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## Controlling the fate of two triplet states: solid-state annihilator design for photon upconversion

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Photon upconversion, the process of converting low-energy light into higher-energy photons, offers transformative opportunities for energy conversion and optoelectronics. In this Perspective, we examine the molecular design principles of solid-state annihilators, emphasizing a unified excitonic framework that links upconversion with related technologies such as organic light-emitting diodes and singlet fission. We discuss key challenges, including controlling triplet exciton diffusion, maximizing singlet formation efficiency, and suppressing loss channels such as excimer and trap-state formation. Strategies that leverage precise intermolecular packing and tailored electronic coupling are highlighted as critical levers for dictating excited-state dynamics and optimizing photophysical outcomes. Looking forward, we propose that future breakthroughs will surpass the "solution-first approach" and hinge on integrating data-driven machine learning approaches with phonon engineering to rationally design materials with enhanced light emission and energy conversion efficiency. This framework provides guiding principles for the next generation of high-performance solid-state upconversion systems.

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Associate Professor. Her group has pioneered solid-state perovskite-sensitized photon upconversion using a variety of tetracene and anthracene derivatives. A particular focus is placed on understanding the role of nanoscale structure on ensemble material properties. The combination of optical spectroscopy and scanning probe microscopy employed in her lab enables a unique understanding of the complex photophysical processes occurring in these systems.



# 1. Introduction

Photon upconversion based on triplet–triplet annihilation (TTA-UC) is deeply interconnected with singlet fission (SF), organic light-emitting diodes (OLEDs), room-temperature phosphorescence (RTP), and related areas of organic electronics that exploit spin-dependent excited-state dynamics. Rather than being isolated phenomena, these fields share common physical principles involving triplet generation, triplet pairing, and the control of singlet and triplet energy manifolds through molecular packing and electronic coupling. This Perspective positions solid-state TTA-UC annihilator design squarely within the broader excitonic landscape.

TTA and SF represent complementary pathways that interconvert singlet and triplet excitons through correlated triplet-pair states, placing annihilator chromophores at the same conceptual foundation as SF materials and OLED emitters. In OLEDs, control over triplet harvesting, singlet formation, and excimer or exciplex emission is central to device efficiency, while in RTP materials, suppression or modulation of non-radiative triplet decay governs emission lifetimes and brightness. These same design challenges reappear in solid-state TTA-UC, where interchromophore coupling, energetic alignment, and aggregate structure determine whether triplets undergo productive annihilation, form emissive singlets, stabilize excimers, or funnel into undesired loss channels.

By explicitly unifying TTA-UC with singlet fission, OLED photophysics, RTP, and broader organic electronic materials, this Perspective emphasizes that advances in annihilator design are not incremental refinements of upconversion alone but contribute directly to a shared framework for manipulating spin statistics and excited-state fate in organic solids.

The discussion is intentionally focused on molecular and aggregate-level design principles of annihilators and excludes polymeric films, extended frameworks, and device fabrication strategies, for these topics we refer the interested reader to existing literature.<sup>1–5</sup> Emphasis is placed on transferable design rules that balance triplet generation, diffusion, and annihilation with selective singlet stabilization and emission, offering guidance relevant across upconversion, light emission, and energy conversion technologies.

## 2. Overview of the mechanism of TTA-UC and the critical loss channels in solid state

TTA occurs when two (spin-)triplet excited states come into contact and annihilate to generate a higher excited state and a ground state.<sup>6,7</sup> UC arises when photoexcitation produces triplet states at an energy lower than that of the higher excited state formed through TTA, as shown in Fig. 1. The desired higher excited state is often a singlet state that can relax radiatively, however the upconverted energy can potentially be directly harvested from other species, such as the triplet pair state.<sup>8–11</sup> For TTA to result in a singlet excited state, the



Fig. 1 The TTA-UC cascade that begins by the sensitizers absorbing low energy photons and undergoing intersystem crossing (ISC) to yield excited triplet states. Triplet energy transfer (TET) then occurs between the sensitizer and annihilator. When two triplet excited annihilators come into contact, triplet–triplet annihilation (TTA) may occur, which, through an intermediate triplet pair state, can yield a ground state and an annihilator in its singlet excited state that ultimately emits the upconverted photon.

annihilator chromophore needs to generally satisfy the energetic requirement of:

$$E(S_n) \leq 2 \times E(T_1), \quad (1)$$

where  $E(S_n)$  is the energy of the excited spin-singlet state,  $E(T_1)$  is the energy of the excited spin-triplet state and  $n \geq 1$ . The inequality sign is flipped in eqn (1) in case of SF. However, this energetic requirement can be greatly relaxed in SF compared to TTA due to the entropy contribution from the triplet pair separation.<sup>12,13</sup> We will discuss the implication of this entropic cost on solid-state TTA-UC more in depth later.

