanism of triplet harvesting, used in optoelectronic device applications, by formation of an excited singlet state from two triplet states.

Here, we report two efficient regioisomeric D-A-D emitters, comprising 3,6-di-tert-butyl-9H-carbazole as both donor units and a dibenzo[a,c]phenazine-based acceptor. The molecules differ in donor substitution position, yielding T-shaped (PC8) and Y-shaped (PC16) geometries, the structures are given in Figure 1**.** Time-resolved photoluminescence measurements demonstrate delayed fluorescence (DF) in solution and solid state. Laser power and temperature dependence studies confirm that DF arises from a combination of TADF and TTA. In dilute films, both mechanisms contribute, while in neat films TTA dominates. Notably, PC8 neat films exhibit deep-red emission with only a moderate PLQY reduction compared to dilute films, highlighting its resistance to aggregation-induced quenching. OLED devices were fabricated with PC8 and PC16 as the active emissive layer in neat and CBP host conditions, giving electroluminescence covering green to deep-red. PC8 additionally displays mechanochromic properties. Upon exposure to different external stimuli (grinding, DCM vapour and recrystallisation), the emission colour can be reversibly switched, with PL maxima spanning 597-637 nm. This study allows the exploration of the difference in luminescent properties arising from different positioning of the donor units as well as the demonstration of efficient OLEDs even in the deep-red.

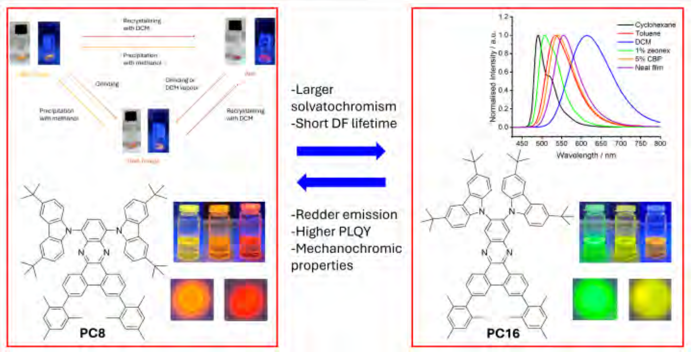

Figure **1**. The structures of PC8 and PC16 and a summary of their luminescent properties.

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Fluorescence Quenching Through Conical Intersections: The inverted energy gap law and Solvent-Induced CI opening

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A novel 'single benzene'-based fluorophore (TGlu) exhibits exceptionally high fluorescence quantum yield (ϕ_F) in solution and in the polycrystalline state. Experimental measurements of four structural analogues showed lower ϕ_F for molecules with higher Franck-Condon energy (FCE), an inversion of the trend predicted by the energy gap law (EGL) derived in Fermi's golden rule, (i.e. the smaller energy gap, the larger k_{nr}). This suggests the presence of a conical intersection (CI) that is accessible to molecules with higher FCE, as it is the case for a family of dicyano-distyrylbenzenes derivatives that was reported by our group before [1]. TGlu is highly emissive in essentially all solvents, with one notable exception, DMSO [2], suggesting a specific interaction of the fluorophore and the solvent that lead to an 'opening' of the CI path that results in the quenching of the fluorescence. Molecular dynamics simulations were performed for TGlu derivatives with alkyl chains of different lengths that effectively 'shielded' the molecule, resulting in a ϕ_F recovery up to 30%.

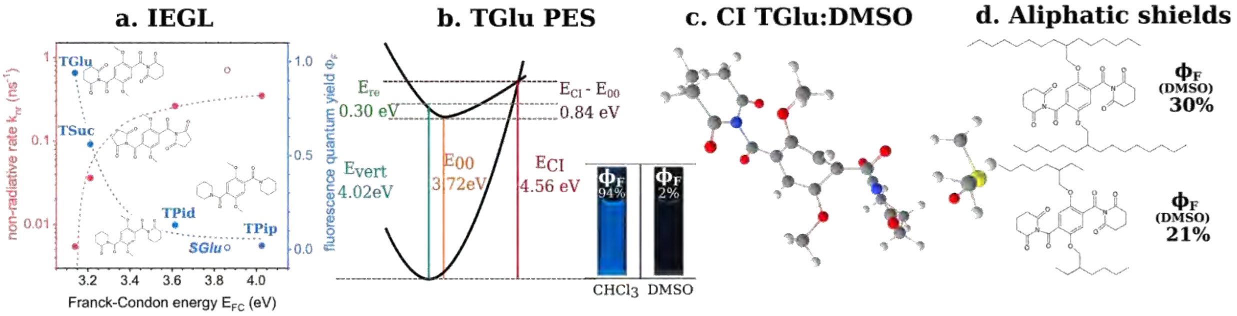

Figure 1. a. Inverse EGL in TGlu and analogues; b. Calculated points of the potential energy surface for TGlu; c. Conical intersection geometry for the TGlu:DMSO system; d. TGlu derivatives with aliphatic chains that partially recover the fluorescence efficiency.

To locate the CIs, we used the Mixed-Reference Spin-Flip TD-DFT formalism, which takes advantage of the formulation of LR-TD-DFT to obtain excited states coupled with the ground state, allowing the location of these nonadiabatic crossings [3]. Our study allowed us to conclude that the geometrical changes induced by the interaction with the solvent, for instance, the deformation of the benzene central ring, open the path to the CI.

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Modelling Thermally Activated Delayed Fluorescence Emitters

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Multi-resonance (MR) and inverted singlet-triplet gap (INVEST) thermally activated delayed fluorescence (TADF) dyes show great potential for applications in organic light-emitting diodes (OLEDs) because of their larger photoluminescence quantum yields (PLQY) and narrower emission profiles as compared to those attained by the traditional TADF dyes whose excited states are long-range charge transfer-based. Instead, the singlet and triplet excited states of MR- and INVEST-TADF emitters possess significant short-range charge transfer (SRCT) characteristics, which lead to negligible and inverted singlet-triplet gaps; respectively; and thereto to more efficient reverse intersystem crossing (RISC) processes. However, accurately predicting their electronic properties remains computationally challenging due to the delicate balance of electronic spin and correlation effects, which usually demand from expensive highly correlated electronic structure calculations, and hence limiting efficient molecular discovery and design for industrial applications. In this presentation, I present benchmark studies for the excited-state decay rate constants calculations of MR- and INVEST-TADF emitters, using our state-of-the-art techniques.[1] Specifically, we calculated the fluorescence, direct and reverse intersystem crossing (RISC) rate constants. Our studies highlight the importance of including Herzberg-Teller effects in the ISC and RISC rate constant calculations.[2] In order to accelerate the molecular discovery, we also developed wavefunction-based descriptors enabling to discern between INVEST and MR-TADF systems, importantly without the need of expensive highly correlated electronic structure calculations.

In addition, to assess the role of higher-lying excited states in the excited state dynamics of TADF dyes, we have developed multistate (four-states and five-states kinetic models) and we implemented them in our code KinLuv. In this regard, the excited state kinetics in TADF dyes is often simplified by a three-state picture (S_0, S_1, T_1) which neglects the role of higher-lying excited states (S_2, T_2). I here also showcase that for several MR-TADF dyes, going beyong the simplified three-state picture may be needed aiming to accurately model in a quantitative manner the PLQY values and the prompt and delayed lifetimes.

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Structural influence on the exciton binding energy of thermally-activated delayed fluorescent molecules

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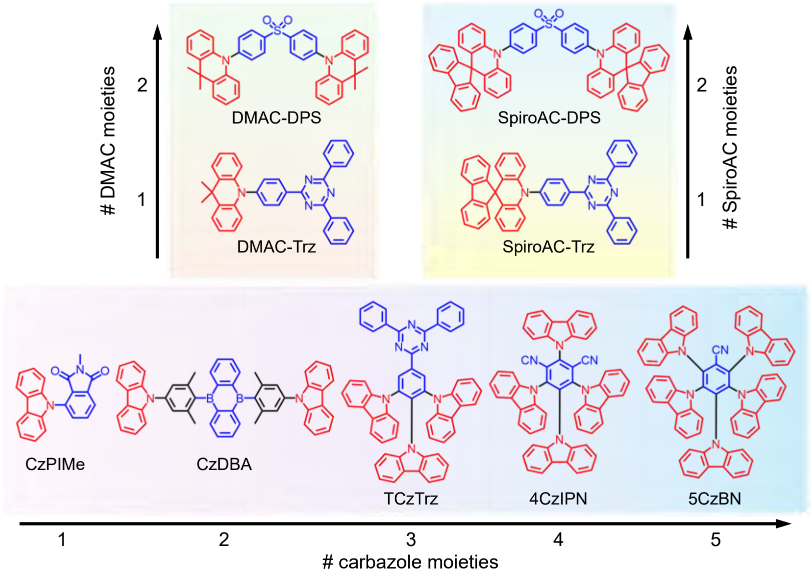
Thermally-activated delayed fluorescence (TADF) materials consist of a donor-acceptor structure to reduce the singlet-triplet energy gap. As a result of the charge-transfer character of the excited states, the exciton binding energies of TADF materials are expected to be lower than that of fluorescent molecules. However, a clear correlation between the exciton binding energy and the type of donor-acceptor structure is not yet known. In this study, we carried out field-induced dissociation (FID) measurements in which the photoluminescence efficiency of TADF materials is measured as a function of the applied electric field in reverse bias. In combination with kinetic Monte Carlo (KMC) simulations, the binding energy of excitons of the TADF emitters can then be estimated. This method has previously been applied to determine exciton binding energies of fluorescent materials [1] and iridium-based phosphorescent materials [2].



We selected various widely-studied TADF emitter molecules consisting of different numbers of carbazole, DMAC and SpiroAC moieties (see the figure). In order to study the validity of the FID method, we have also estimated the exciton binding energies by (1) deducing the frontier orbital energies from exciplex emission spectra of blends in which these TADF materials are combined with several donor or acceptor materials [3], and by (2) determining the singlet energies using optical spectroscopy.

In this presentation, we will discuss the measured material-specific exciton binding energies and the LUMO energy levels of these TADF materials, and their correlation with the molecular structures.

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High-power electrochemiluminescence for optogenetic manipulation of fruit fly larval behaviour

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Electrochemiluminescence (ECL), often referred to as "fluid light," offers strong potential for adaptable light-delivery devices in biophotonics, such as optogenetics, due to its use of fluid media. However, practical applications have been hindered by challenges in brightness (<700 cd/m^2) and stability. Here, we introduce an exciplex-mediated ECL mechanism in which electrochemically generated exciplexes in a toluene-based solution transfer energy to neighbouring terminal emitters.[1] This mechanism significantly improves reaction stability, allowing for relatively high-voltage operation. Additionally, adopting a TADF material that forms charge-transfer excimers can induce hyperfluorescence.[2]

By implementing a biphasic pulse operation strategy, we achieve an optical power density exceeding 100 µW/mm², equivalent to 14300 cd/m^2, sufficient to stimulate transgenic neurons in optogenetic methods. This demonstrates the first-ever ECL-driven optogenetics experiment [3], successfully eliciting avoidance behaviour in fruit fly larvae expressing CsChrimson (Figure 1a). The semi-transparent design of the device permits behavioural imaging through the device from underneath (Figure 1b). This innovation will be a breakthrough in establishing ECL-based light sources as powerful and versatile tools for neuro-optics and various biomedical research applications.

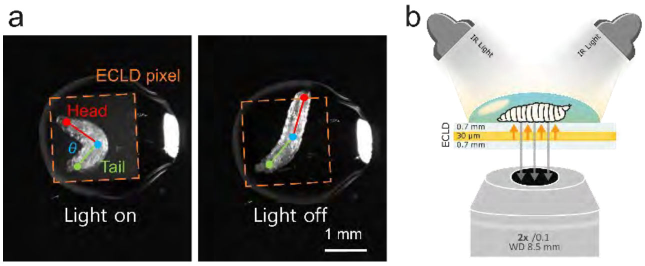

Figure 1. a Optogenetic manipulation of larval behaviours using ECL device placed underneath the larva. **b** Schematic of the inverted microscope setup.

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Polaritonic Light-Emitting Electrochemical Cells

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Polaritonic light-emitting devices make use of strong light-matter coupling to form hybrid exciton-photon quasiparticles—i.e., polaritons—with different properties from its constituents, offering a route to narrowband and potentially angle-independent emission and direct control of energy levels involved.[1] Polariton formation can be achieved, for example, by confining light emission between two mirrors which can also simultaneously serve as electrodes. The light-emitting electrochemical cell (LEC) is a natural candidate for this approach since its structure comprises only a single active layer sandwiched between two electrodes. This simplicity is possible thanks to its unique operation mechanism: the dynamic *p-i-n* junction, driven by mobile ions, that forms under bias.[2] Here, we present unpublished work of what is, to our knowledge, the first polaritonic LEC (p-LEC), realized by embedding a broadband-emitting polymer (Super Yellow) and an electrolyte within an optical microcavity operating from the strong coupling regime. Angular-resolved photoluminescence (PL), electroluminescence (EL), and reflectivity measurements confirm a polariton emission from the lower polariton branch. By tuning the cavity condition, we fabricate narrowband green- to red-emitting p-LECs (~20 nm FWHM, c.f. Figure) with efficacies comparable to those of their reference LEC counterpart. We further discuss how the mixed ionic-electronic nature of the LEC—such as the spatial overlap between the position of the dynamic emission zone and the cavity antinode—modulates the strength of the light-matter interaction and, thus, the device performance.These results establish a proof-of-concept of polaritonic LECs and opens a new path toward light-emitting sustainable technologies where polariton strategies might offer greater advantages, including TADF-based LECs to mitigate triplet-triplet and triplet-polaron quenching.

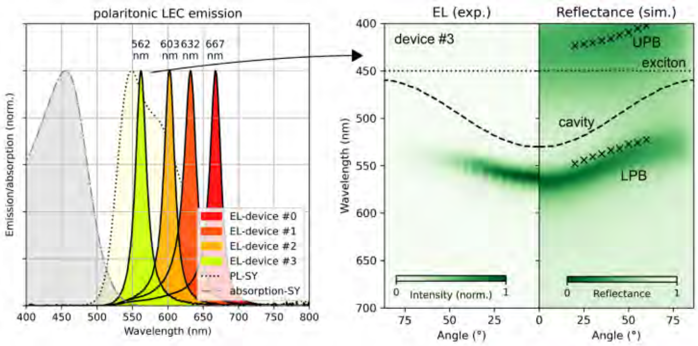

Figure 3. Left: Emission from the different polariton LECs with differently tuned cavities and the absorption and PL spectra of the emitter (SY). Right: Angle-resolved EL (experimental) and simulated reflectance for device #3. The lines show the cavity mode (dash) and exciton energy (dots). The upper and lower polariton branches (UPB, LPB) are indicated. The crosses show the minima positions in the measured reflectivity spectra.

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Low-Threshold Lasing in Photonic Crystals via Epsilon-Near-Zero Band Engineering

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Photonic crystals (PCs) offer a versatile platform for engineering electromagnetic environments through the control of their dispersion properties. Independently, near-zero-index (NZI) media—characterized by an effective refractive index approaching zero—exhibit unusual light–matter interaction regimes. Depending on whether the electric permittivity or the magnetic permeability vanishes, NZI media are classified as epsilon-near-zero (ENZ) or mu-near-zero (MNZ), respectively. Under specific dispersion conditions, PCs can support bands that effectively mimic such NZI responses, establishing a direct connection between photonic band engineering and NZI physics [1].

In this work, we investigate how these two mechanisms interplay in the context of laser operation. Using an analytical approach based on Maxwell–Bloch rate equations [2], complemented by finite-difference time-domain simulations, we study the influence of ENZ and MNZ environments on laser dynamics. We first show that, within a homogeneous-medium description, assimilating the active region to an ENZ environment leads to a reduction of the lasing threshold compared to conventional dielectric media.

We then extend this analysis to structured systems. In two- and three-dimensional PCs, dispersion regimes associated with a vanishing group velocity ($v_g \rightarrow 0$) are known to enhance light-matter interaction and reduce the lasing threshold [3]. Here, we demonstrate that the extent of this reduction strongly depends on the electromagnetic nature of the photonic band. In particular, ENZ-like bands lead to a lower threshold than MNZ-like bands, even within comparable slow-light regimes. This difference originates from the distinct modification of the stimulated emission process induced by the ENZ or MNZ character of the band.

These results show that low-threshold PC lasers cannot be attributed solely to slow-light effects but require careful engineering of ENZ bands. This work provides clear physical guidelines for designing low-threshold PC laser architectures.

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Towards Circularly Polarised Luminescence from Inherently Chiral Inverted Singlet-Triplet Dyes

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Recent years have seen rising interest in molecules that violate Hund's rule, where the first excited singlet state lies below the triplet ($\Delta E_{ST} < 0$), accelerating reverse intersystem crossing, a key process in thermally activated delayed fluorescence. Such molecules hold potential for optoelectronic applications as OLEDs and photocatalysis.[1] Despite growing interest, no single-molecule emission from a chiral dye with inverted gap has been reported, and only one case has shown such emission from supramolecular aggregates.[2] We present a computational study on such inverted singlet-triplet (IST) molecules modified for chirality to enable Circularly Polarised Luminescence (CPL), an unexplored direction for IST emitters.

We show the first circularly polarised light emission (CPL) from a chiral molecule exhibiting inverted singlet-triplet gap. Our design is based on the achiral heptazine core, functionalised with chiral substituents. Photophysical characterisation, including temperature-dependent optical spectra and photoluminescence decay profiles confirms the inverted gap. Chiroptical properties show dissymmetry factor g~10^{-3} comparable to other chromophores functionalised with chiral groups. Combined with promising photoluminescence quantum yields, these findings highlight the potential of such materials for circularly polarised OLED devices.