TTA and SF are considered the reverse reactions of each other and can be presented under a unified kinetic model:<sup>14,15</sup>



where  $T_1$  is a triplet state localized on a single chromophore,  $[T_1 \cdots T_1]$  is a weakly bound triplet pair state with spin coherence,  ${}^1(TT)$  is a correlated triplet pair with both electronic and spin coherence, and  $S_1$  and  $S_0$  are the excited-state and ground-state singlets, respectively. In solid-state TTA-UC systems the upconverted emission can be considered to occur from this electronically coupled dimer, while the nature and strength of this coupling will differ greatly in different annihilators and largely decide the fate of the generated excited singlet.<sup>16</sup> Eqn (1) is often further modified for solution-based TTA-UC by including the localization of the singlet excited state ( $S_1 S_0 \rightleftharpoons S_1 + S_0$ ) to individual chromophores, however in solid state, as we will discuss below, the probability of such localization is reduced to a great extent.

Excited triplet states in TTA-UC are typically produced by separate chromophores called (photo)sensitizers due to the spin-forbidden nature of the direct transition to the spin-triplet state (Fig. 1). Historically, sensitizers have been molecular chromophores that undergo efficient intersystem crossing (ISC) to produce excited triplet states from singlet excited states that can be directly excited.<sup>17</sup> However, the use of molecular photosensitizers in solid-state TTA-UC is often hampered by aggregation-induced losses that compete with triplet energy



Table 1 Examples of different types of TTA-UC systems that represent the state of the art

Sensitizer	Annihilator	$\Phi_{UC}$ (%)	$I_{th}$ (mW cm <sup>-2</sup> )	$\Delta E^a$ (eV)	Ref.
WSe <sub>2</sub>	TIPS-An	1.2	110	1.12	31
PYT1:PBQ-TCl	Rub:DBP	2.2	10	0.5	45
MA <sub>0.15</sub> FA <sub>0.85</sub> PbI <sub>3</sub>	Rub:DBP	0.11	61	0.44	46
PdPc	DPP <sub>EH</sub> -tBu	1.5	16 200	0.43	47

<sup>a</sup> Apparent anti-Stokes shift.

transfer (TET) to the annihilator.<sup>18–21</sup> More recently, new classes of photosensitizers have been developed, such as semiconductor quantum dots that possess spin-mixed excited states, alleviating large exchange energy losses.<sup>22</sup>

Intriguingly for solid-state applications, inspiration has also been drawn from solar cell technologies through the development of layered TTA-UC devices, where the triplet excited states are generated by charge recombination. The triplet generation can occur either in the photosensitizer bulk, for example at an organic donor–acceptor heterojunction, or at the interface between the annihilator and the photosensitizer, such as bulk halide perovskites,<sup>23</sup> transition metal dichalcogenides<sup>24</sup> or organic semiconductors,<sup>25–27</sup> resulting in direct triplet generation in the annihilator layer. The emergence of these layered TTA-UC devices has greatly boosted solid-state upconversion efficiencies.<sup>28</sup> However, triplet generation by interfacial charge recombination requires band alignment between the valence band of the sensitizer and the highest occupied molecular orbital (HOMO) of the annihilator,<sup>23,29–32</sup> which imposes stricter constraints on the choice of annihilators beyond the rudimentary energetic requirement discussed above (eqn (1)).

As hinted above with eqn (1), TTA-UC can result in a higher-lying excited singlet state. An archetypal example of such an annihilator is Zn-tetraphenylporphyrin, where low energy excitation of the S<sub>1</sub> results in efficient ISC to T<sub>1</sub> and subsequent TTA to S<sub>2</sub>.<sup>33–35</sup> As the sensitizer and the annihilator are the same chromophore, this process is called homomolecular TTA (HTTA). In addition to being interesting systems from a fundamental photophysical and photochemical perspective, realization of efficient HTTA-UC systems would streamline the design of solid-state TTA-UC. As singlet fission can also occur from higher singlet excited states,<sup>36,37</sup> such materials can offer insight into developing more efficient HTTA materials along with other chromophores that break Kasha's rule.<sup>38,39</sup> In the solid state, altered relaxation pathways and energy landscapes can make radiative decay from higher excited states competitive; consequently, restricted molecular motion, reduced vibrational energy dissipation, and strong intermolecular interactions slow internal conversion, increasing the likelihood of Kasha's rule breakdown.

The efficiency of TTA-UC can be represented with three figures of merit: (1) the apparent anti-Stokes shift,<sup>40</sup> (2) the quantum yield of upconversion ( $\Phi_{UC}$ )<sup>41</sup> and (3) the intensity threshold ( $I_{th}$ )<sup>42,43</sup> at which TTA becomes the primary triplet relaxation pathway. The apparent anti-Stokes shift is the energy difference between the excitation wavelength and upconverted emission in a TTA-UC system.  $\Phi_{UC}$  is often decomposed into the individual efficiencies of the processes that participate in the TTA-UC cascade (Fig. 1):

$$\Phi_{UC} = \frac{1}{2}\Phi_{ISC}\Phi_{TET}\Phi_{TTA}f\Phi_f, \quad (3)$$

where  $\Phi_{ISC}$  is the efficiency of intersystem crossing,  $\Phi_{TET}$  is the efficiency of triplet energy transfer from the photosensitizer to the annihilator,  $\Phi_{TTA}$  is the efficiency of TTA,  $f$  is the spin-statistical factor, *i.e.*, the fraction of annihilating triplet pairs that produce the desired excited singlet state, and  $\Phi_f$  is the quantum yield of fluorescence of the annihilator.

As TTA is a bimolecular process that occurs between metastable states,  $\Phi_{UC}$  is a function of the triplet population and thus the excitation intensity. The maximum  $\Phi_{UC}$  is reached at excitation intensities where the triplet decay is dominated by TTA over the unimolecular or spontaneous triplet decay. The  $I_{th}$  is the excitation intensity at which the rate of TTA and the rate of spontaneous triplet decay are equal and is typically defined as<sup>44</sup>

$$I_{th} = \frac{(k_T)^2}{\Phi_{TET}\alpha k_{TTA}}, \quad (4)$$

where  $k_T$  is the rate of spontaneous triplet decay,  $\alpha$  is the absorption coefficient of the photosensitizer and  $k_{TTA}$  is the rate constant of TTA.

Typically, the performance goals for UC systems are to maximize the apparent anti-Stokes shift and  $\Phi_{UC}$ , while minimizing the  $I_{th}$ . To illustrate some of the recent advances in the field, we have highlighted TTA-UC systems that are among the state of the art in Table 1.

However, we would like to offer a counterpoint that as the field of TTA-UC matures and becomes more application-oriented, these goals may change.<sup>5</sup> For example in photocatalytic applications, maximizing the brightness of the UC system or the reaction rate at the achievable excitation intensity may be more important than as high and low as possible  $\Phi_{UC}$  and  $I_{th}$ , respectively.<sup>8,48</sup> Accordingly, the focus of this Perspective is to offer annihilator design guidelines for tuning the properties of annihilators to best suit the application at hand.

### 3. Maximizing singlet and fluorescence yields

As eqn (3) shows, achieving high  $\Phi_{UC}$  requires annihilators with high probability of singlet formation upon TTA ( $f$ ) and  $\Phi_f$ . In this section we will investigate the various annihilator attributes to maximize the production of upconverted photons.

#### 3.1 How to (statistically) make two triplets into one singlet

Eqn (1) shows the most rudimentary energetic conditions for TTA-UC to occur, *i.e.*, to yield an upconverted singlet state. 9,10-



Bis(phenylethynyl)anthracene (BPEA, Fig. 2) is a common annihilator as well as SF material since it fulfils the energy requirements of both SF and TTA:  $2 \times E(T_1) \cong E(S_1)$ .<sup>49,50</sup> Gray *et al.* have shown that the free rotation of the phenyl groups and consequent change in  $\pi$ -conjugation alters the energies of the excited triplet and singlet state.<sup>51</sup> Thus, only certain conformations of BPEA have sufficiently high triplet energy to annihilate into a singlet excited state and results in poor  $\Phi_{UC}$  with BPEA in solution phase. In a similar vein, the groups of Campos and Congreve have engineered diketopyrrolopyrrole (DPP, Fig. 2), tetracene, anthracene and perylene annihilators by relatively decreasing the singlet energy compared to the triplet energy and therefore increasing the energetic driving force of singlet formation upon TTA and  $\Phi_{UC}$ .<sup>52,53</sup> While these results were obtained in solution-based TTA-UC, this approach was shown to work in solid-state TTA-UC by Radiunas *et al.* in rubrene-based annihilators.<sup>54</sup>

Alternatively, the relative triplet and singlet can be altered in the solid state without modifying the chemical structure of the chromophore. Ye *et al.*<sup>55</sup> boosted the TTA efficiency of a DPP annihilator by coupling its singlet state to a polaritonic state, thus providing larger energy overhead for accessing an excited

radiative state upon TTA. Aggregation may also lower the singlet excited state energy, ultimately facilitating TTA-UC.<sup>56</sup> For example, Nienhaus and co-workers have demonstrated that TTA is boosted in naphtho[2,3-*a*]pyrene (NaPy, Fig. 2) aggregates due to the redshift of the excited singlet state in strongly coupled dimer states.<sup>57,58</sup> A similar strategy has been employed to turn on thermally activated delayed fluorescence by reducing the  $S_1$ - $T_1$  energy gap.<sup>59</sup> As such, the selective tuning of the singlet and triplet energies either through synthetic methods, light-matter interactions or intermolecular coupling is a viable strategy to tip the scale towards singlet generation in TTA-UC.