We finally explored inherently chiral chromophores, focusing on extended triangulenes resembling helicenes,[3] known for their strong CPL. Substituents enabling enantiomer separation were introduced, and racemisation barriers were evaluated. When inversion was lost, structures were further optimised, leading to a promising substrate combining a high barrier enabling enantiomer separation, strong CPL activity, and inverted singlet–triplet energetics, making it suitable for CP-OLED applications.

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Good and bad electronic disorder in mixed halide perovskite semiconductors for light emitting devices

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Halide perovskites are a flexible platform for the development of performant Light Emitting Devices (LEDs), due to a unique compositional flexibility which has no analogues among conventional semiconductors. The pivotal work of Noh et al. indeed demonstrated full compositional miscibility for lead-based, iodine/bromine compositions, highlighting gradual tuning of the absorption and emission wavelength from 780 nm to 530 nm, which ultimately paves the way for obtaining LEDs with tunable color [1].

Still a fundamental question raises, as, with chemical inhomogeneity representing a source of disorder, it is hence expected to negatively impact on the electronic properties of this class of semiconductors. To clarify this point, we performed electronic structure simulations of pure- as well as mixed-halide iodide/bromide lead-based perovskites, aiming at discriminating the impact from different sources of disorder. The emerging picture is that finely intermixed bromide/iodide solid state solutions show comparable behavior of their pure halide analogues, with electronic waves comparably delocalizing over both the halides species (Figure 1), and disorder stemming mainly from a similar homogeneous contribution as for pure halide compositions. In turn, halide segregated domains feature both enhanced disorder from inhomogeneous source, potentially associated with interfacial states at the domain boundaries (Figure1). Large-gap (bromine) domains also behave as hole blocking layers, hence affecting the transport properties of these compounds. Overall, we find that compositional disorder in the halide is not negative for mixed halide LEDs, "per-se", but suffer from halide segregation [2-3].

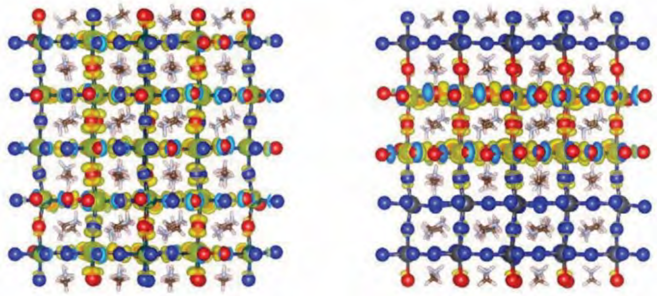

Figure 1. isosurface associated with the valence band edge for a finely intermixed iodide/bromide solid state solution (left panel) and with halide segregated domain (right panel)

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Toward Integrated Perovskite Laser Diodes

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Metal-halide perovskites have rapidly emerged as potential gain materials for thin-film lasers, owing to their exceptional optical gain, narrow emission linewidths, and bandgap tunability across the visible/near-infrared spectrum. Their solution processability and compatibility with a wide range of substrates, including those used in silicon photonics and CMOS electronics, position them as strong candidates for next-generation compact light sources. Despite these advantages, realizing an electrically injected perovskite laser diode remains an elusive milestone. Key challenges include severe Joule heating under high current densities, rapid material and interface degradation during electrical excitation, and substantial optical losses introduced by conventional metal electrodes that impede the formation of low-threshold, high-Q cavities.

In this presentation, we showcase recent experimental progress aimed at addressing these limitations and moving perovskite devices closer to true lasing under electrical injection. We focus on three complementary strategies. First, we employ nanosecond-scale electrical excitation at cryogenic temperatures to suppress Joule heating and stabilize the perovskite active layer during high-current operation. This approach enables carrier densities exceeding 10^{17} cm^{-3} and allows external quantum efficiencies above 3% to be maintained at current densities beyond 3 kA/cm^2, values that approach the regime required for population inversion.[1] Second, we engineer low-loss transparent conducting electrodes based on optimized indium tin oxide (ITO) structures.[2] By minimizing free carrier absorption by metal electrodes, we mitigate one of the dominant optical loss channels present in devices using metal contacts. This results in improved modal confinement and reduces the gain threshold increase due to absorption losses. Third, we demonstrate high-quality optical cavities with quality factors compatible with stimulated emission at low thresholds, while maintaining fabrication routes that are fully compatible with mainstream CMOS processing.[3] These cavities combine low scattering losses with strong optical confinement, enabling a platform that can be integrated with both planar photonic structures and electrically injected architectures. Finally, we outline a clear roadmap toward achieving full electrically driven lasing in perovskite devices and demonstrate that several of the critical performance metrics are now within reach.

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Mixed-Solvent Strategy for Efficient and Stable Quantum Dot Light-Emitting Diodes

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Colloidal quantum dots (QDs) are highly attractive emissive materials for next-generation optoelectronic devices owing to their size-tunable bandgap, narrow emission linewidth, high color purity, and compatibility with solution-based processing. These advantages have enabled substantial progress in quantum dot light-emitting diodes (QLEDs); however, device performance and operational stability remain strongly influenced by the quality of the emissive layer. In particular, the role of QD film uniformity in governing charge injection and device stability has not been systematically explored.

Here, we investigate the influence of QD layer uniformity on QLED performance and demonstrate a mixed-solvent strategy to enhance QD film homogeneity. By combining solvents with complementary evaporation characteristics, we achieve homogeneously packed QD films with significantly improved packing periodicity compared to single-solvent systems, as confirmed by atomic force microscopy and grazing-incidence small-angle X-ray scattering. The improved film uniformity leads to enhanced carrier injection and transport, effectively suppressing parasitic leakage pathways. As a result, QLEDs fabricated with mixed-solvent-processed QD films exhibit enhanced electroluminescent performance and prolonged operational stability relative to single-solvent counterparts.

These results highlight QD packing homogeneity as a key factor governing carrier dynamics in QLEDs and demonstrate its impact on enhanced device performance, while providing practical guidelines for improving the efficiency and reliability of solution-processed optoelectronic devices.

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Kinetic Formalisms for Triplet-Mediated Organic Optoelectronics: From One-Component TTA to All-Photonic Synapses

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The performance of many organic optoelectronic systems is set by a complex photophysical process rather than a single molecular parameter. This complexity impeded the establish of the structure-property of materials resulting limitation of high-performance materials. While kinetic methods have been extensively employed in chemical reaction studies, their application in photophysics has remained largely supplemental. In our work, focusing on triplet-triplet annihilation (TTA) systems and all photonic synapse (APS) materials, we demonstrate that kinetic analysis can effectively elucidate intricate photophysical processes, uncover underlying performance mechanisms, identify decisive factors, and ultimately establish structure-property guidelines for the directed screening of advanced materials. TTA is widely used for efficient exciton utilization and photon up conversion. Conventionally, the change of slope in the double logarithmic relation between emission intensity and excitation intensity from 2 to 1 is treated as evidence of TTA. However, recent experiments on many one component organic TTA systems do not exhibit this canonical slope transition [1]. By classifying one component TTA systems according to dominant emissive singlet state ($S_1 \rightarrow S_0$ vs $S_n \rightarrow S_0$), oxygen participation, and the involvement of higher excited states, we formulate two generic kinetic models that cover eleven practical photophysical cases [2]. From these models we derive a general steady state formalism, which consistently describes both typical and previously anomalous systems beyond traditional treatments. The model predicts two distinct turning points in the $\log I_{\mathrm{em}}$ versus $\log k_{\mathrm{ex}}$ behaviour, and a monotonic increase of the luminescence quantum yield Φ_{em} toward saturation, in agreement with steady state spectral measurements. Importantly, the evolution of Φ_{em} provides a more universal criterion for identifying TTA than the slope changes alone, enabling reliable diagnosis of kinetic regimes that are difficult to capture with conventional analysis. We further apply kinetic reasoning to organic APS devices, where optical memory and accumulation effects are observed but have remained mechanistically unclear. We establish a three-step mechanism that explains the emergence of these behaviours. For APS materials based on long persistence luminescence (LPL), especially host guest systems, the kinetic framework links LPL and accumulation to charge transfer and separation dynamics. We identify a key requirement for high quality phosphorescent synapses: the generation of charge separated states from charge transfer states should not overwhelmingly exceed the generation of local excited states, and the dissociation of charge separated states should be slow. Guided by this mechanism, we connect molecular level energetics to synaptic performance and obtain a structure property relationship: a smaller host guest energy descriptor $\mathrm{U}_{\mathrm{T}}^{\mathrm{L}}$ leads to improved linearity and higher recognition accuracy. Overall, these works demonstrate that kinetic formalisms can turn complex photophysics into actionable mechanistic rules and practical descriptors for screening high performance organic optoelectronic and neuromorphic materials.

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Zn(II) Complexes as Efficient TADF and OLED Emitters

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The investigation of 3d transition metal compounds as substitutes for precious metal complexes in photonic applications is a very timely topic.[1] One of the reasons is the comparably costly and energy-intensive production of 4d and 5d elements that are typically employed to facilitate and make use of photoinduced spin-forbidden processes due to their strong spin-orbit coupling (SOC). Another motivation is the search for new combinations of photophysical and photochemical properties and modes to control them, with manifold applications in photo-induced energy (EnT) and electron transfer (ET), sensing, light-emitting devices, and as responsive smart materials. Although Cu^{I} complexes with a d^{10} electron configuration that exhibit thermally activated delayed fluorescence (TADF) are currently being considered as the prime choice among the 3d elements for luminescent device applications,[2] we recently demonstrated that a TADF mechanism with exceptional radiative rate constants k_{TADF} of $1.2*10^{6}$ s^{-1} can be achieved in Zn^{II} complexes, surpassing the brightness of commercial Ir^{III} and Pt^{II} based emitters.[3] In this talk, the latest developments of luminescent Zn^{II} complexes, their OLED application and single-photon source properties will be discussed.

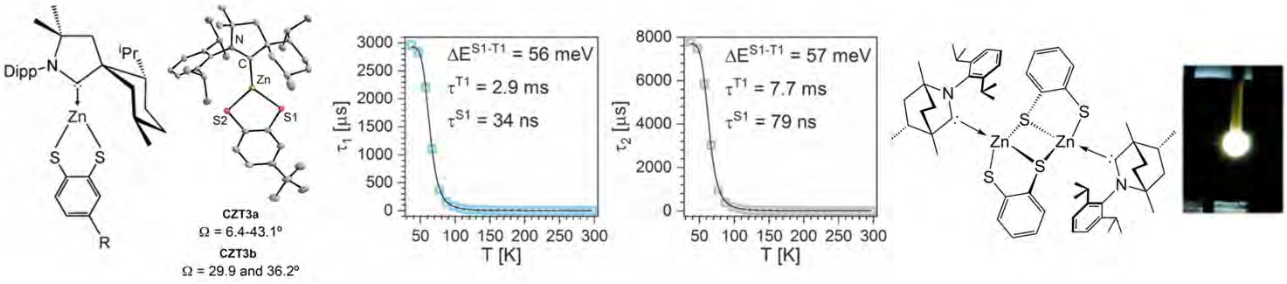

Figure 4. TADF properties and OLED application of selected carbene Zn^{II} thiolate (CZT) complexes.

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Placing Iridium Complexes Among TADFs: Evidence for Thermally Activated Delayed Fluorescence in Iridium(III) Complexes

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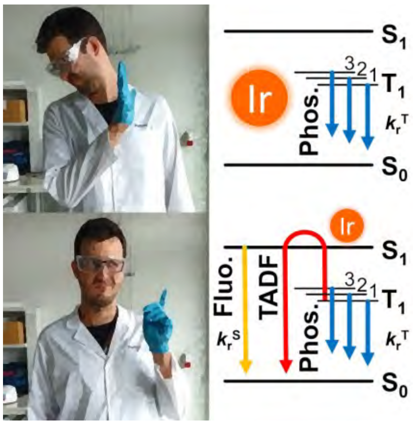

Iridium(III) complexes play a pivotal role in research and technology. The popularity of Ir(III) complexes in OLEDs remains somewhat uncontested, despite the low earth abundance of this metal and enthusiastic efforts to identify alternatives. Although they are widespread, have we really understood fully the excited-state properties of Ir(III) complexes?

In this work we report the second ever example of a fully experimentally confirmed thermally activated delayed fluorescence (TADF) in a dinuclear Ir(III) complex. The said complex displays a singlet-triplet gap ΔE_{ST} = 28 ± 5 meV. We also demonstrate a proof-of-concept solution-processed OLED, achieving EQE of up to ~10% and maximum luminance of 18 000 cd m^{-2}.

Our findings are complemented by a detailed consideration of spectral signs of TADF in the already known Ir(III) complexes. In this study, we have scrutinized literature data on iridium(III) complexes that show significant overlap between absorption and PL, and we conclude that a small singlet-triplet energy gap ΔE_{ST} in these complexes results in a TADF contribution to their emission. We use computations to clarify the nature of the excited states in these complexes, demonstrating that the distinctive S_1 and T_1 character of states can be identified as well as confirming that ΔE_{ST} is small enough for TADF to occur at room temperature.

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The sweet spot of energy level alignment in hyperfluorescent OLEDs

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Using a combined experimental and simulation-based approach, we investigated loss mechanisms in hyperfluorescent organic light-emitting diodes (HF-OLEDs) with the emissive layer consisting of a host, a thermally activated delayed fluorescence (TADF) sensitizer and a terminal emitter (TE). We compared devices with two different TEs to understand how the energy level alignment between the TADF sensitizer and the TE affects device efficiency and roll-off. Device-scale kinetic Monte Carlo simulations indicate that the formation and subsequent dissociation of an intermolecular charge-transfer state reduce the device quantum efficiency (EQE). Such dissociation can be prevented if the energy of the intermolecular state lies at least 150 meV above the lowest singlet energy level (typically on the TE). Furthermore, we show that using a multi-resonant TADF TE significantly reduces residual triplet-related losses, compared to a device with a non-multi-resonant TE. In conclusion, we provide guidelines for selecting TEs and optimizing energy level alignment to address loss pathways related to intermolecular charge-transfer states in HF-OLEDs.

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Heptazine-Assisted Multi-Resonance TADF Emitters with Fast Reverse Intersystem Crossing for Efficient Solution-Processed OLEDs

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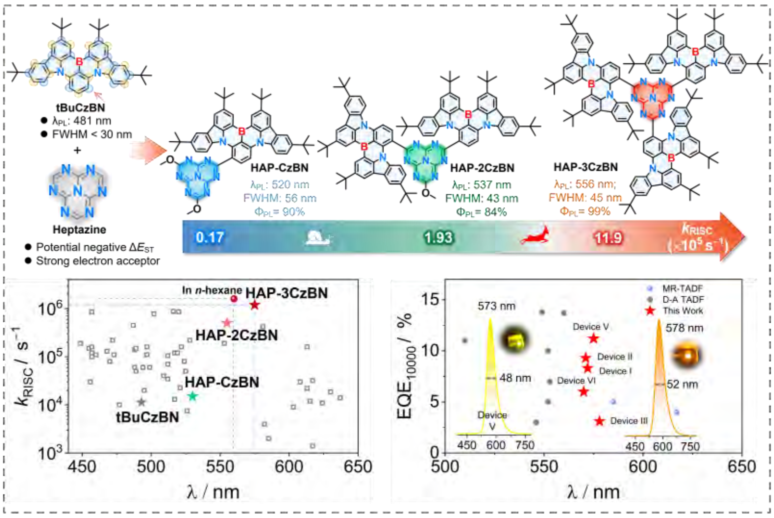
The development of solution-processed organic light-emitting diodes (SP-OLEDs) with narrowband emission, high brightness, and minimal efficiency roll-off remains a significant challenge. Herein, we report a series of heptazine-assisted multi-resonance thermally activated delayed fluorescence (MR-TADF) emitters for high-performance SP-OLEDs. By integrating a heptazine core with one to three MR units (tBuCzBN), we synthesized three emitters (**HAP-CzBN**, **HAP-2CzBN**, and **HAP-3CzBN**) exhibiting excellent photoluminescence quantum yields and progressively reduced singlet–triplet energy gaps (ΔE_{ST}) with increasing MR content. Among these, **HAP-2CzBN** and **HAP-3CzBN** show green and yellow emission at 537 nm and 556 nm with small full width at half maximum (FWHM) of 43 and 45 nm in toluene, respectively. Notably, both emitters exhibit concentration- and temperature-dependent dual emission with TADF behavior in n-hexane, suggesting potential for optical temperature sensing. In the solid state, **HAP-3CzBN** achieves the shortest reported delayed lifetime of 0.92 μs and a record-high reverse intersystem crossing rate constant of 1.19×10^6 s^{-1} among MR-TADF emitters without heavy atoms with long-wavelength emission. SP-OLEDs based on **HAP-3CzBN** exhibit a peak external quantum efficiency (EQE) of 15.5%, negligible roll-off at 1000 cd m^{-2} (EQE_{1000}= 15.4%) and maintain 11.2% EQE at 10,000 cd m^{-2}, setting a new benchmark for high brightness MR-TADF devices via solution processing. An OLED employing a trap-free transport layer configuration further increases the EQE_{max} to 20.3%, along with exceptional current efficiencies of 90.2 cd A^{-1}.



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POSTER SESSION

1st DAY

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Band Alignment and Interfacial Hybridization in Carbazole-Based 2D Hybrid Perovskites

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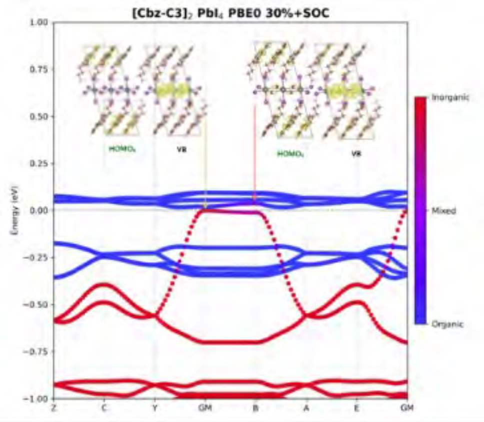
Two-dimensional hybrid organic–inorganic perovskites (2D HOIPs) are promising materials for light-emitting and photovoltaic devices, spatial and dielectric confinement leading to the formation of stable electron-hole pairs. On the other hand, the incorporation of π-conjugated organic moieties in the 2D lattice appears as an effective approach to further extend the functionalities of these compounds, via the possible energy and charge transfer effects between the inorganic and organic components. Here, we investigate a series of newly synthesized 2D HOIPs containing carbazole-based alkylammonium cations (Cbz-C_x, with x = 2, 3, 4), in which the alkylammonium chain is anchored to the benzene ring of the carbazole unit and incorporated into the lead-iodide framework.

Using state-of-the-art hybrid Density Functional Theory (DFT) calculations including spin-orbit-coupling, we studied the electronic structure and band alignment in these compounds. The increase in the length of the alkylammonium anchoring group goes together with a transition from type I alignment (Cbz-C_2) to type II one (Cbz-C_4). The CbzC_3 in particular features a close resonance between the valence band edge of the PbI4 lattice and the HOMO bands of the organic molecule enable partial hybridization between these states, with an estimated 30 meV electronic coupling. The fundamental band gap opening from Cbz-C_2 and Cbz-C_4 to Cbz-C_3 nicely follows the blue shift from reflectance spectroscopy. These in turn both disagree with the trend in the optical gap measured for thin films, indicating that the optical properties of these compounds are sensitive with respect to material morphology.



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Chiral Substituted Polyfluorene-TADF Polymers for Circularly Polarized OLEDs

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Organic light-emitting diodes (OLEDs) capable of emitting high levels of circularly polarized (CP) light attract strong attention due to their potential in advanced technologies, such as power-efficient displays, optical spintronics, and chiral sensing. Such devices require chiral emitters to simultaneously display high luminescence efficiency and strong chiroptical characteristics. However, developing CP-OLEDs that meet these criteria remains a significant challenge due to intrinsic trade-offs. The majority of current small-molecule chiral emitters, including the state-of-the-art triplet-harvesting thermally activated delayed fluorescence (TADF) materials, display outstanding emissive properties but often suffer from low levels of CP-(electro)luminescence. In contrast, π-conjugated polymers can form chiral supramolecular assemblies, providing a promising class of materials to meet the application requirements. Our work attempts to combine the best of both worlds by exploring TADF polymers that incorporate chirally substituted fluorene monomers, known for their amplified chiroptical properties.[1] By integrating small fractions of an acridine-benzophenone (ABP) co-monomer, we aim to enhance luminescence efficiency via Förster resonance energy transfer (FRET), while retaining the potential to adopt a helical conformation.[2,3] Structural variations are made on both the emissive and chiral motifs of the polymer to investigate their respective impacts on the (chir)optical performance. Optimized annealed films achieve dissymmetry values in absorption (g_{abs}) and photoluminescence (g_{lum}) within the 10^{-1} - 10^{-2} range, representing a promising strategy for efficient dissymmetric emission.

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Optimising CPL of Inverted Singlet-Triplet dyes by Substitution of the Heptazine Core

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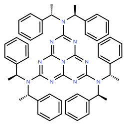
Recent years have seen rising interest in molecules that violate Hund's rule, where the first excited singlet state lies below the triplet (ΔEST < 0), accelerating reverse intersystem crossing, a key process in thermally activated delayed fluorescence. Such molecules hold potential for optoelectronics applications as OLEDs and photocatalysis. In those molecules, the $S_1 \rightarrow S_0$ transition is symmetry forbidden, thus showing low oscillator strength. Despite growing interest, strong emitting substrates have not been reported yet. Recent advances in chiral IST dyes emitting Circularly Polarised Light provide new opportunities to enhance OLEDs performance.[1,2] We present a combined computational and experimental study on such inverted singlet–triplet (IST) molecules, starting from substrates already prepared and characterised in ref. [1]. We introduced several modifications to the heptazine, breaking symmetry, introducing interacting units. We demonstrated that such functionalisations do not alter the IST nature of the dyes, and result in improved oscillator strength, as demonstrated via MRSF-TDDFT calculations. Experimental characterisation through fluorescence and CPL confirms computational results.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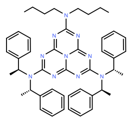
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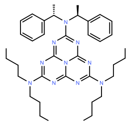
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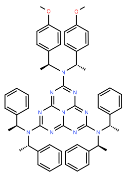
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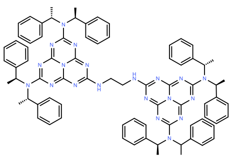
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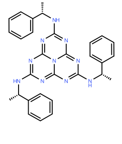
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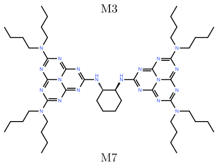
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Aggregation-Dependent MMLCT and Emission Characteristics in Polymorphic Pt(II) Complexes

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Aggregation-induced metal-metal-to-ligand charge transfer (MMLCT) is frequently invoked to rationalize the red-shifted and broadened emission observed in polymorphic Pt(II) complexes. However, the putative MMLCT character and its microscopic origin in the solid state remains unclear. In this work, we present a theoretical investigation on Pt(II) complexes [1] exhibiting multiple solid-state packing motifs with distinct emission behaviors. Monomer, dimer, and trimer models were constructed from crystal structures and treated using different QM/MM schemes and exchange-correlation functionals [2]. Simulations of the phosphorescence spectra from the first triplet excited states have been performed taking into account the vibronic coupling effects. Our results reveal that dimers do not exhibit MMLCT characteristics, whereas trimers induce Pt⋯Pt interactions in some of the studied polymorphs, leading to enhanced low-energy absorption and red-shifted, featureless phosphorescence. The emergence of MMLCT is accompanied by reduced reorganization energies and suppressed high-frequency vibrational coupling. These findings demonstrate that MMLCT is an aggregation-threshold-dependent phenomenon rather than a simple dimer effect and provide a mechanistic explanation for the polymorphism-dependent emission observed experimentally.

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Eu(II) in OLED: On the Interplay of Intrametallic Emitters and Hosts

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Eu(II) emitters offer a compelling route to deep-blue OLEDs [1], yet implementation has remained limited by the coupled requirements of vacuum processability and pure blue emission. After overcoming this challenge by introducing carborate ligands yielding EuCrown and EuCovCrown (see Figure), we encountered a second and far less explored bottleneck: Host compatibility is fundamentally different for Eu(II)-based than for traditional organic π-emitters [1,2].

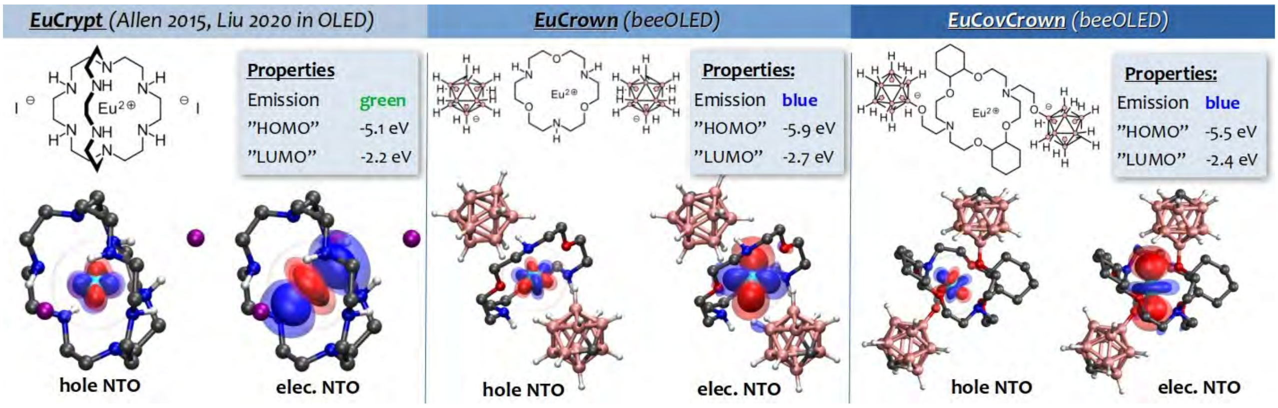

***Figure:** beeOLED's carborate-based intrametallic Eu(II) emitters compared to literature known materials.*

This talk shows why the conventional HOMO/LUMO concept does not apply to intrametallic emitters, where the excited electron of the highly localized $4f - 5d$ exciton resides in a spatially diffuse state (Figure) that is unbound in the neutral ground state. By combining host-dependent photoluminescence experiments with state-of-the-art DFT, we translate the conventional concepts into criteria applicable to intrametallic emitters that separate electronic host compatibility from chemical host compatibility [3]. Based on these criteria, this talk provides a rationale for the development of robust, high-performance Eu(II)-based OLEDs.

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Anti-Kasha electroluminescence in carbene-gold-arylacetylide complexes

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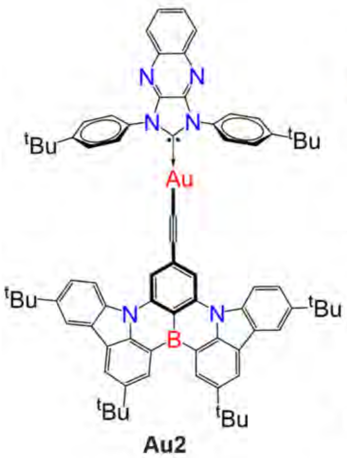
We report carbene-gold-arylacetylide complex **Au2** which coordinates a (carbene)gold(I) moiety to a multiple resonance chromophore using an acetylide linker. This molecular design spatially separates the frontier molecular orbitals of the complex, leading to a dark long-range charge transfer S_1 state and a brightly emissive short-range charge transfer S_2 state. In-depth optical spectroscopy and theory confirm that the bright, narrow emission at 495 nm originates from this S_2 state as Anti-Kasha photoluminescence.

This Anti-Kasha emission is retained in electroluminescence. Proof-of-concept solution-processed energy transfer OLEDs fabricated using **Au2** exhibit the same bright sky blue emission (CIE coordinate 0.16, 0.52). These devices achieve 20.4% maximum external quantum efficiency (EQE) and show suppressed roll-off at high luminance with 13% EQE at 10,000 cd m^{-2}.



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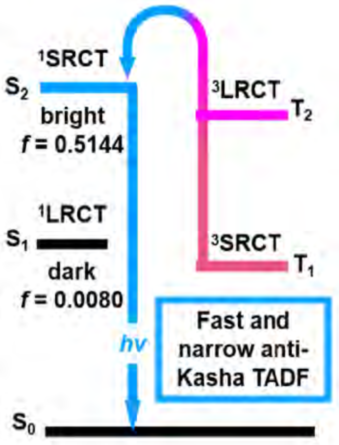

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Suppressing Exciton–Polaron Quenching in TADF OLEDs through Host-Induced Spontaneous Orientation Polarization

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Spontaneous orientation polarization (SOP) in vacuum-deposited organic films arises from the partial alignment of permanent molecular dipoles and can modify the internal electrostatic potential in OLEDs, leading to exciton quenching even below the turn-on voltage [1,2]. However, the influence of SOP on internal charge transport and exciton–polaron interactions in TADF architectures has not been systematically explored. In this work, we show that the SOP of a polar host in the emissive layer, combined with a polar electron-transport layer, electrostatically modulates internal fields to suppress exciton–polaron quenching by limiting hole penetration into the emissive layer.

OLEDs with the architecture TCTA / EML / TPBi were investigated, where the emissive layer (EML) consisted of 4CzIPN doped into either a nonpolar host (mCBP) or a polar host (BCPO). Impedance spectroscopy revealed that in devices incorporating the polar host, charge accumulation region is shifted from the EML/ETL interface toward the HTL/EML interface. Bias-dependent photoluminescence (PL) measurements indicate that PL quenching correlates with excess hole density within the emissive layer. In nonpolar-host devices, significant hole accumulation occurs inside the EML, resulting in pronounced quenching, whereas SOP in BCPO confines interface charges at the HTL/EML interface, substantially reducing exciton–polaron interactions. Displacement current measurements coupled with simultaneous PL (DCM-PL) directly link the onset of PL quenching to the presence of excess holes in the EML, confirming exciton–polaron quenching as the dominant nonradiative pathway. By controlling the spatial distribution of holes through host-induced SOP, devices achieve a threefold increase in external quantum efficiency.

These findings establish host polarization as an effective electrostatic design parameter for tuning charge distribution and mitigating exciton–polaron interactions in TADF OLEDs, providing an additional degree of freedom for optimizing device performance and stability.

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Phosphorescent Exciplexes

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The steady state and time dependent photoluminescence spectra have been studied to determine whether the formation of a charge transfer state occurs between pairs of various organic molecules at both room temperature and the low temperature of 80 K. Samples of these molecules were prepared on transparent quartz substrates in the form of thin films of the desired molecules which were prepared by dissolving in toluene, mixed in the desired ratios, pipetted onto the substrate and heated in a vacuum oven. The use of a fluorometer fluorolog, cryostat and ultra-fast 4 PICOS gated iCCD camera system with pulsed Nd:YAG laser at 355 nm were used for the steady state measurements, the cooling of the samples and the time dependent measurements respectively with the aim of creating an organic exciplex system which displayed signs of phosphorescent emission. Various ratios of acceptor to donor volume were tested in ratios of 80 : 20, 70 : 30, 50 : 50 and the reverse. Evidence of charge transfer formation was found across several of the pairs of organic acceptor and donor molecules tested via the redshift and broadening of their emission peaks compared to their individual emission peaks. Only one sample, 0,10-Dimethyl-9,10-dihydroanthracen-9-on (DMA) mixed with 1- (tert-butyl)-10H-phenothiazine (PTZ-tBu) displayed firm evidence of strong phosphorescence emission. In addition, the samples showing evidence of a charge transfer state were compared to the same component molecules covalently bonded together to determine the difference in photophysical properties. It was concluded that charge transfer states display evidence of different photophysical properties, and hence different singlet and triplet energy levels.

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Spin Coupling in Symmetric and Asymmetric Allyl and Phenalenyl Diradicals Bridged by an Inverted Singlet-Triplet System

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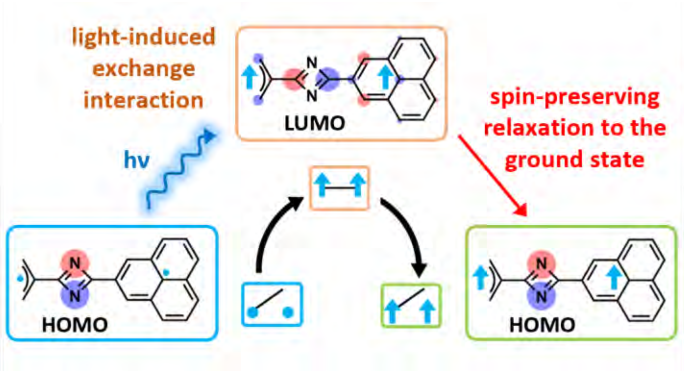
Optically addressable molecular spins are promising candidates for quantum sensing and information processing.[1,2] While metal-free organic diradicals offer high chemical tunability, realizing robust optically detected magnetic resonance (ODMR) functionality requires precise, light-driven control over spin-spin interactions.[1,2]

In this work, we present a comprehensive theoretical investigation of symmetric and asymmetric disjoint diradicals bridged by an inverted singlet-triplet (InveST) core. Specifically, we focus on a 1,3-diazete bridge coupled to allyl and phenalenyl radical units.[3] Employing the Pariser-Parr-Pople (PPP) Hamiltonian within a Restricted Active Space (RASCI) scheme, validated by multireference ab initio CASSCF/QD-NEVPT2 calculations, we demonstrate that these systems possess disjoint ground states with effectively degenerate singlet and triplet levels, indicating fully decoupled spins. However, the population of the bridge LUMO trough optical excitation triggers a finite exchange interaction that stabilizes the triplet excited state below the corresponding singlet. Crucially, we demonstrate that thermally accessible torsional fluctuations at the bridge-radical junctions break molecular planarity, activating the spin-orbit coupling (SOC) that mediates intersystem crossing (ISC), thereby driving the robust population of the T1 state from the excited singlet manifold.[3]

These findings highlight InveST-bridged diradicals as a robust, metal-free paradigm for room-temperature molecular qubits and spin-optical interfaces.[2,3]



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Computation of vibrationally resolved spectra of organic radicals: from benchmarks to applied systems

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Organic radicals, with properties such as unpaired electron spins, redox versatility, and magnetic behavior, hold significant potential for breakthroughs in organic electronics, photoredox catalysis, magnetic materials, and biomedical imaging.[1] While these properties make organic radicals highly promising, their effective integration into novel technologies remains challenging due to their instability at room temperature and typically weak emission. Recently,[2] the potential of open-shell neutral organic radicals as efficient OLED emitters has emerged. These radicals, emitting through spin-allowed doublet transitions ($D_0 \rightarrow D_1$), can overcome the 25% efficiency limit imposed by spin statistics in closed-shell organic emitters, which rely on intersystem crossing to a triplet state. Examples of the core structures of these radicals are provided in Figure 1. From a computational perspective, several studies have sought to elucidate the photophysical properties of these radicals, however, this task is challenging due to issues such as spin contamination, which limits the straightforward application of Density Functional Theory (DFT).