In the early days of the TTA-UC renaissance in the 2000s, there were conflicting conceptions whether two annihilating triplets can produce a singlet state encounter complex with either a 1/9 (~11%) or ~40% probability.<sup>17,60</sup> Both of these limits were first challenged by Schmidt *et al.* by observing higher singlet yields in TTA in rubrene.<sup>61-63</sup> Followed by their initial discoveries, several pathways of boosting  $f$ , and consequently  $\Phi_{UC}$ , have been identified. Here, we break them into three individual mechanisms: (1) relative energetics of the higher triplet and singlet excited states, (2) inter-chromophore orientation and distance and (3) changing the singlet character of the triplet pair state by tuning the triplet-triplet coupling.

Above, we discussed how altering the singlet and triplet energies can lead to higher singlet yields. However, states of higher multiplicity than singlets, namely higher excited triplet states ( $T_n$ ,  $n \geq 2$ ), can also be generated upon TTA. Accessing these higher triplets can be considered a loss channel for TTA as the  $T_n$  undergoes rapid internal conversion to  $T_1$ .<sup>64,65</sup> Similarly, close energetic alignment of  $T_n$  and  $S_1$  is considered detrimental for SF as a single triplet state may be generated *via* ISC instead of two triplets *via* SF in such chromophores.<sup>66,67</sup> Considerable efforts, mostly using computational methods, have been made to discover annihilators,<sup>68-73</sup> TTA-OLED<sup>74</sup> and SF materials<sup>75-83</sup> where  $T_n$  is not energetically accessible, *i.e.*,  $2 \times E(T_1) < E(T_n)$ . However, as most of these studies are performed using isolated molecules, their predictive capability has been limited in solid-state systems, where the complex chromophore-chromophore interactions complicate the model.<sup>84</sup> It will be interesting to see how quickly new data-driven methods, such as machine learning,<sup>85</sup> can start producing translatable predictions for solid-state TTA and SF materials.

In contrast to the assumption stated above that energetically accessible  $T_n$  states are outright adverse for high  $f$  and consequently  $\Phi_{UC}$ , Xu *et al.*<sup>86</sup> discovered in 2019 that closely matched  $S_1$  and  $T_2$  energy levels in an anthracene-based emitter increased the efficiency of TTA-OLEDs and demonstrated that  $T_2 \rightarrow S_1$  ISC occurred and was the likely cause for the boost. Since then, this high-level 'reverse' intersystem crossing (HL-RISC, Fig. 3) has been identified as an active channel in increasing  $f$  rubrene<sup>87-89</sup> and in a structurally diverse set of TTA-OLED materials.<sup>90-96</sup> Since the discovery of HL-RISC as an active channel in TTA is recent, we expect that its mechanism and existence in other annihilators, such as TIPS-naphthalene,<sup>97</sup> that surpass the 'conventional' limit of  $f = 0.4$  will be investigated. For example, the high  $f > 0.4$  in 9,10-diphenylanthracene (DPA) has been attributed to  $T_2 \rightarrow S_1$  HL-RISC by Miyashita



Fig. 2 Molecular structures of some of the annihilators discussed in this Perspective. (a) Rubrene is the prototypical solid-state annihilator that has delightfully seen some challengers recently. (b) Increasing the steric bulk of annihilators is an emerging approach to improve solid-state TTA-UC performance.





Fig. 3 Summary of some of the molecular interactions and processes that influence the spin statistical factor ( $f$ ) of TTA. Rotating clockwise from top left: the intermolecular arrangement, both in displacement and rotation changes, for example, the orbital overlap and thus the exchange interaction between the annihilators. The triplet pair may be strongly ( $J \neq 0$ ,  $J$  is the exchange energy within the triplet pair) or weakly ( $J \approx 0$ ) coupled and this coupling can change dynamically as the triplets for example hop. The magnetic field ( $B$ ) effect on TTA can be used to elucidate the spin interactions in the triplet pair. The closely matched energies of the triplet pair, the higher lying triplet states ( $T_n$ ) and the singlet excited state and the couplings between these states can give rise to high-level 'reverse' intersystem crossing (HL-RISC), which may deactivate the triplet loss channel from the triplet pair to the lowest triplet state, therefore increasing  $f$ . HL-RISC may occur directly from the triplet pair or proceed via the higher lying triplet state ( $T_n$  mediated HL-RISC), highlighting the urgent need for more mechanistic studies for different annihilators.