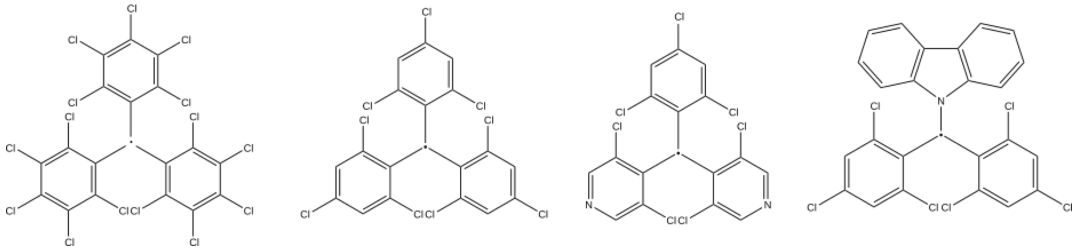

Figure 1: Example of radicals species used as emitters in OLED.

In this study, we build on these efforts by computing the vibrationally resolved absorption and emission spectra of selected radicals, a relatively unexplored aspect of their photophysical behavior. Using DFT and the harmonic model within the FCclass software,[3] we aim to establish best practices for accurately modeling these spectra by directly comparing computational predictions with experimental data from the literature. Our approach involves identifying optimal density functional approximations, selecting suitable vibrational models for the potential energy surfaces, and assessing the role of Herzberg-Teller effects. For absorption spectra, we conduct a preliminary analysis on a set of small benchmark radicals, while for emission, we examine the radiative and non-radiative constants of the radicals depicted in Figure 1, along with some of their most promising derivatives.

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Organic triradicals molecules to obtain high-spin ground state populations

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Recent studies, [1,2,3], have shown that light irradiation can enhance the quartet ground-state population of triradical molecules, making them promising candidates for magnetic sensing and quantum information applications. Here, we focus on π-conjugated triradicals to investigate radical–radical interactions in both ground and excited states through molecular structure tuning.

We present a theoretical-computational study of photoactive high-spin triradicals, analyzing the excited-state relaxation pathways responsible for quartet-state population. Excited-state properties are examined using the Pariser–Parr–Pople (PPP) model. To address the strong electron correlation characterizing these systems, we diagonalize the PPP Hamiltonian within a Configuration Interaction (CI) framework and compare the results with a Restricted Active Space CI (RASCI) approach based on tailored active spaces.

Given the multiconfigurational nature of the electronic states, we further benchmark our results against *ab initio* CASSCF-QD-NEVPT2 calculations. Our findings highlight the key role of frontier orbitals and molecular structure in governing radical interactions and demonstrate that the PPP-RASCI approach provides an effective balance between accuracy and computational cost for modelling excited states in organic triradicals.

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Wavefunction-based Descriptor for Thermally Activated Delayed Fluorescence Emitters

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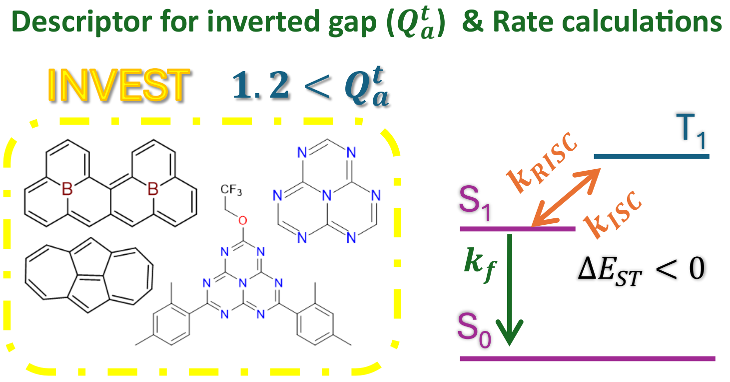
Thermally activated delayed fluorescence (TADF) systems, including multi-resonance (MR) and inverted singlet-triplet gap (INVEST), show great potential for applications such as organic light-emitting diodes due to their high emission efficiency. However, accurately predicting their electronic properties remains computationally challenging due to the delicate balance of electronic excited states involved, limiting efficient molecular discovery and design for industrial applications. This study investigates two aspects of MR/INVEST emitters: their electronic structure and excited-state rate constants. First, we study the relationship between the electronic structure of MR/INVEST emitters and their singlet-triplet energy gaps using wavefunction-based descriptor. This descriptor (Q_a^t), originally proposed for ionic states, measure the distribution of charges in atomic centers based on the 1-electron transition density matrix. Here, we directly analyze the transition density matrix connecting singlet and triplet excited states involved in TADF. Our findings reveal a correlation between the descriptor and the singlet-triplet energy gap, with smaller (more negative) gaps corresponding to higher descriptor values, leading to a separation between INVEST and MR-TADF systems. Thus, the descriptor can be used to predict singlet–triplet gap inversion. The descriptor also distinguishes excited states involved in TADF within the triplet manifold. Then, we identified the potential deactivation pathways using excited-state decay rate constants calculations. We calculated the fluorescence, direct and reverse intersystem crossing (RISC) rate constants, and we assessed the influence of Herzberg-Teller effects and potential energy surface model, among other parameters. Optimized structures, Hessians, and SOCMEs were obtained at TDA-DFT/CAM-B3LYP, and excitation energies were calculated using SCS-CC2 and ADC(2) to ensure accurate energy values for rate constant calculations. We found that the favorable thermodynamics for the RISC in INVEST systems leads to $k_{RISC} > k_{ISC}$, with k_{RISC} values typically exceeding 10^6 s^{-1}.



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Photoinduced transient structure in an organic light-emitting material

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Organic light-emitting diodes are self-emissive devices that are thin, lightweight, and capable of reproducing a wide and vivid color; therefore, they have been applied in displays and lighting. Thermally activated delayed fluorescence (TADF) materials have attracted significant attention owing to their high emission efficiency. They utilize reverse intersystem crossing (RISC) to convert energy from the lowest triplet excited state (T_1), which can undergo thermal deactivation, to the lowest singlet excited state (S_1) [1]. The rate constants of nonradiative transitions between S_1 and T_1 have been studied in previous reports. Molecular structural changes have also been predicted to affect these processes [2]. However, the transient structure in the excited state has never been directly observed. In this study, we employed ultrafast time-resolved electron diffraction measurements to elucidate the transient structure of photoexcited 4CzIPN single crystals. Our results reveal that 4CzIPN molecules undergo rotational motion of the carbazolyl groups in the excited state. The time constant of this intramolecular structural change is consistent with the results obtained using time-resolved photoluminescence and infrared spectroscopy. Quantum chemical calculations further suggest that 4CzIPN crystals rapidly transition from S_1 to a structurally stable T_1 state upon photoexcitation. These findings are expected to contribute to the design and development of novel organic light-emitting materials.

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Dibenzofuran-Based Hosts for Stable Blue TADF-OLEDs: the Role of Charge Trapping

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Organic light-emitting device (OLED) technology has become dominant in the display sector owing to its high energy efficiency and fabrication versatility. Although thermally activated delayed fluorescence (TADF) emitters enable near-unity internal quantum efficiency, the realization of stable and efficient blue devices remains limited by the availability of suitable high-triplet-energy host materials. Device stability is particularly sensitive to the host response under electrical stress. Moreover, many widely used hosts contain weak C–N bonds that are susceptible to dissociation in the anionic state [1]. Thus, the rational design of host materials that combine high triplet energy with balanced charge transport and robust bonding is essential for further progress in blue TADF OLEDs.

Here, we report four chemically robust dibenzofuran–biphenyl (DBF-BPh) hosts designed to systematically probe the effects of DBF linkage position (2 vs 4) and tert-butyl substitution on material properties and device performance. All hosts exhibit high neat-film triplet energies (T_1 = 2.77–2.87 eV) and strong multi-state bond dissociation energies (BDE > 2.3 eV). In blue TADF OLEDs, the 4-linked host delivers the best overall performance, achieving EQE_{max} up to 23.5% with low roll-off and LT_{50} = 17.5 h at 1000 cd m^{-2}. In contrast, tert-butyl-substituted analogues exhibit 2–4x shorter operational lifetimes despite comparable energetics and BDE. Impedance spectroscopy and equivalent-circuit analysis reveal >5x higher characteristic parallel resistance in OLEDs with tert-butyl-substituted hosts, implying enhanced charge trapping, consistent with increased carrier accumulation and exciton-polaron annihilation-induced losses under electrical operation.

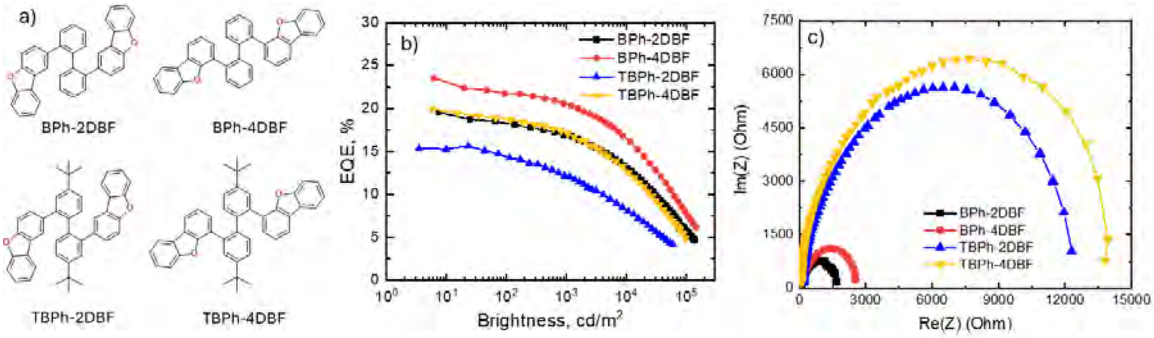

Fig 1. (a) Molecule structures of new hosts, (b) EQE – brightness characteristics of (BPh-DBF) host-based blue TADF OLEDs, (c) impedance spectroscopy results of the OLEDs: Cole–Cole plots measured at 7V.

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Detuning-Dependent Electroluminescence in TADF Polariton OLEDs

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Controlling electroluminescence through light-matter hybridization in organic microcavities is a promising strategy for next-generation optoelectronic devices [1, 2].

Here, we investigate the detuning-dependent emission behavior of blue thermally activated delayed fluorescence (TADF) polariton organic light-emitting diodes (POLEDs) by incorporating an assistant strong coupling layer (A-SCL) containing absorbers with different exciton energies. Two coupling materials, BSBCz and v-DABNA, with different absorption onsets were employed within a mixed A-SCL, while the cavity thickness was adjusted to modify the optical mode condition. Angle-resolved electroluminescence at 100 cd/m² reveals distinct dispersion and angular emission characteristics depending on the coupling material and cavity thickness. For the sky-blue device, the BSBCz-based POLED 1 device achieves an EQE of 18%, compared to 12.3% for the v-DABNA device (POLED 2), accompanied by broader angular spectral dispersion. In contrast, a green-emission device incorporating v-DABNA (POLED 2) reaches an EQE of 29.6%, exceeding the POLED 1 (24.9%) while maintaining comparable angular stability.

The results demonstrate that exciton-energy engineering in the strong coupling layer provides an effective approach to modulate electroluminescence in TADF POLEDs and can be utilized to enhance the performance of narrowband and angle-stable blue OLEDs for display applications.

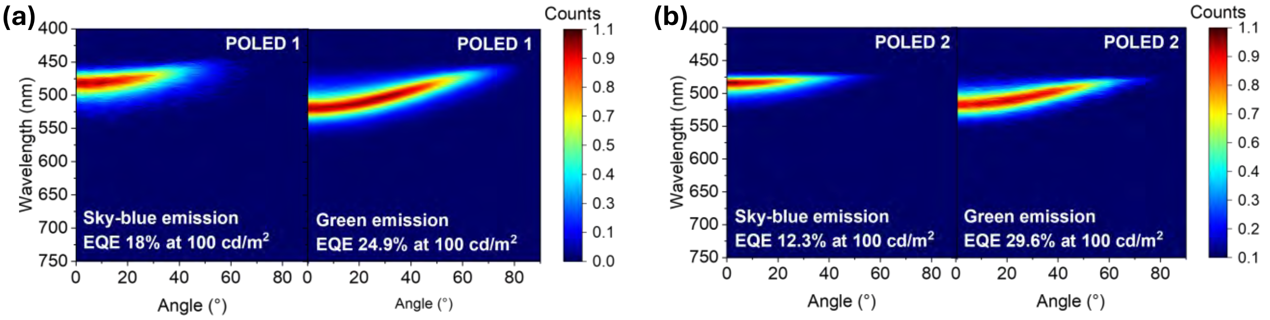

Figure 1. Angle-resolved electroluminescence spectra of POLEDs at 100 cd/m^2 with different absorbers in the A-SCL (a) BSBCz-based POLED 1 and (b) v-DABNA-based POLED2, each showing sky-blue and green emission. The devices exhibit distinct angular dispersion behavior and EQEs of 18% / 24.9% in POLED 1 and 12.3% / 29.6% in POLED 2, respectively.

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From unconventional CT-TADF scaffolds to spin-flip engineering in MR-TADF NIR-emitting materials: A molecular design approach

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Historically, the development of organic NIR-TADF emitters has centered on donor-acceptor architectures, utilizing large, pyrazine-derived acceptor cores to achieve the desired red-shift. However, these particular systems often suffer from broad emission profiles, poor processability, and low photoluminescence quantum yields (PLQYs), presenting a significant bottleneck [1]. Moving beyond these conventional scaffolds, researchers have pivoted toward the design of compact but highly electron-deficient acceptor moieties. While not straightforward, our investigation into these alternative structures remains active and ongoing [2]. Parallel to these efforts, and following the seminal work by the group of Duan *et al.*, a new strategy was adopted focused on multi-resonant (MR) NIR-TADF frameworks [3]. While MR architectures already offer exceptional emission performance, efficiently reaching longer wavelengths requires overcoming their small Stokes shifts and slow spin-flip kinetics. Our work explores a systematic molecular design approach aimed at modulating the excited-state dynamics through two key design rules: the integration of heavy atoms to enhance spin-orbit coupling, and the incorporation of ring-strain to induce structural distortions. These modifications are intended to modulate the energy landscape between the S_1 and T_1 states, providing a tunable platform for triplet exciton management. By breaking the planarity typically associated with MR systems, we aim to accelerate k_{RISC} and suppress the quenching mechanisms inherent to long-wavelength emitters. Furthermore, we explore molecular motifs that limit the overall size of the emitter, ensuring high solubility and ease of processing for both vacuum-deposited and solution-processed devices. As we progress from the synthesis phase to comprehensive photophysical benchmarking, we invite potential collaborators with expertise in device engineering and NIR-OLED architectures to discuss the integration of these novel NIR-MR-TADF materials into high-performance optoelectronic devices.

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Beyond The RISC Rate: A Figure of Merit for MR-TADF Materials and the Path to High Efficiency OLEDs Having Minimal Efficiency Roll-Off and High Stability

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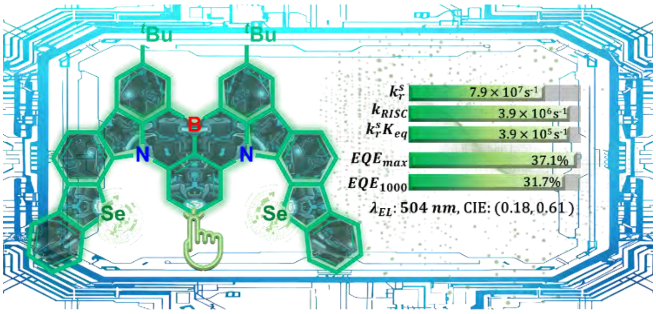
The relatively slow reverse intersystem cross rate constant (k_{RISC}) of multi-resonant thermally activated delayed fluorescence (MR-TADF) emitters has been recognized as perhaps the most significant factor governing the rather significant efficiency roll-off in MR-TADF organic light-emitting diodes (OLEDs). A recent study identified a figure of merit for TADF materials, [1] which captures the relevant exciton dynamics processes and correlates these with efficiency roll-off in the resulting device. Two MR-TADF emitters **tBTCzBN** and **tSeCzBN,** containing, respectively, dibenzothiophenocarbazole and dibenzoselenophenocarbazoles were designed. [2] Their rigid p- and n-doped nanographene structures, incorporating heavy chalcogen atoms at optimal locations, result in fast k_r^Ss of 1.7×10^8 and 7.7×10^7 s^{-1}, k_{RISC} values of 2.6×10^5 and 3.9×10^6 s$^{-1,}$ and FOMs of 1.8×10^5 and 3.9×10^5 s^{-1} for **tBTCzBN** and **tSeCzBN**, respectively. The sensitizer-free OLEDs with **tBTCzBN** and **tSeCzBN** exhibited green electroluminescence [CIE coordinates of (0.14, 0.61), and (0.18, 0.61)]. Notably, the device with **tSeCzBN** delivered very high maximum external quantum efficiencies ($\mathrm{EQE_{max}}$) of 37.1%, with $\mathrm{EQE_{1000}}$ of 31.7%, which is one of the highest reported $\mathrm{EQE_{1000}}$ values, and reflects a remarkably low efficiency roll-off of 14%, especially compared to other MR-TADF OLEDs. [2] This work highlights the distinct benefits and the importance of judicious incorporation of heavy atoms within MR-TADF emitter structures to facilitate efficient exciton harvesting and enhance device performance.



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Dual-Chromophore Isolation Strategies for Efficient Upconversion in TADF Emitters via Rigid, Covalent Bridges

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The development of high-efficiency organic light-emitting diodes (OLEDs) hinges on the precise control of excited-state dynamics in thermally activated delayed fluorescence (TADF) emitters. A promising approach involves the use of dual-chromophore architectures, in which multiple chromophores are integrated into a single emitter molecule [1]. The degree of conjugation between these chromophores inherently governs the emitter's optical and electronic properties, with recent studies indicating that a reduction in conjugation enhances device performance.

In this study, we investigate a dual-chromophore TADF emitter linked by a series of rigid, covalent bridges (Figure 1). These bridges systematically modulate the degree of conjugation and through-space coupling, significantly influencing key photophysical properties, including the singlet-triplet gap and the associated emission pathways available.

Our findings demonstrate that sterically hindered and electronically decoupling bridges effectively reduce conjugation, leading to distinct emission profiles, and ultimately aiming to enhance exciton utilisation and improve device efficiency. This work offers a rational framework for the next generation of OLED devices, emphasising the pivotal role of bridge-mediated tuning of TADF emitters for optimised performance and efficiency.

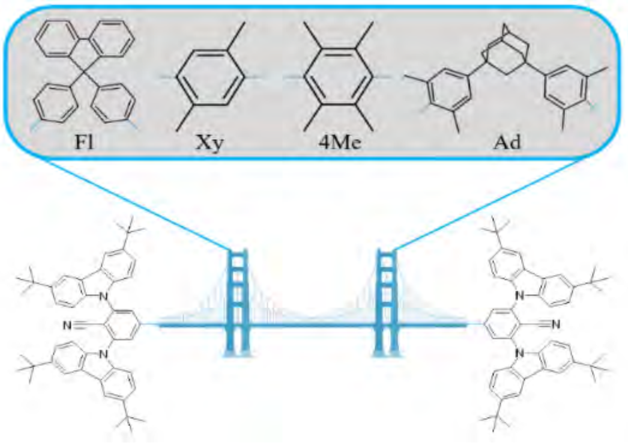

Figure 1: Structural representation of dual-chromophore system for TADF emitters, illustrating the different bridges investigated.

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Effect of chlorine atom on spectral parameters in molecules exhibiting thermally activated delayed fluorescence

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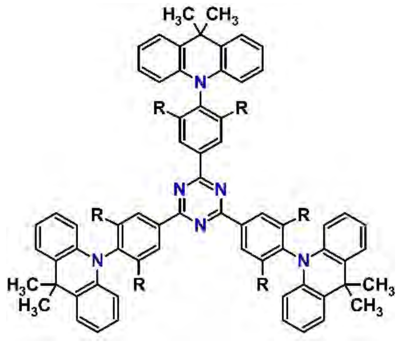
Thermally activated delayed fluorescence (TADF) is a phenomenon occurring in molecules. It enables the increase of efficiency and stability of organic light-emitting diodes (OLEDs), that are used in modern displays and lighting. The key parameter to design a high performing TADF emitter is fast reverse intersystem crossing (rISC), which requires a balance between singlet–triplet energy gap (ΔE_{ST}) and high spin–orbit coupling (SOC). However, these two parameters are typically reverse correlated. In this work we propose a molecular design strategy based on introducing a moderate heavy-atom substitution (chlorine), which reduces ΔE_{ST} and strengthens SOC, thereby accelerating rISC and improving overall emitter performance.[1]

We report a comparative study of triDMAC-TRZ [2] and its chlorinated analogue triDMAC-diCl-TRZ to reveal how selective halogen substitution modulates TADF. To assess the potential for various applications, including OLEDs, we tested both emitters in the crystalline state and dispersed in host matrices of varying polarity (BCPO, mCBP-CN, and ZEONEX®). Detailed photophysical investigations revealed that, e.g. in ZEONEX® films, the delayed fluorescence lifetime shortens from 50 µs in triDMAC-TRZ to 0.4 µs in triDMAC-diCl-TRZ, as k_{rISC} increases from $3*10^4$ to $8*10^6$ s^{-1}, respectively. The reasons of such improvement is extremally low activation energy (E_a) 13 meV and simultaneous increase of SOC.



R = H (triDMAC-TRZ),
R = Cl (triDMAC-diCl-TRZ)

In the crystalline state, triDMAC-diCl-TRZ shows a pronounced bathochromic shift and altered excited-state dynamics. Single-crystal XRD reveals strong π–π interactions between chlorinated acceptor units, forming dimers that stabilize the S_1 state and modify triplet harvesting. Such interactions are absent in the non-chlorinated analogue.

Density functional theory (DFT) calculations confirm that, chlorine substitution enforces orthogonal D–A geometry and enhances SOC through static and vibrational heavy-atom effects, especially through coupling of S_1 with higher-lying locally-excited triplet states. Such a selective single-atom modification enables efficient rISC even in rigid crystals, providing a robust design strategy for high-performance, fast-response materials for light-emitting applications.

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Azepine Donors as Conformational Control Elements for Tailored Charge-Transfer States in Organic Emitters

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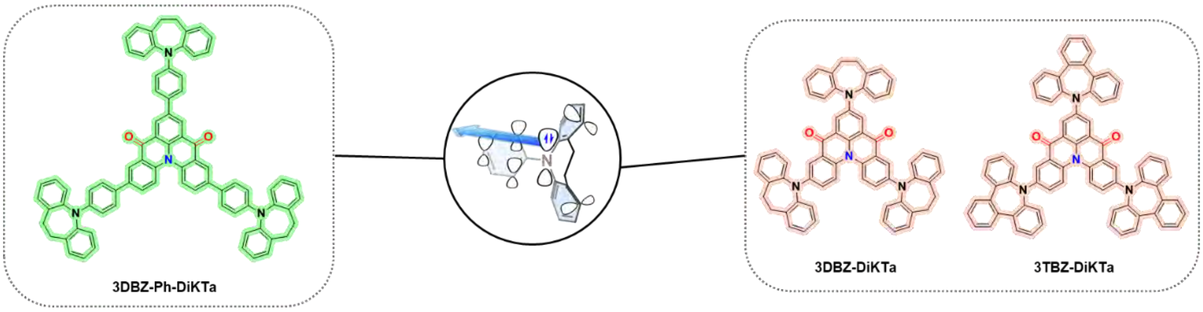

Molecular donor conformation is a decisive but underutilized parameter for controlling excited-state topology in donor-decorated MR-TADF frameworks. We introduce azepine donors as conformational control units that enforce quasi-axial donor geometries to systematically modulate charge-transfer character and singlet–triplet energies. Dibenzoazepine (DBZ) donors were first connected to **DiKTa** MR-TADF cores via a phenylene bridge and benchmarked against twisted TPA and HMAT donor-analogues. The quasi-axial geometry of the azepine enforces a distinct donor–acceptor orientation, enabling systematic tuning between short-range (SRCT) and long-range charge transfer (LRCT). Moreover, direct azepine–**DiKTa** coupling yields red emitters with substantially prolonged prompt lifetimes (>20 ns). This translates into enhanced contrast in fluorescence lifetime imaging microscopy (FLIM), underscoring their potential as lifetime-encoded probes. Azepine donors thus emerge as structural design elements for programmable excited-state landscapes across emission color, lifetime, and ΔE_{ST}.

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1,6-Diazapyrene: A Novel, Well-Defined, Small-Size Prototype System for Nitrogen-Containing PAHs

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Nitrogen doped polycyclic aromatic hydrocarbons (N-PAHs) are interesting materials to tune the electronic, optical and photophysical properties of PAHs, graphene, and carbon dots in (opto)electronic, (photo)-catalytic and biochemical and biomedical applications. Among them, diazapyrene (DAP) appears as a small-size prototype system to understand the relationship between the structure and the resulting photophysical and photochemical properties, such as deactivation pathways, which are crucial for the functionality in the different applications. In particular derivatives of the 2,7-isomer (DAP27) were studied for the purpose of organic electronics, as well as model systems for N-PAHs and carbon dots. [1, 2] In the case of solvothermally synthesized carbon dots, it has been shown that N-PAHs are responsible for their photoluminescence, even though the presence of specific DAPs has not been detected.

In the present study, a novel, simple, and small compound,1,6-diazapyrene (DAP16), was synthesized. In-depth analysis, employing optical spectroscopy and (time-dependent) density functional theory, (TD-)DFT, elucidates the optical excitations on the basis of MO symmetry, energy, and topology considerations, unveiling the photophysical and photochemical deactivation kinetics after photoexcitation. The new compound dramatically changes the optical excitation, and subsequent photophysics and -chemistry compared to pyrene and the well-studied 2,7-diazapyrene. The high sensitivity of the aza-substitution position to generate such changes is considered as highly relevant for the targeted design of N-doped PAHs in general. [3]

Furthermore, because of its unique photophysics, DAP16 shows an extreme sensitivity against oxygen, leading to reversible peroxide formation. The activity of DAP16 in the presence of oxygen is being further investigated for possible bioapplications.

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From Donor Substitution to Distance-Controlled TADF dimers: Curcuminoid derivatives for OLED applications

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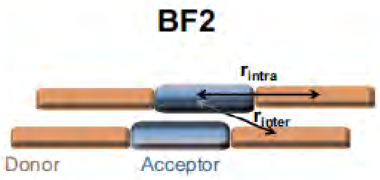
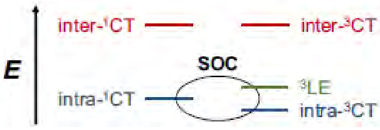
Curcuminoids constitute of a class of materials which has shown interest in bioimaging and organic light-emitting diodes (OLEDs) applications. In particular, BF2, a curcuminoid derivative containing a difluoroboron group as acceptor and two diphenylamine electron donors, has attracted some attention for its near infrared light emission. The curcuminoid core exhibit a large versatility in their synthesis allowing to vary the nature of the electron donor and acceptor to tune the optoelectronic properties of these materials. A systematic investigation of twelve donor molecules derived from BF2 to evaluate how chemical substitution affects the electronic nature and vertical excitation energies of the lower-lying singlet (S_1) and triplet (T_1) states. To this end, excited-state calculations has been carried out at the SCS-ADC(2)/def2-TZVP level. S_1 and T_1 nature was analysed using difference-density-based descriptors ($\Delta\rho$), together with the amount of charge displaced during excitation (q_{CT}) and CT distance between positive and negative barycenters (D-index). These metrics allows us to rationalize the evolution of the singlet-triplet energy gap ΔE_{S-T} and the SOC between S_1 and T_1, which governs driving RISC process at the single molecule level. Our calculations reveal that the ΔE_{S-T} is too large and the SOC too small to promote RISC at the singlet molecule level for all compounds investigated. However, our results indicate that T_2 state is nearly degenerate with the S_1 state and therefore T_2 state could serve as a doorway state to repopulate the singlet manifold. We next investigated the singlet and triplet dimer excited states for two representative molecules of the series using optimally ω-tuned LC-ωhPBE, with tuning based on Koopmans-compliant procedures to ensure correct separation of short- and long-range exchange contributions [1]. For the two selected dimers, the dependence of the excited-state landscape on intermolecular distance has been explicitly investigated, following the strategy reported for BF_2 dimers [2]. A near-degeneracy between ^{1}CT and ^{3}CT states is observed at specific intermolecular separation, a condition under which spin interconversion is no longer expected to be driven by SOC, but instead through HFI mechanism. These findings shed light on the structural and electronic factors driving CT-mediated TADF in donor dimers and outline the conditions under which HFI-driven RISC becomes operative.





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Fluorescence Efficiency Regulation in Conjugated Organic Materials

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Conjugated organic chromophores have found immense interest in current materials research, and rapid progress has been seen over the past years. In any case, the quest for sustainable research demands pre-synthesis tailor-made targeted design beyond experimental (and computational) trial-and-error strategies. This can only be achieved by a thorough understanding of the underlying photophysical process combined with spectroscopic and computational techniques. [1]

A central figure of merit is the fluorescence quantum yield Φ_F of the compounds, which is decided by the competition of radiative vs. nonradiative processes. [1] This is not only key for obvious applications like OLEDs, OLETs, lasing, sensing, or bio-imaging, but also e.g. for photovoltaics.

In solution, nonradiative decay is mainly driven by internal conversion (IC; and subsequent vibrational relaxation; VR); this is frequently tackled via a 'Fermi's Golden Rule' (FGR) approach.[1] However, in the last years, it has become increasingly evident that FGR may break down both in a quantitative as well as in a qualitative manner, in particular for systems with very effective IC. This was especially shown for compound families which establish an 'inverted energy gap law', contrasting the prediction of FGR in a simple view. Instead, this can be well understood in the framework of conical intersections (CIs), which provides an accurate description of IC. [2,3]

In molecular solids, IC becomes a minor pathway in most cases, as the access to the CI often involves large amplitude motions which are effectively blocked in rigid environments; [2,3] this gives subsequently rise to 'Solid State Luminescence Enhancement' (SLE). [1,2] On the other hand, examples of active CIs in solid state samples have been identified, due to the absence of large amplitude motions on the path to the CI, [3] so that fluorescence quenching may persist across solution and molecular solids.

Nevertheless, the most crucial quenching pathway in molecular solids is trapping (at surfaces/interfaces), which becomes notorious in polycrystalline samples, while single crystals of the same materials are commonly highly luminescent. [1] The central role of trapping is largely underestimated in the community, and strategies how to achieve highly luminescent polycrystalline samples are therefore addressed.

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Unbiased Atomistic QM/MM Modelling of Crystal Emission Spectra of Conjugated Organic Molecules at Cryogenic Temperatures

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In the study and development of organic conjugated materials for optoelectronic applications, an understanding of vibronic coupling plays a key role. This property governs the shape and position of their spectra, allowing for color-control. At room temperature, complex vibronic patterns are commonly obscured by environmental broadening, which prevents detailed insight into the underlying mechanisms of coupling. On the other hand, at liquid helium temperatures in confined environments, a rich pattern of progressions and intercombination bands becomes visible. For isolated molecules, this can be achieved in Shpolskii matrices [1], while for aggregated systems, it is accessible via single crystals [2,3], as demonstrated, for instance, with distyrylbenzene (DSB) derivatives in our group over the years [1-3].

Nevertheless, the complexity of the vibronic pattern does not allow for a detailed Franck-Condon (FC) analysis from experiment alone. This demands explicit quantum-chemical calculations, particularly within the framework of (time-dependent) density functional theory, (TD)DFT. Especially for the emission process, the application of unbiased models results in more precise spectra—for example, using atomistic approaches via QM/MM techniques, as pioneered in our group [3]. This allows for a detailed dissection of intramolecular and intermolecular FC couplings, as well as aggregate-type Herzberg-Teller couplings [3].

However, such calculations still pose challenges, particularly for molecules with strongly distorted backbones, such as cyano-substituted DSB variants (DCS), which may persist even in single-crystal environments [7,8]. In fact, in this case, linear and quadratic coupling cannot be separated, as mode-mixing is effective; this imposes technical challenges in calculating full vibronic coupling for both Shpolskii-embedded single molecules and single crystals. Consequently, this project aims to tackle these challenges using experimentally available cryogenic (1.4 K) emission data of molecules and crystals with varying degrees of backbone distortion. This will allow us to disentangle intra- and intermolecular contributions to excited-state structural reorganization, as well as static structural inhomogeneities, both of which are of central importance to understanding the complex photophysics of conjugated organic molecules

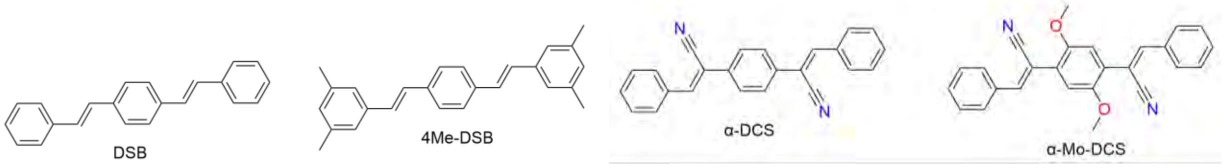

Figure 1: Molecular structures of DSB derivatives

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Nanomechanical Behavior of π-Conjugated Systems: From Single Molecule to Polymer Thin Films

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π-conjugated systems are central in organic electronics whose optoelectronic properties are tuned by molecular design to improve the efficiencies of devices. Besides, their nanoscale mechanical properties are key for the development of flexible devices.

In this contribution, we will discuss the mechanical properties for three different systems at different length scales using molecular dynamics (MD) simulations. We first investigated a PDI dimer where the two molecules interact through non-bonded interactions. Here, we unraveled the mechanism for disrupting the π stacking of the two PDIs as observed in atomic force microscopy (AFM) pulling experiments and linked it to concerted relative rotation and sliding of the two PDIs.

We next explored the impact of the addition of linear alkyl chains on the mechanical response of small molecule organic semiconductors. We focused on DNTT and its alkyl derivative C8-DNTT-C8, largely used in organic field-effect transistors.[1] Combining MD and AFM, we showed that while the side chains provide more flexibility along the backbone of the molecule, C8-DNTT-C8 becomes stiffer in the conduction plane as compared to bare DNTT.

Finally, we investigated two polymers, PBTTT, a semi-crystalline polymer, and IDTBT, with a near amorphous morphology that exhibit contrasting mechanical behaviors.[2] Indeed, atomic force microscopy (AFM) mapping reveals a heterogeneous Young's modulus in PBTTT, compared with a more uniform one in IDTBT. To gain insight behind these disparities, we use molecular dynamics (MD) simulations to correlate microstructure with mechanical response and highlights the role of the anisotropy of mechanical responses.

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Temperature-Dependent Exciton Dynamics and Energy Funneling in MAPbBr3 Nanocrystals

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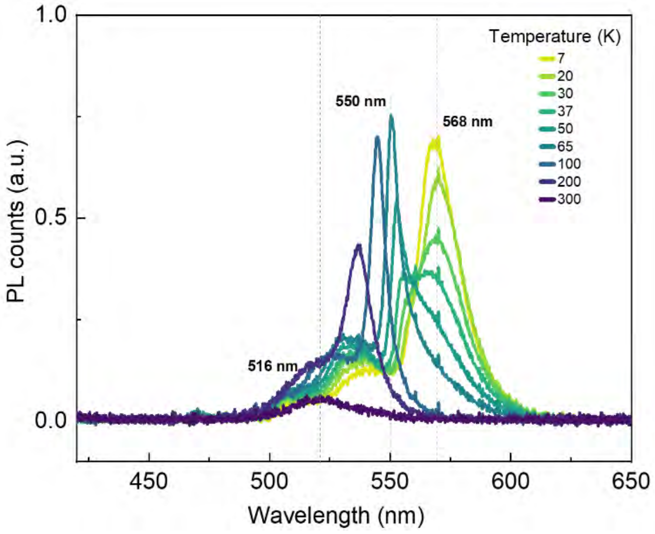
$MAPbBr_3$ nanocrystals exhibit size-dependent optoelectronic properties modulated by quantum confinement and defect-related states. At room temperature, layered nanocrystals show a photoluminescence band-edge emission at 516 nm. As the temperature decreases, two additional red-shifted emission peaks appear at 550 nm and 568 nm. This temperature-dependent optical properties indicates a substantial contribution of energy funneling toward lower-energy emissive states. The nanocrystal substructure further modulates this process by enabling exciton transfer to bulk-like or defect-associated energy minimum. These findings highlight the critical role of temperature, nanocrystal substructure, and energy funneling in controlling excitonic populations and recombination dynamics across different $MAPbBr_3$ morphologies.