*et al.*,<sup>98</sup> whereas Shao *et al.*<sup>99</sup> concluded it results from direct ISC from  $^3(\text{TT})$  to  $S_1$ . This underlines the need for more in-depth mechanistic studies for different annihilators to elucidate the mechanism.

Efficient HL-RISC naturally requires close energetic alignment between  $T_n$  and  $S_1$  and large spin-orbit coupling (SOC) to compete with the often rapid  $T_n \rightarrow T_1$  internal conversion. Kim *et al.*<sup>100</sup> demonstrated *in silico* that introducing electron-donating and withdrawing functional groups, heavy atoms and geometric distortions enhances  $T_2$ - $S_1$  SOC and presumably HL-RISC. They also postulate that since the  $T_2 \rightarrow T_1$  internal conversion requires significant geometric reorganization due to the large  $T_2$ - $T_1$  energy gap, in solid-state  $T_2 \rightarrow S_1$  HL-RISC may offer significant competition to  $T_2 \rightarrow T_1$  internal conversion and contribute to achieving high  $f$ . However, we would like to cautiously note that the requirements for efficient HL-RISC, *i.e.*, a small energy gap between  $T_n$  and  $S_1$  and significant SOC may be at odds with the other desired attributes for annihilators, such as high  $\Phi_f$  and small  $k_T$ . Thus, systematic experimental studies are needed to balance the outcome to create new efficient annihilators.

We now turn our investigation from energetics to the spin-character triplet pair state and its influence on  $f$ . The spin interactions between two triplets, A and B, can be expressed with a Hamiltonian that, without spin-orbit coupling, can be approximated as<sup>88,101</sup>

$$\hat{H} = \hat{H}_{\text{exchange}} + \hat{H}_{\text{inter}} + \sum_{i=A,B} (\hat{H}_{\text{Zeeman}} + \hat{H}_{\text{ZFS}}) \quad (5)$$

where  $H_{\text{inter}}$  is the spin-dipole interaction between the two triplets and the summed term accounts for the intra-triplet spin interaction, *i.e.* zero-field splitting (ZFS) and Zeeman effect when an external magnetic field is applied. The triplet pair can be both strongly and weakly (exchange) coupled (Fig. 3).<sup>101,102</sup> For the weakly coupled triplet pair, the exchange interaction is weaker than the dipole-dipole interaction or zero-field-splitting in the triplets in  $[T_1 \cdots T_1]$  (see eqn (2)).<sup>103</sup> This becomes evident from the fact that Zeeman effect induced by an external magnetic field ( $<1$  T) alters the singlet yield, *i.e.*,  $f$ , to some degree upon TTA.<sup>104,105</sup> In the absence of an external magnetic field, the spin-character of the weakly coupled triplet pair depends on the orientation of the chromophores,<sup>106</sup> and more crucially for  $f$ , the singlet-character is maximal in parallel chromophores and can reach up to  $2/3$  (Fig. 3).<sup>88,107,108</sup> Despite the seemingly alluring simplicity of this rule, translating it to a real annihilator design is naturally complicated by the fact that the spin Hamiltonian is dominated by the exchange interaction, that not only depends on the interchromophore angle but on the orbital overlap in the strongly coupled triplet pair. Thus, it may be challenging to deconvolve the contribution of  $f$  and  $\Phi_{\text{TTA}}$  to  $\Phi_{\text{UC}}$ , which will require thorough kinetic analysis and the use of magnetic field effects. Luckily for readers that are only concerned about maximizing  $\Phi_{\text{UC}}$ , both  $f$  and  $\Phi_{\text{TTA}}$  seem to benefit from this parallel alignment,<sup>109</sup> as we will discuss below.

From a purely spin-character perspective, the strongly coupled triplet pair is not expected to have an angular dependence on  $f$ . However, the exchange interaction and thus the triplet-triplet coupling depends on the orbital overlap that is a function of the overall chromophore distance and alignment (Fig. 3),<sup>110,111</sup> which will influence the branching ratios between singlet formation and other competing processes occurring in the triplet pair, such as internal conversion to an individual triplet ( $^3(\text{TT}) \rightarrow T_n$ )<sup>88</sup> or dissociation from the strongly to the weakly coupled triplet pair ( $^1(\text{TT}) \rightarrow [T_1 \cdots T_1]$ ),<sup>107,112,113</sup> which can have a significant effect on  $f$ .<sup>64</sup>