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POSTER SESSION

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Low optical-loss design toward perovskite injection lasing

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Metal halide perovskites have emerged as promising candidates for lasers owing to their high optical gain, near-unity photoluminescence quantum yield, and low stimulated emission thresholds. While indirectly electrical driven perovskite lasers have been demonstrated [1], achieving an electrically pumped perovskite laser remains a significant challenge. A major limitation arises from the high optical losses associated with proximate metallic electrodes. Transparent conductive oxides such as indium tin oxide (ITO) offer a potential alternative, and net optical gain in perovskite devices with ITO electrodes under optical pumping has been reported [2].

In this work, we report on perovskite light-emitting diodes (PeLEDs) with both cathode and anode made of ITO based on a state-of-the-art conventional stack [3] (Fig. 1a). By optimizing the hole injection layer (HIL), we reduce the threshold of optically pumped amplified spontaneous emission (ASE) more than 4 times (Fig. 1b) while improving the electrical performance of the device under direct current (DC) injection (Fig. 1c). We also operate the optimized device under nanosecond electrical pulsing in the kA.cm^{-2} range. These results provide new insights into stack design strategies and represent an important step toward the realization of perovskite injection lasers.

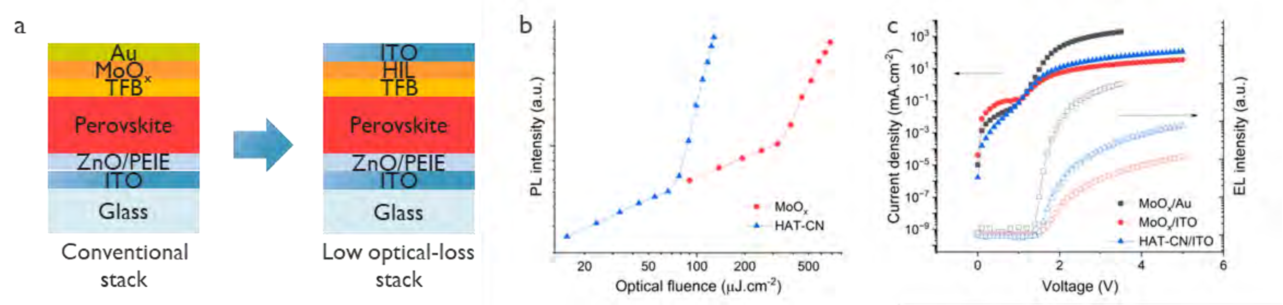

Fig. 1. (a) Schematic of conventional and low optical-loss device stacks. (b) Dependence of photoluminescent (PL) intensity on input laser fluence. (c) Dependence of current density and electroluminescent (EL) intensity on voltage.

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Loss Modeling of Diameter-Dependent Thresholds in Perovskite-on-SiN WGM Lasers

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Metal-halide perovskites have rapidly advanced as promising gain materials for compact laser sources, owing to their high optical gain, spectral tunability, and easy processing [1,2]. In this work, we investigate the dependence of lasing threshold on diameter in hybrid perovskite-on-SiN whispering-gallery-mode (WGM) resonators and introduce an analytical model to interpret the observed scaling. Threshold measurements across a wide range of diameters reveal two distinct operational regimes. In the small-radius limit, the threshold is dominated by curvature-induced radiative losses, which impose a steep geometric penalty on modal confinement [3]. Beyond a characteristic diameter, further enlargement of the cavity doesn’t impact threshold reduction, indicating that scattering associated with the perovskite gain layer sets a diameter-independent loss floor. To capture these behaviors, we formulate the total attenuation as the sum of a radius-dependent bending-loss term and a constant scattering contribution. This phenomenological representation accurately reproduces the experimental threshold evolution and enables quantitative separation of the loss channels. The model provides a direct basis for optimizing WGM resonators' dimensions and highlights material-scattering mitigation as the primary route to threshold reduction in the large-diameter regime.

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Computational modelling of chiral additive-induced Circularly Polarized Luminescence in π-conjugated polymers for Organic Light-Emitting Diodes applications

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Organic light-emitting diodes (OLEDs) are complex devices made in a multilayer structure. The external quantum efficiency (EQE) of such a device is the product of the internal QE (IQE) quantifying the percentage of electrons and holes leading to recombination in emissive excited states, and a light outcoupling parameter characterizing the light transmission through the OLED structure. OLEDs are usually equipped with an anti-glare filter. This filter is usually a chiral photonic structure that on one hand hinders incoming ambient light from entering the OLEDs stack to avoid visibility issues and on the other hand, blocks fifty percents of the usually unpolarized light generated in the OLED emitting layer thus severely limiting the EQE. [1] To circumvent this latter issue, organic π-conjugated materials exhibiting (either left- or right-handed) circularly polarized luminescence (CPL) were developed to improve light outcoupling. Since organic molecules show very small dissymmetry factors g_{lum} around 10^{-3}, the CPL they produce yields a negligible improvement to the light outcoupling. Using polymers and chiral dopants, the polymers can assemble in chiral superstructures, resulting in a massive increase of g_{lum} reaching 0.8 [2] for fluorene-based copolymers.

This work will focus on the modelling of both the vibrational circular dichroism (VCD) of the structures and their chirality index as defined by Solymosi. [3] Within this framework, our two model systems are poly(9,9-di-*n*-octylfluorene) (PFO) and poly(9,9-di-*n*-octylfluorene-alt-benzothiadiazole) (F8BT), two fluorene-based polymers known for exhibiting high photoluminescence in the green and blue regions, respectively.

Comparing our results with the studies carried out by our experimentalist collaborators, we can analyze the structure these polymers adopt in a thin film and how the chirality of the structure can affect the luminescence properties of these materials.

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Activation of TADF in Photon Upconverting Crystals of Dinuclear Cu(I)-Iodide Complexes by Ligand Engineering

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Cu(I)-halide based emitters have emerged as a potential alternative to the traditional semiconductors and quantum dots in the field of optoelectronics and non-linear optics in recent times. The emission mechanism of these emitters is interpreted mostly as an admixture of two pathways, emissive decay from (metal+halide)-to-ligand charge transfer ((M+X)LCT) states and triplet cluster-centered (^{3}CC) states. Several complexes and their emission mechanism have been reported but, segregation and correlation between (M+X)LCT and ^{3}CC emission are lacking in the previous literature. Despite having prominent charge transfer excited states, non-linear optical properties of these systems also remain unexplored.

To eradicate these lacunae, we have prepared two novel Cu(I)-iodide di-nuclear complexes coordinated with pyridine-based and triphenylphosphine ligands in this work. The photophysical properties have been studied and the contributions of two emissive states in the total emission process have been explored with several experimental methodologies. The Cu…Cu distance was sequentially tuned in three complexes to show the correlation between these two emissive states. The complex with highest extent of Cu⋯Cu interaction, exhibited mixed triplet (M+X)LCT and ^{3}CC emission whereas the other complex without Cu⋯Cu interaction exhibited simultaneous thermally activated delayed fluorescence (TADF) from (M+X)LCT states. The excited states have been characterized by DFT calculations, and it was also found that increased ^{3}CC emission can cause a large suppression of the TADF process from the low-lying (M+X)LCT state. Moreover, the complexes in their crystalline state were found to manifest third-harmonic up-conversion, which has potential applications in the field of laser technologies and quantum information science.

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Design of efficient, NIR-luminescent Pd/Pt(0) complexes

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At the doorstep to the near infrared region (NIR), the energy gap law greets. It states that the nonradiative decay rate k_{nr} increases exponentially with decreasing energy difference. Unfortunately, the radiative rate shrinks cubically with the energy gap. Additionally, non-adiabatic coupling and direct spin—orbit coupling (SOC) can affect k_{nr}. Efficient luminescence requires thus a) weak direct coupling to the ground state S0, but b) sizeable transition dipole moments to achieve sufficient radiative rates.

A reliable prediction of NIR luminescent molecules requires a quantitative description of the electronic state landscape, for which we use the DFT/MRCI method.[1] It combines the description of dynamic correlation via density functional theory (DFT) and static correlation via the multireference configuration interaction (MRCI) component. SOC is described in SOCI, which treats spin-free and spin-dependant operators on the same footing.[2]

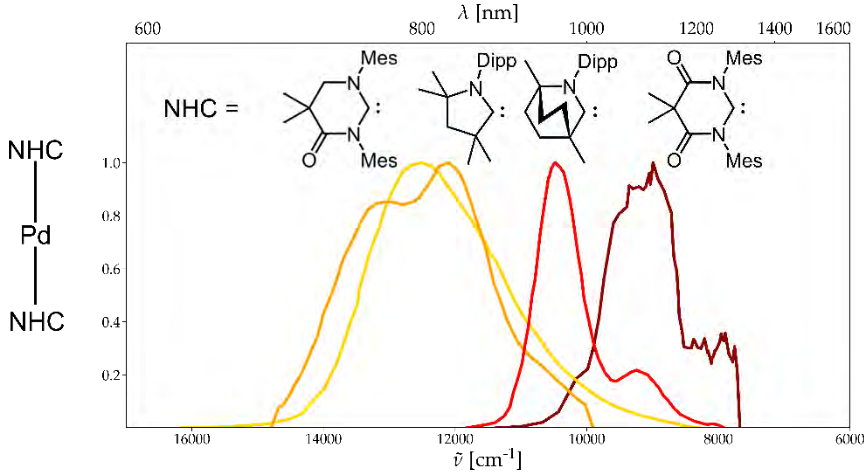

Figure 5: Emission spectra of the respective bis-carbene Pd(0) complexes

Counterintuitively, metal to ligand charge transfer (MLCT) states of neutral d10-complexes may fulfil all listed requirements, provided that the underlying complex is designed well. Linear bis-carbene complexes can possess low direct coupling to S0 and sizeable radiation rates, but at first sight, their linearity conflicts with low-lying carbene orbitals and NIR luminescent states. Careful construction of the employed carbenes can overcome the challenges and enable efficient IR-luminescence. Literature and own results support the underlying theoretical model for the design guidelines.[3]

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Development of High-Efficiency and Stable Deep-Blue Phosphorescent Pt(II) Dopants for OLED Applications

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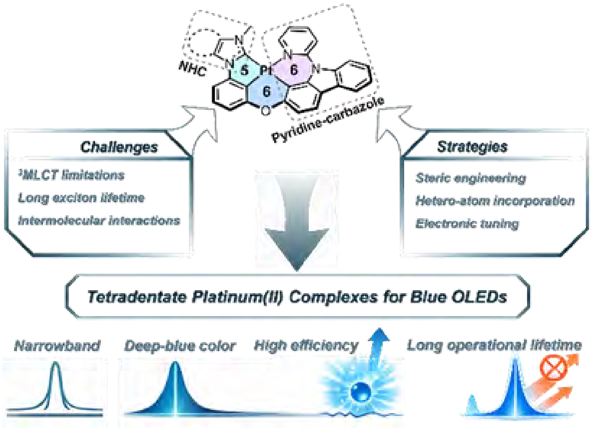
Deep-blue phosphorescent emitters are critical for achieving high-resolution and energy-efficient OLED displays; however, realizing simultaneous high efficiency and long operational lifetime in this spectral region remains challenging. The high triplet energy required for deep-blue emission often leads to accelerated efficiency roll-off and material degradation under high-brightness operation. In this work, we report the development of Pt(II)-based deep-blue phosphorescent dopants designed to address these limitations. Through systematic molecular design and coordination environment control, the electronic structure and emissive characteristics of the complexes were tuned to support efficient deep-blue emission while enhancing material stability. The synthesized complexes exhibit deep-blue photoluminescence with favorable spectral properties suitable for high-color-gamut display applications. Photophysical and electrochemical analyses indicate high radiative efficiency and stable excited-state behavior. Initial device evaluations demonstrate promising external quantum efficiency and improved operational durability compared with representative blue phosphorescent systems. These results underscore the potential of Pt(II) complexes as robust deep-blue emitters and provide practical design directions for achieving efficient and long-lifetime OLED materials.



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Dual TADF and TTA Emission in D-A-D molecules from Green to Deep Red with Mechanochromic Properties

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Materials which display thermally activated delayed fluorescence (TADF) have been widely employed in organic light emitting diode (OLED) applications. This is because of their ability to harvest light from the triplet state, T_1 allowing devices to have theoretical internal quantum efficiencies (IQEs) of 100%. Donor-acceptor-donor (D-A-D) molecules have been shown to be good candidates for TADF and efficient OLEDs [1,2]. However, obtaining efficient deep-red emitters remains a challenge due to the energy gap law as non-radiative decay is enhanced [3]. Triplet-triplet annihilation (TTA) is another mechanism of triplet harvesting, used in optoelectronic device applications, by formation of an excited singlet state from two triplet states.

Here, we report two efficient regioisomeric D-A-D emitters, comprising 3,6-di-tert-butyl-9H-carbazole as both donor units and a dibenzo[a,c]phenazine-based acceptor. The molecules differ in donor substitution position, yielding T-shaped (PC8) and Y-shaped (PC16) geometries, the structures are given in Figure 1**.** Time-resolved photoluminescence measurements demonstrate delayed fluorescence (DF) in solution and solid state. Laser power and temperature dependence studies confirm that DF arises from a combination of TADF and TTA. In dilute films, both mechanisms contribute, while in neat films TTA dominates. Notably, PC8 neat films exhibit deep-red emission with only a moderate PLQY reduction compared to dilute films, highlighting its resistance to aggregation-induced quenching. OLED devices were fabricated with PC8 and PC16 as the active emissive layer in neat and CBP host conditions, giving electroluminescence covering green to deep-red. PC8 additionally displays mechanochromic properties. Upon exposure to different external stimuli (grinding, DCM vapour and recrystallisation), the emission colour can be reversibly switched, with PL maxima spanning 597-637 nm. This study allows the exploration of the difference in luminescent properties arising from different positioning of the donor units as well as the demonstration of efficient OLEDs even in the deep-red.

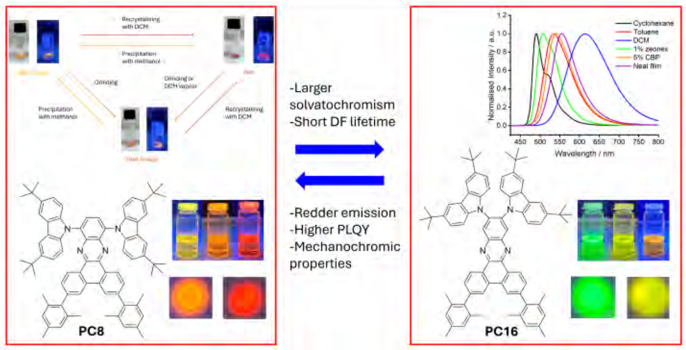

Figure **1**. The structures of PC8 and PC16 and a summary of their luminescent properties.

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Coupling Chromophores to Open-Shell Systems: From Organic Radicals to Direct Triplet Phosphorescence in Lanthanide-Doped Nanocrystals

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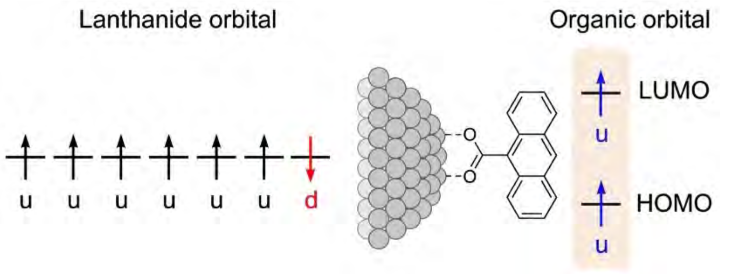
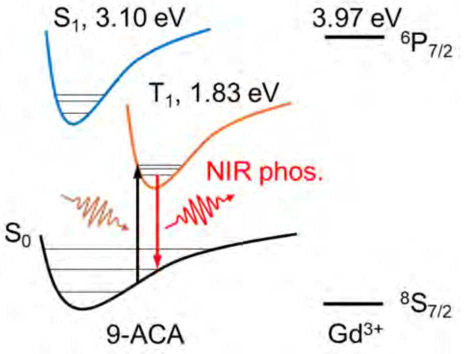
Chromophores linked to open-shell systems represent innovative molecular designs that allow exchange interactions between unpaired electrons, drastically influencing the properties of the chromophore's excited states. As demonstrated by S. Gorgon et al. [1,2], a chromophore's triplet state can couple with an adjacent radical system's unpaired electron, splitting into a trip-doublet $^2[D_0T_1]$ and a high spin quartet $^4[D_0T_1]$ state. Because these addressable high-spin excited states satisfy the DiVincenzo criteria, they hold great promise for quantum information science. The exchange coupling strength is typically in the thermal k_BT range and many possible designs pairing bright radicals with selected chromophores, or dark radicals like TEMPO with TADF/INVEST chromophores, can be developed. While overall spin multiplicity is conserved via a double spin-flip mechanism, the $^2[D_0T_1]$ state typically remains optically dark in investigated pure organic systems. However, we show how this could be overcome in organic chromophores attached to lanthanide-doped nanocrystals with unpaired f-orbital electrons [3]. Spin-exchange coupling between the lanthanide's 4f unpaired electrons and the organic molecule unlocks direct photoexcitation of the triplet from the ground state, enabling room-temperature, visible-to-near-infrared phosphorescence in solution and films. Our multiconfigurational computational studies on 9-anthracenecarboxylic acid (9-ACA)-Gd^{3+} complexes reveal the luminescent lower-spin excited state is a formal octet, like the ground state. Its wavefunction contains a sizeable (~20%) contribution where a local Ms = +/-1 triplet is balanced by a counter spin-flip in the 4f-orbitals. By preserving the overall octet spin state, this double spin-flip mechanism renders direct optical absorption into the triplet formally spin-allowed, while the coupled system simultaneously borrows optical intensity from the bright singlet state.





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Modeling Bridge and Substituent Effects on the Electronic Structure and Excited States of TTM-Based Diradicals

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Tris(2,4,6-trichlorophenyl)methyl (TTM)-based diradicals are promising open-shell systems with potential applications in molecular spintronics and optoelectronic devices due to their tunable magnetic coupling and rich excited-state photophysics. [1,2] In this work, we computationally model a family of TTM-based diradicals to investigate how structural modifications influence their ground- and excited-state electronic structures. We explore systems where two TTM units are connected through different molecular bridges, as well as the effect of anchoring electron-donating (D) and electron-accepting (A) substituents to the radical centers. In particular, we analyze a series of donor-acceptor patterns including X-TTM-bridge-TTM-X, X = D or A, architectures. Additionally, we investigate the limiting case where two TTM units are directly connected through a single C-C bond without a molecular bridge. Ground-state geometries and spin distributions were first characterized using unrestricted density functional theory (DFT) within the MGGA DFT theory. Exchange interactions between radical centers were estimated from triplet and broken-symmetry singlet configurations. To obtain a reliable description of excited states in these open-shell systems, screened optimally tuned range-separated hybrid (OT-SRSH) functionals were employed, including solvent effects through the polarizable continuum model (PCM). Excited-state properties were investigated using Tamm-Dancoff TD-DFT, spin-flip TD-DFT and mixed-reference spin-flip approaches, complemented by multireference CASSCF/QDNEVPT2 calculations. The calculations reveal that both the nature of the bridging unit and the presence of donor or acceptor substituents strongly influence spin distribution, exchange coupling and the character of low-lying excited states. Natural transition orbital analysis highlights the interplay between local excitations and charge-transfer contributions across the diradical framework. This study provides insights into structure-property relationships in TTM-based diradicals and offer guidelines for the rational design of open-shell molecular systems with tailored magnetic and photophysical properties.

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Theoretical analysis of non-radiative decay rates in π-conjugated molecules

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Non-radiative decay processes play a central role in the photophysics of organic molecules. The non-radiative decay rate (k_{nr}) directly governs excited-state lifetimes, photoluminescence quantum yields, and the magnitude of radiative and non-radiative voltage losses in organic optoelectronic devices. Understanding k_{nr} is therefore essential for the design of efficient emitters, stable open-shell radicals, and high-performance non-fullerene acceptors (NFAs) for organic photovoltaics. Despite its importance, rationalizing k_{nr} remains challenging. To address this issue, we performed a two-stage theoretical analysis.

First, we calculated k_{nr} values and compared them with the available experimental data for different materials, mainly radicals, together with NFAs and thermally activated delayed fluorescence (TADF) emitters [2]. A fair agreement between calculated and measured rates was obtained, providing a solid basis for further analysis of the molecular factors governing non-radiative decay.

Second, we investigated the relationship between k_{nr} and the high-frequency reorganization energy (λ_{h}). Recent studies [2] have suggested that NFAs exhibit higher non-radiative decay rates than radicals because they are more strongly coupled to high-frequency vibrations and therefore display larger λ_{h}. However, when comparing k_{nr} against λ_{h} across our full dataset, no correlation is found; NFAs even show an anticorrelation, indicating that high-frequency vibrational coupling is not the main factor controlling the rate, contrary to previous proposals [2].

Instead, a clear trend emerges with the ionicity of the excited state, quantified through the excited-state dipole moment: molecules with larger dipole moments systematically display smaller k_{nr}. This behaviour is directly connected to the non-adiabatic couplings (NACs) [3], since larger dipoles are associated with weaker electronic coupling. TADF emitters show a smaller sum of squared NACs over all vibrational modes than NFAs, which explains their much lower k_{nr}. An almost linear relationship is observed between k_{nr} and the sum of squared NACs, indicating that changes in the electronic wavefunction dominate the rate, while vibrational contributions remain secondary, although not negligible.

Overall, this study provides a coherent theoretical picture consistent with experimental observations [2] and clarifies the relative roles of electronic and vibrational factors in determining non-radiative losses in radicals, NFAs, and TADF emitters.

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Boron-substituted xanthene dyes for bioimaging applications

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Xanthene dyes such as fluoresceins and rhodamines have been intensively studied since their first respective synthesis in 1871 and 1887. An interesting way of increasing their absorption and emission wavelengths is to substitute the central oxygen by a group 14, 15 or 16 element such as Si, P, C or S.[1,2] Boron-substituted xanthenes have already been synthesised but are yet to be furtherly investigated. Tricoordinated boron-fluoresceins displayed the largest wavelength shifts amongst other studied heteroatoms, allowing emission in the near-infrared range, despite low fluorescence quantum yields.[3] The vacant p orbital of the tricoordinated boron atom allows p-π* interactions, greatly stabilising the LUMO, which results in an increase of the wavelength. This is needed to enter the range of the therapeutic window, where light can penetrate deeper into living tissues, allowing the use of weaker LASERs and thus reducing the cytotoxicity of the process.

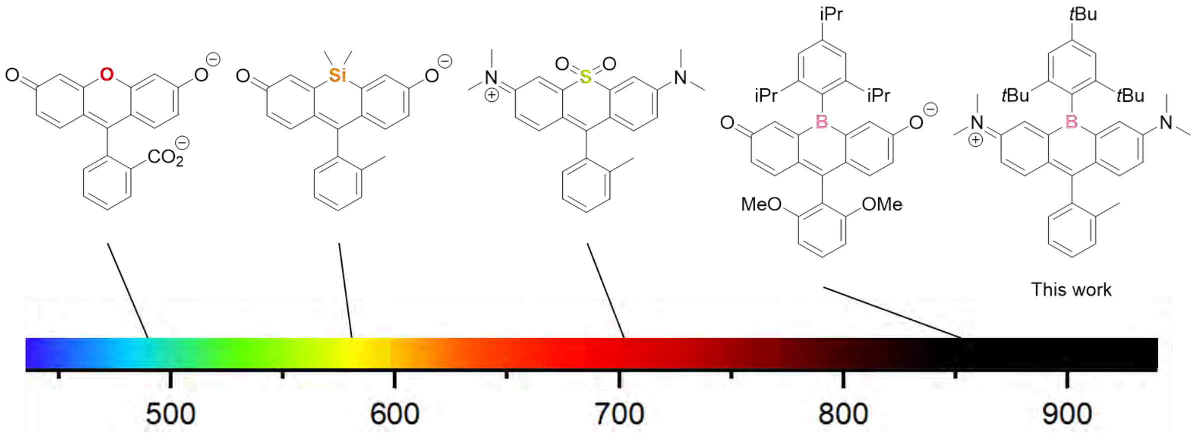

Figure: Several known xanthene fluorophores and their experimental absorption wavelength

Improving the synthesis, increasing the quantum yields and extending the process to rhodamines and rhodols opens a path towards several applications such as bioimaging or in-vivo imaging, TADF, pH sensors...

In this poster, we will present the advances in the synthesis of new boron-substituted xanthene dyes.

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Mechanistic modelling of exciton-polaron quenching in thermally activated delayed fluorescence emitters

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A major source of efficiency loss in organic light emitting devices (OLEDs) are so-called ‘quenching’ losses, which scale with the density of charge carriers present in the device. Exciton quenching occurs when charged molecules (holding either a hole or electron) can absorb excitonic species which would otherwise have emitted light. This reduces device efficiency and contributes towards device degradation. Potentially, the role of quenching can be reduced when using thermally-activated fluorescent (TADF) emitters, with emissive lifetimes that can be much shorter than that of phosphorescent emitters. In previous studies [1,2], quenching in TADF-based devices has been studied using a phenomenological (rate-equation) model. However, the various approximations that are made using such approaches limit their applicability and do not allow a comparison with results of first-principles (quantum-chemical) methods. Here, we develop a mechanistic description of the efficiency loss due to TPQ for the prototypical blue-green TADF emitter material DMAC-TRZ, by analyzing the current-density dependence of the time-resolved photoluminescence (TRPL) of single-layer hole-only (see Figure 1) and electron-only devices. The system is modelled using kinetic Monte Carlo simulations to analyse the observed quenching. For hole-only devices (see Figure 1), the delayed component of the TRPL is found to be most strongly affected, indicating that triplets are quenched more strongly than singlets. The KMC analysis is used to obtain the rate of Dexter-type triplet-hole quenching. The validity of the approach is demonstrated by making a comparison with the quenching in films in which DMAC-TRZ is blended with a high-energy gap spacer material.

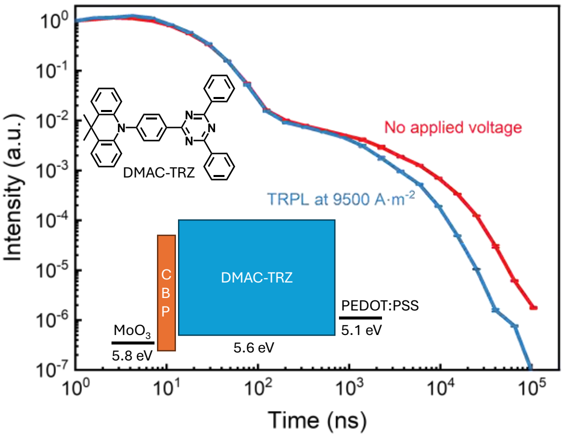

Figure 6*:* Time resolved photoluminescence of a 170 nm DMAC-TRZ neat film device, sandwiched in between hole-injecting and extracting electrodes. The two curves show the normalized TRPL intensity in the absence of a current and at a large current density.

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A strategy for red-shifting the emission of D-A TADF and MR-TADF emitters with bora-triptycene Lewis acids

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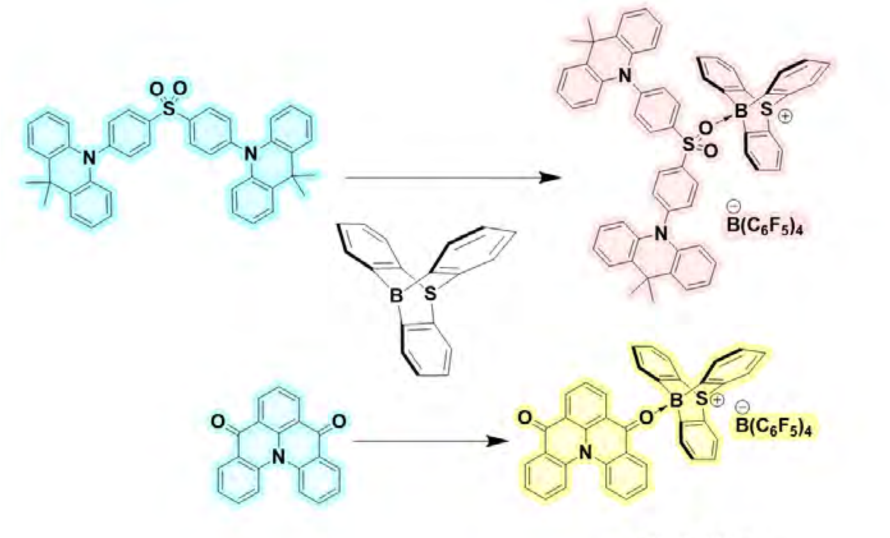
There are now thousands of examples thermally activated delayed fluorescent (TADF) molecules that emit across the visible light spectrum.[1] Compared to blue and green emitters, there are far fewer exemples of red and near-IR TADF emitters, linked to a deficit of design strategies targeting red-emissive compounds. Current methodologies typically require the use of strong donor and/or acceptor groups.[2]

Herein, we present a photophysical study on bench-stable Lewis Adducts, formed between D-A TADF and MR-TADF emitters and a boron-based Lewis acid.[3] The resulting adducts are bench stable, and demonstrate bathochromically shifted emssion maxima of over 100 nm. Importantly, time-resolved photoluminescence measurements reveal that the presence of the Lewis acid does not adversely affect the TADF properties.



Bench stable
Maintains TADF
DA & MR-TADF examples

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Novel Potential MR-TADF Emitters Based on Fused Phenothiazines

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Due to their unique alternating electron distribution in fused polycyclic systems, multi-resonance thermally activated delayed fluorescence (MR-TADF) materials based on electron deficient carbonyl groups and electron donating nitrogen atoms are investigated for their use as novel emitters in organic light-emitting diodes (OLEDs).[1] The MR effect is enhanced by a *para*-substitution of the corresponding groups which leads to a spatial separation of the frontier orbitals and results in a small energy gap between the excited singlet and triplet state.[2] Due to the rigid framework and the short-ranged reorganization of the electron density when returning to the ground state, MR-TADF emitters usually show narrowband emission.[2] The introduction of a phenothiazine moiety can enlarge the spin-orbit coupling by utilizing the heavy atom effect of the sulfur atom and thereby enhance the device performance.[3] Oxidation to the sulfone introduces another acceptor to the system to enhance the MR effect and manipulate the electronic structure (Fig. 1, Part A).

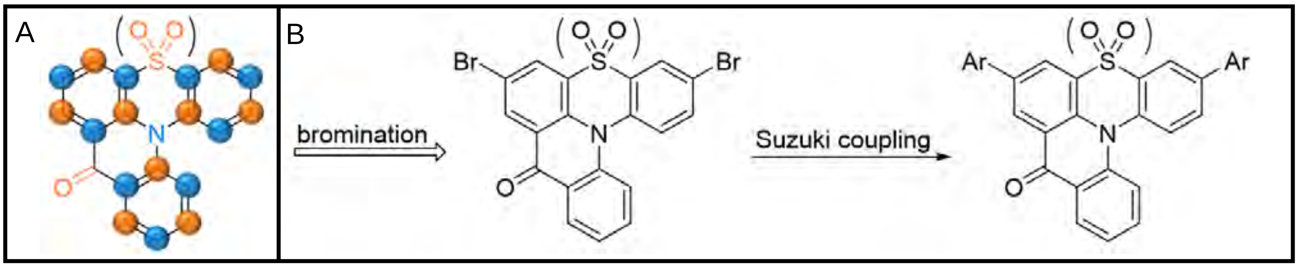

Figure 7: A: HOMO-LUMO separation in the phenothiazine-based frameworks of QPO (thioether) and QP3O (sulfone). B: Modification by bromination and subsequent Suzuki coupling.

Bromination of the pentacyclic scaffold enables the extension of the π-system via Suzuki coupling (Fig. 1, Part B). The photophysical properties of newly synthesized emitters were investigated in the solid state and in solution. The oxidized sulfone derivatives show a blue-shifted emission, smaller Stokes shifts and narrower FWHMs.

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Theoretical Insights into Nonlinear Optical Read-Write Mechanisms in Multistate DHA-SP Molecular Switches

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Molecular switches are promising candidates for high-density data storage devices, in which photochromic molecules serve as key functional units and form the logic devices, with their switching states corresponding to distinct information bits. Increasing information storage density requires: (i) multistate systems storing multiple bits per molecule and (ii) high-resolution read-and-write strategies. Nonlinear optical (NLO) responses offer an attractive and powerful solution, combining molecular selectivity with high spatial resolution due to the nature of light-matter interactions.

Here, we present a time-dependent density functional theory investigation of the read-and-write ability of an eight-state Dihydroazulene-Spiropyran (DHA-SP) molecular switch [1,2]. On the one hand, the writing process is driven by the two-photon absorption (TPA) in the near-infrared spectral region. On the other hand, the reading process is performed by using the second harmonic generation (SHG) responses, a nondestructive readout method.

We show that TPA efficiently induces switching from the DHA-E-MCH to the VHF-E-MCH form, with TPA cross-sections of ~2500 GM. These two states exhibit distinct SHG responses, with the DHA-E-MCH amplitude being 1.5 times larger than that of VHF-E-MCH, enabling optical discrimination. In contrast to one-photon absorption, TPA spectra of the dyads show non-additive behavior of their constitutive units, highlighting cooperative effects in the most active form.

Overall, we demonstrate the promising potential of the DHA-SP multistate multifunctional molecular switch for NLO read-and-write applications in optical memory storage.

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Orthogonal biaryl systems as potential TADF-emitters in OLED-application

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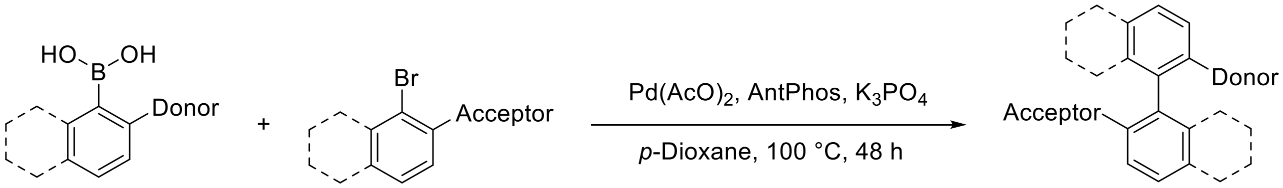
Since the introduction of the first organic light-emitting diode (OLED) in 1987 by *Tang* and *VanSlyke*, different generations of OLEDs were established depending on which mechanism luminescence is generated.[1] Phosphorescence emitters were the first attempt of improving OLEDs and form the second generation of OLEDs. Those emitters rely on the usage of rare earth metals like iridium and platinum, which are expensive and unsustainable. In contrast to that Adachi *et al*. developed the first thermally activated delayed fluorescence (TADF) emitters in 2009, which are forming the third generation of OLEDs, and further improved the structural design in 2012 to achieve a theoretical fluorescence quantum yield of 100% without using any metals.[2,3]

We have developed novel orthogonal biaryl based donor-acceptor-systems as potential TADF-emitters. The aim of this work is to develop donor and acceptor units independently and later couple them via cross-coupling. Usually, the donor is used as boronic acid source and the acceptor acts as bromide source to than be coupled via Suzuki-coupling. The donor and acceptor units are attached to either a naphthalene or a methylated phenyl ring to further increase the steric hindrance and the rotational barrier. This also leaves room for introducing functional groups in the backbone and further improve specific properties of the emitter. Since donor and acceptor moieties are synthesized independently it is easy to achieve a broad spectrum of different emitters with only one reaction.