Going beyond the exchange interaction in the triplet pair, Naimovičius *et al.*<sup>114</sup> have suggested that silylethynyl (often referred to as 'TIPS') functionalization of perylene (Fig. 2) more than doubled its singlet yield from 18% to almost 40% by introducing significant charge transfer character to the annihilator  $S_0S_1$  dimer. Similarly, charge transfer character in the dimer has been shown to increase the coupling between  $S_0S_1$  and  $^1(\text{TT})$  in singlet fission.<sup>115</sup> The involvement of charge transfer states in boosting  $f$  could be probed by, for example, changing solvent polarity (in solution-based TTA-UC),<sup>116-118</sup> or by applying an external electric field (in solid-state TTA-UC).<sup>119,120</sup> Another interesting method for controlling the dielectric properties of solids is co-crystallization,<sup>121,122</sup> although disentangling changes in annihilator coupling from purely dielectric stabilization of the charge transfer state may be challenging.

In summary, the seminal work of Bossanyi *et al.*<sup>88</sup> using rubrene indicates that  $f$  can be dominated by the spin character of the weakly coupled triplet pair and HL-RISC, however we eagerly wait for equally thorough studies on other solid-state



annihilators beyond rubrene to expand and generalize these rules. DPPs are synthetically straightforward to functionalize and are both SF<sup>123</sup> and TTA<sup>47</sup> active, thus offering a highly tuneable platform for systematic studies. Some covalently linked annihilator dimers have shown improved  $f$  over their monomers and thus offer a precisely tuneable platform for studying the exchange interaction and its role in determining  $f$ .<sup>124,125</sup>

### 3.2 The fate of the singlet excited state

Having outlined, in a somewhat shaky fashion that perhaps reflects the current level of certainty in the field, the design factors that contribute to  $f$ , we turn our focus to the newly generated excited singlet state. The two annihilators, one in a singlet excited state and the other in singlet ground state, are inherently coupled, and the nature and extent of this coupling determines the fate of the singlet excited state. As we mentioned in Section 2, the goal for TTA-UC systems is often to yield a  $S_n$  that would emit as high-energy photon with as high probability as possible.

Above we discussed how aggregation can be used to modify the singlet energy of the annihilator in respect to the triplet. In these aggregates,  $S_1$  was red-shifted in respect to the monomer, which is often attributed to J-type aggregation (Fig. 4a) that also tends to enhance the radiative decay rate and thus  $\Phi_r$ .<sup>56,126</sup> On the other hand, H-type aggregation (Fig. 4a) is often associated with blue-shifted emission but at a cost of quenched emission compared to the monomer.<sup>127</sup> Based on this rather simple comparison, it would be most beneficial for TTA-UC to realize aggregates that bear the benefits of both types of aggregates, *i.e.*, enhanced and blue-shifted emission. Considering that the chromophore couplings that lead to the aggregate properties are an ensemble of coulombic and charge transfer interactions that can have opposite signs, systems that exhibit both H- and J-type (called HH, HJ, JH and JJ-aggregates<sup>128</sup> or more recently

referred to I aggregates<sup>58,129,130</sup>) properties can be realized. As an example, by carefully balancing the exciton and charge transfer (CT) coupling, aggregates that exhibit both high carrier mobilities (often associated with H-type aggregates due to co-facial stacking motifs) and high emissivity can be designed (Fig. 4).<sup>131</sup> Disorder may also relax these rules to some extent.<sup>132</sup> These factors naturally carry great importance to the design of annihilators, not only in terms of their emissivity and singlet energies, but also enhancing triplet diffusion, which we will discuss later.

The mention of CT coupling naturally brings about another possible decay pathway for  $S_n$ , which is the formation of an excited state dimer (excimer, Fig. 4b) where the exciton is shared between two chromophores through coulombic coupling and stabilized through charge transfer interaction. Historically, excimer and TTA research have advanced together and, in many systems, excimers have been identified as a direct and thus competing product of TTA instead of a monomeric  $S_n$ .<sup>133–135</sup> Excimers have also been identified as either an intermediate or a product state in SF, underlying the importance of understanding the mechanism and control of excimer formation in TTA-UC. Further, excimers can serve as (defect) trap states to which excitons can migrate rapidly over long distances even if the dominant crystal structure of the annihilator is not conducive for excimer formation.