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Stability Enhancement in Blue TADF-OLEDs via Anionic Bond Strength Tuning in Carbazole-Biphenyl Hosts

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Achieving stable and efficient blue thermally activated delayed fluorescence (TADF) OLEDs remains challenging due to high-energy excitons and polarons that induce bond cleavage, limiting the operational lifetime. We develop a series of carbazole–biphenyl host materials (Figure 1) with tuned charge transport (from ambipolar to strongly electron-transporting) while maintaining high triplet energies (2.77–2.85 eV in neat films), enabling a systematic probe of charge balance and degradation mechanisms in blue TADF-OLEDs.[1] Devices incorporating blue TADF emitters with different triplet energies (2.79 eV and 2.62 eV) and optimized dopant concentrations (7–40 wt%) reach maximum external quantum efficiencies up to 18% with low efficiency roll-off for the most suitable host–dopant combinations. Operational stability tests at 1000 cd m^{-2} show that, within the same device architecture and fabrication protocol, OLEDs using the N-phenylated host consistently outperform non-phenylated analogues by factors of 1.6–12 in device lifetime (LT_{50}). Density functional theory calculations link this improvement to an increased anionic-state bond dissociation energy of the weakest exocyclic C–N bond (2.22 eV vs. 0.73–0.75 eV in the non-phenylated hosts), enabled by shifting LUMO density away from the carbazole core via N-phenyl substitution. These results identify anionic-state C–N bond strength as a key molecular parameter for robust high-triplet-energy hosts and provide chemically grounded design guidelines to mitigate polaron-induced degradation while retaining high efficiency under the studied conditions.

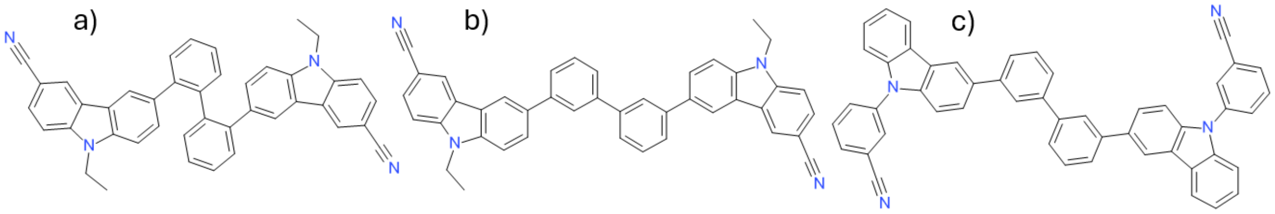

Figure 1. a) oCzB-2CN, b) mCzB-2CN, c) mCzB-2PhCN.

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Effect of molecular anisotropy on emitter orientation in solution-processed host-guest systems

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Preferential horizontal orientation of the emissive transition dipole moment (TDM) can substantially enhance light outcoupling efficiency of organic light-emitting diodes (OLEDs) [1]. While there are many studies about molecular orientation in vacuum-deposited systems [2], comparatively little is known about the factors governing the orientation in solution processed films. Even though solution processing offers significant advantages in terms of lower fabrication cost and simpler, scalable manufacturing, controlling the alignment of small-molecule emitters in solution-processed films remains challenging. This becomes more difficult considering that many emissive layers are host-guest systems. As a result, a systematic understanding of how host-emitter interactions influence TDM orientation in these systems is still lacking.

Here, we use variable-angle spectroscopic ellipsometry and angle-resolved photoluminescence spectroscopy to investigate how the molecular anisotropy of a series of fluorescent and thermally activated delayed fluorescence (TADF)-based emitters guides their TDM orientation in solution-processed host-guest films. Namely, the newly synthesized fluorene-benzothiadiazole-based oligomer $(F6)_2$-BT-$(F6)_2$ [3]and the OLED small-molecule emitters C545T, CzDBA and TBRb were doped into films of the hosts TPBi and poly(N-vinylcarbazole) (PVK) via spin-coating. We have further studied the effect of spin speed as a fabrication-related parameter on the emitter TDM orientation. Our results indicate that the increasing emitter length in thinner films leads to an improved horizontal orientation, with $(F6)_2$-BT-$(F6)_2$ achieving >80% horizontal TDM orientation even in the small-molecule host TPBi. Our comprehensive study on the effect of the molecular geometry, host characteristics, and spin-coating-related parameters on emitter TDM orientation contributes to a more systematic understanding of molecular orientation in solution-processed OLED films. This is expected to provide guidance for improving light outcoupling in cost-effective device architectures.

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Effect of torsion-inducing methyl substituents on the delayed luminescence of star-shaped emitters

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The efficiency of thermally activated delayed fluorescence (TADF) in donor-acceptor (D-A) molecules is governed by a well-stablished paradox: small spatial overlap between HOMO and LUMO leads to a decrease in the energy gap between S_1 and T_1 (ΔE_{S1-T1}). However, this also causes a reduction of the fluorescence radiative decay rate [1]. To further investigate this, we studied the TADF properties of a series of emitters composed of carbazole and *sym*-triazine as donor and acceptor moieties, respectively, connected via phenylene bridge. We probed the impact of *meta* versus *para* substitution pattern, as well as of methyl substitution of the phenylene linkers, on key TADF parameters, such as ΔE_{S1-T1}, the photoluminescence quantum yield (PLQY) and delayed fluorescence lifetime (τ_{DF}). We found that the TADF properties change dramatically upon these structural modifications: Due to deteriorated oscillator strength, the PLQY drops sharply when torsion comes very close to orthogonality upon double methyl substitution; only *para* bridging allows coexistence of delayed fluorescence with room temperature phosphorescence in the solid; the smallest singlet-triplet energy gap (ΔE_{S-T}) and the fastest TADF result from methyl-substituted *meta*-bridges, whereas by far the greatest emission quantum yields are observed upon methyl-substituted *para*-bridging.

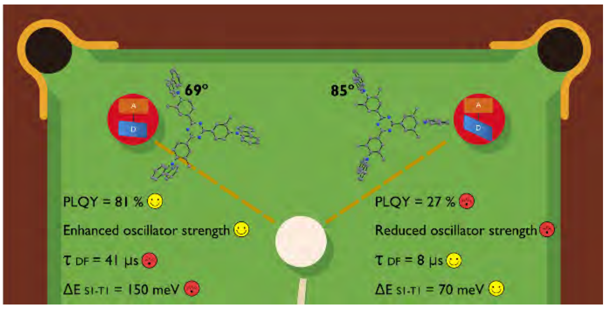

Figure 8: Diagram summarizing the impact of structural modifications of star-shaped emitters on the TADF.

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Optimization of polariton organic light-emitting diodes structure for achieving high device performance

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Organic light-emitting diodes (OLEDs) have been developed actively due to their commercial advantages, including low power consumption, fast response times, high color purity, and mechanical flexibility. Recently, polariton OLEDs (POLEDs) have emerged as a promising extention to improve OLED display performance. By inserting materials that enable strong light–matter coupling into an OLED with a high-quality microcavity, POLEDs offer a potential solution to the angle-dependent color shift that limits color purity in conventional OLED displays. In 2023, Mischok *et al.* reported ultralow angular dispersion POLEDs exhibiting spectral shifts below 10 nm at a viewing angle of 60° and external quantum efficiencies above 10%, thereby representing the first POLEDs with a practically relevant efficiency. However, the correlation between device efficiency and angle dependent spectral variation in POLEDs has not yet been clearly established. In this work, we computationally investigated the correlation of outcoupling efficiency angular variation in EL spectrum, by quantifying differences in peak wavelength ($\Delta\lambda_{peak}$) and full width at half maximum ($\Delta FWHM$) at 0° and 70°, for blue, green, and red SCL POLEDs through transfer matrix method simulations combined with a coupled oscillator Hamiltonian model. Finally, we suggested an optimized device structure with material property to achieve improved device performance.

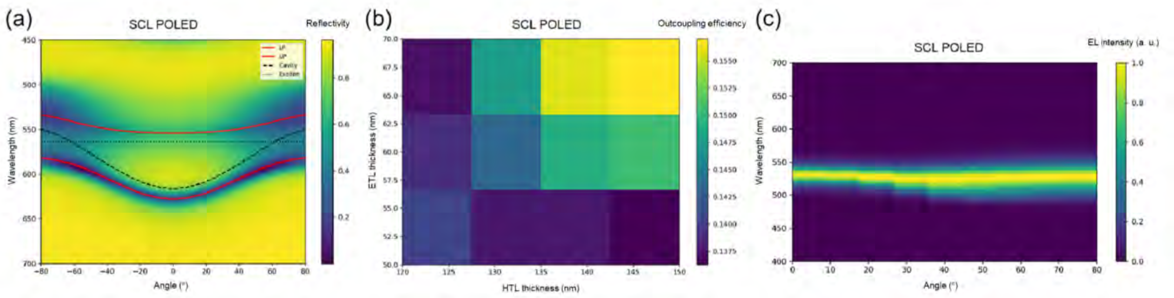

Figure 1. Optical simulation results. (a) Reflectivity spectra. (b) Heat map of outcoupling efficiency according to thickness of hole and electron transport layer. (c) Angle-resolved electroluminescence spectra at the minimized $\Delta FWHM$ value at 0° and 70° angle.

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Improving OLED efficiency through plasmon engineering: a 3D finite element method approach

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Plasmon coupling is traditionally depicted as a major loss channel limiting the efficiency of organic light-emitting diodes (OLEDs). Recent works have however exploited controlled plasmon coupling as a route to enhance OLED efficiency and stability [1,2]. Nevertheless, the systematic optimization of such strategies remains challenging due to the strong sensitivity of plasmonic resonances to geometrical and material parameters, as well as the complexity and diversity of the competing mechanisms involved (total internal reflections in substrate and organic layers, quenching, and ohmic losses in metallic electrodes). In this context, electromagnetic numerical modeling becomes essential to quantitatively analyze light-matter interaction, plasmon energy redistribution, and establish predictive design guidelines for efficiency enhancement. In this work, a three-dimensional finite-element model (FEM) is developed to quantify outcoupling efficiency and plasmon coupling in OLED stacks. For benchmarking, the outcoupling efficiency was calculated by integrating the far-field intensity over the light escape cone, showing agreement within 2% against analytical results for a typical OLED architecture. This validated 3D FEM provides a powerful platform for quantitative analysis of plasmonic coupling in realistic device geometries. It is the method of choice to derive design guidelines for efficiency enhancement in plasmonic OLED architectures.

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Kinetic Monte Carlo modelling of organic light-emitting diodes and photodiodes for optical communication

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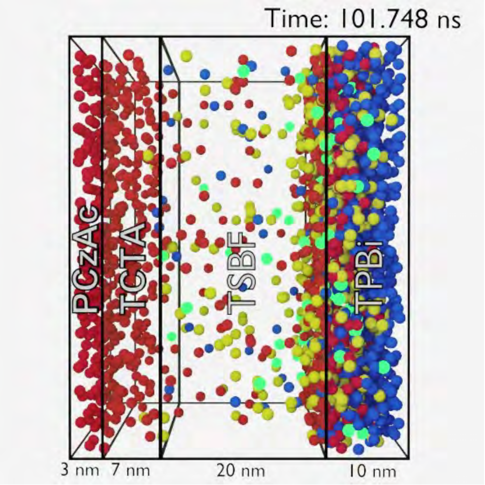
Organic light emitting diodes (OLEDs) and photodiodes (OPDs) present compelling alternatives to their inorganic counterparts in optical communication owing to their spectral tunability and the absence of toxic or resource critical elements. A possible downside could be the low charge-carrier mobility of organic semiconductors. However, when high bias voltages are applied one can profit from the strong field enhancement of the mobility. Current modelling of organic optoelectronic devices predominantly relies on rate equation or drift-diffusion approaches, which are insufficient in describing the coupled charge transport and excitonic processes occurring at the molecular up to the device scale. Mechanistic Kinetic Monte Carlo (kMC) simulations can capture all these processes at all relevant scales, and are therefore perfectly suitable to explore the fundamental mechanisms that ultimately constrain data rates and device performance. In this work, we employ kMC simulations to analyse the reported transient behaviour of an OLED [1] and an OPD [2] driven by a short (nanosecond-scale) voltage or optical pulse, respectively. By systematically varying the pulse width and key device and material parameters, we study their impact on the luminescence and photocurrent transients, as well as on the spatiotemporal evolution of excitons and charges inside the devices (see figure). We find that the time scale of the transients in both devices can be greatly reduced by increasing the bias voltage, demonstrating the feasibility of using OLEDs and OPDs in optical communication with speeds that can compete with their inorganic analogs.



Snapshot of a kMC simulation of the OLED in Ref. [1] driven by a 5 ns voltage pulse of 20 V starting at 100 ns. Red: holes. Blue: electrons. Green: singlet excitons. Yellow: triplet excitons. Courtesy to Christian McDonald for the visualization.

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Correlation Effects in Molecular Singlet-Triplet Energy Gaps

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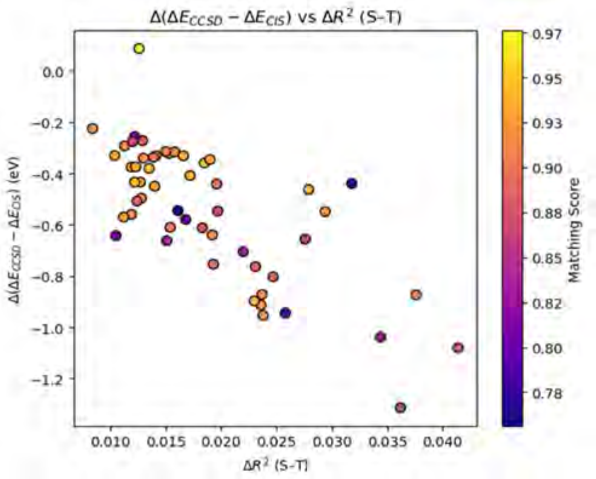
Accurate prediction of singlet–triplet energy gaps (ΔE_{ST}) is critical for understanding excited-state processes in light-driven materials, particularly in systems with significant electron correlation such as inverted singlet–triplet (INVEST) [1, 2] molecules. Conventional single-excitation methods often struggle to describe states with substantial double-excitation character, leading to method-dependent discrepancies. In this work, we investigate the relationship between double-excitation character and excited-state energetics across a chemically diverse set of molecules using multiple correlated electronic structure methods. A matching-score protocol is employed to ensure consistent state identification across methods. By correlating excitation energies and singlet-triplet gaps with a quantitative measure of double-excitation character, we explore how exchange and correlation effects collectively influence excited-state properties across different molecular frameworks.



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The High-throughput Virtual Screening and Design of Organic Photofunctional Materials

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The excited-state property with charge transfer (CT) or local excitation (LE) determines the occurrence of photophysical behavior in organic materials including the thermally activated delayed fluorescence (TADF), organic room-temperature phosphorescence (ORTP) emitters, and triplet photosensitizers (PSs), invert singlet-triplet (IST) gap molecules. We have developed a fragment frontier molecular orbital (FFMO) model for the donor-acceptor-type systems and constructed molecular descriptors of the excited-state property based on the orbital information on constituent D and A fragments. Applying these descriptors, we rapidly screened CT or LE molecules from 2500 molecules generated by the binding of 50 donors and 50 acceptors. For IST systems, we developed a four-orbital model (FOM) to elucidate the roles of double excitations in the IST formation, and establish two molecular descriptors (K_S and O_D) based on exchange integral and molecular orbital energy. By these descriptors, we rapidly identify 41 IST candidates out of 3,486 molecules. The descriptors-aided approach achieves a screening success rate of 90% and reduces computational costs by 13 times compared to full post-HF calculations. Importantly, we predicted a series of excellent non-traditional near-infrared IST emitters from adataset of 1028 compounds with emission wavelengths ranging from 852.2 to 1002.3nm.

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Round-Robin Test of a Light-emitting Electrochemical Cell: Establishing a(n Interlaboratory) Standard for Quality Research

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The light-emitting electrochemical cell (LEC) is a promising candidate for low-cost, solution-processed lighting devices [1]. It comprises a single active layer in which mobile ions are mixed with an organic semiconductor, enabling ohmic charge-carrier injection and low transport resistance due to electrochemical doping. To date, however, the research field has lacked a common benchmark device for comparative studies. Here, we report the results of the first round-robin test of an LEC system, in which nine international laboratories followed a unified protocol to fabricate and test nominally identical devices. The experiments were conducted in 2025. This contribution presents our unpublished results and compares key performance metrics between the participating labs. We demonstrate that LECs can be fabricated with consistent and reproducible results, and we identify common pitfalls and critical sources of variability. Furthermore, we discuss the importance of standardized fabrication and testing practices. The system introduced in this work serves as a common baseline for future systematic, reproducible LEC research, enabling reliable comparison of key performance parameters and quantitative assessment of device improvements.

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