Excimer formation is often associated with H-type aggregation (Fig. 4) as strong CT coupling typically requires  $\pi$ - $\pi$  overlap.<sup>56</sup> However, in some closely spaced  $\pi$ -stacks, excimer formation is suppressed, which can result from, for example, the balanced coulombic and CT coupling<sup>136</sup> and intermolecular vibrational modes.<sup>137</sup> Thus, transient methods, such as ultrafast Raman,<sup>138,139</sup> multidimensional electronic spectroscopy<sup>140</sup> and ultrafast electron diffraction,<sup>141</sup> that provide time-resolved vibrational or structural dynamics can be valuable tools for untangling the conformational changes that contribute to excimer formation and thus provide insight into molecular/aggregate design. This vibronic coupling highlights the fact that excimers depend on intermolecular reorganization and can provide a prominent handle for tuning the fate of the singlet exciton.<sup>142,143</sup>

As mentioned, excimer formation often occurs in closely spaced cofacial dimers. Thus, adding steric bulk has often been the method for preserving monomeric emission.<sup>144,145</sup> Naturally, this may come at the cost of for example reduced  $f$  or  $\Phi_{TTA}$  but balancing these effects is possible as TTA can occur at larger intermolecular distances than excimer formation.<sup>146,147</sup>

We have used in the discussion above the 'classical' definitions, *i.e.* H and J-aggregation as they often satisfactorily explain the aggregate properties. However, there are naturally other aggregation or stacking modes, such as magic angle and crossing stacking, that do not follow these models, and we refer the interested reader to these recent reviews.<sup>148,149</sup>

There is a wealth of physical insight into controlling the fate of the singlet excited states in molecular aggregates and crystals. This is evident for example in covalently linked dimers where the interchromophore couplings can be tuned to a remarkable degree.<sup>150</sup> However, translating these results into



Fig. 4 (a) The 'conventional' or coulombic coupling-based ( $V$ ) definitions of H and J-aggregates.  $V$  depends on the angle ( $\theta$ ,  $\theta_m$  is the magic angle) between the monomer transition dipole moments ( $\mu$ ). However, the monomers may also couple through charge transfer interaction, which can lead to aggregates that exhibit ensemble properties that are conventionally associated exclusively to H or J-aggregates. (b) Excited dimer or excimer formation is closely associated with TTA-UC and often occurs in cofacially arranged molecules. Controlling excimer formation is one of the outstanding challenges in solid state TTA-UC as they are often considered detrimental due to their considerably redshifted emission.



solid-state systems can be hit-or-miss. The unfortunate reality is that *ab initio* design of organic crystals with predetermined optical properties is very challenging from first principles. As with energetic prediction, we are hopeful that machine learning methods that utilize large crystal databases as training materials will soon yield tangible results.<sup>151,152</sup>

Meanwhile, reverse engineering viable annihilators from known efficient solid-state emitters may be a feasible strategy. Chromophores that exhibit aggregation-induced emission (AIE) show weak or no emission in solution, whereas in the aggregate states they become emissive.<sup>153</sup> This enhancement of radiative decay is often attributed to the inactivation of vibrational or rotational modes that can lead to large conformational changes and provide access to non-radiative relaxation pathways such as minimum energy crossing points between excited and ground state manifolds.<sup>154</sup> As TTA-UC research often follows the “solution first” principle due to the relative ease of solution-based measurements, annihilators that possess for example rotatable bonds have been naturally overlooked. However, there have been a few reports of solid state TTA-UC systems that employ AIE-active annihilators, which serve as encouraging examples of the potential viability of this approach for annihilator design.<sup>155–157</sup> To further this point, we would like to point out indigoid dyes (Fig. 5) as an example of potentially overlooked annihilator class. Indigoids are typically associated as photo-switches as they tend to undergo *Z*-to-*E* isomerization upon photoexcitation.<sup>158</sup> As expected, their  $\Phi_f$  tend to be low in solution but increase in crystals or rigid matrix.<sup>159–161</sup> Indigo also has a low-lying triplet excited state ( $E(T_1) \approx 1$  eV)<sup>162</sup> and thus has been identified as a potential SF material by Michl *et al.*,<sup>66</sup> while isoindigos have been shown to undergo singlet fission.<sup>163</sup> Additionally, indigo exhibits high electron and hole mobilities,<sup>164</sup> whose importance will be discussed in the next section.

While the physical principles of maximizing the fluorescence yield from an annihilator are clear, optimizing the singlet yield upon TTA still requires more fundamental research. The need for further research becomes even more evident, as the applications of TTA-UC often requires optimizing both. In the light of

current evidence, these requirements may be somewhat at odds as, for example, maximal *f* is achieved in parallel chromophore configurations, while simultaneously this arrangement is conducive of excimer formation. Thus, it may be more desirable for applications of TTA-UC to find molecular systems that offer a suitable balance between high singlet and fluorescence yields.

## 4. Triplet diffusion

For two triplet states to come into contact in solid-state devices, they will likely need to migrate over some distance from their sensitization sites. Maximizing this diffusion distance carries two-fold significance for TTA-UC efficiency, as both high  $\Phi_{TTA}$  and low  $I_{th}$  require highly mobile triplet excitons.<sup>165–167</sup> The triplet diffusion length can be expressed as<sup>168</sup>

$$L_T = \sqrt{2Z\tau_T D_T}, \quad (6)$$

where *Z* is the material dimensionality (1, 2 or 3),  $\tau_T$  is the triplet lifetime and  $D_T$  is the diffusion coefficient. It becomes evident that long lived and highly mobile (diffusive) triplets are beneficial for long diffusion lengths and thus efficient solid-state TTA-UC. We will therefore focus in this section on design aspects that ensure these factors (Fig. 6).

Conventional annihilators based on polyaromatic hydrocarbons such as acenes, perylene and pyrene tend to have long intrinsic  $\tau_T$  due to lack of heteroatoms (either those with non-bonding orbitals to invoke El-Sayed type spin-orbit coupling<sup>169</sup> or heavy atoms). However, as the library of annihilators is becoming more chemically diverse beyond hydrocarbons, more sophisticated strategies to extend  $\tau_T$  are required.

Though the  $T_1 \rightarrow S_0$  transition is spin-forbidden, vibrational coupling between different spin manifolds cannot be neglected.<sup>170</sup> For example, the isotope effect on triplet lifetimes has been known since the 1960s when it was discovered that

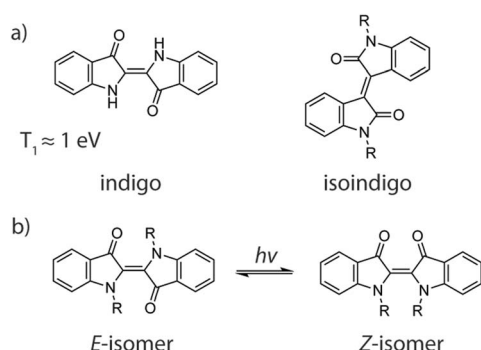


Fig. 5 (a) (Iso)indigos are a potential underexplored annihilator class with suitable energetics for both SF and TTA-UC. (b) Indigos are known as photo-switches as they can isomerize under photoexcitation, which is an excited state decay pathway instead of fluorescence. However, in solid state the isomerization around the C=C bond is hindered, leading to potential aggregation-induced emission properties.

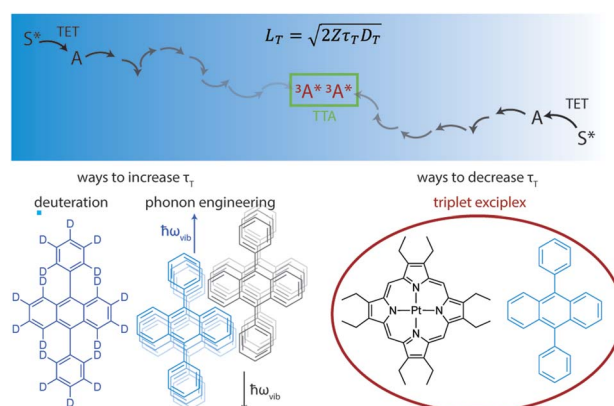


Fig. 6 Top: Efficient solid-state TTA-UC requires triplets that can diffuse over long distances. The diffusion length ( $L_T$ ) can be enhanced by either increasing the diffusion coefficient ( $D_T$ ) or triplet lifetime ( $\tau_T$ ). Bottom:  $\tau_T$  is a crucial parameter for efficient annihilators and it can be increased, for example, by tuning the intramolecular and intermolecular vibrational modes (deuteration and phonon engineering, respectively) or ensuring that triplet excimers/exciplexes are not formed.



deuteration of polyaromatic hydrocarbons, such as naphthalene,<sup>171,172</sup> increases their triplet lifetimes by reducing the frequency of the C–H(D) stretching modes. More recently, Danos *et al.*<sup>173</sup> showed that perdeuteration indeed increased  $\tau_T$  of perylene and thus improved its TTA-UC efficiency at lower excitation intensities in agreement with eqn (4). Similarly, deuteration has been used to increase the efficiency of thermally activated delayed fluorescence<sup>174</sup> and room temperature phosphorescence dyes.<sup>175</sup>

Despite its proven efficacy, we are not advocating for everyone to start deuteration their annihilators, as other tools to achieve similar results exist at a much lower cost factor. These approaches are sometimes summarized under the term ‘phonon engineering’.<sup>176</sup> As vibrational motion cannot be completely suppressed at typical operating conditions of most TTA-UC systems (room temperature or even higher), identifying and isolating modes that contribute to the triplet decay become paramount. Such modes are those that for example enhance the  $T_1$ – $S_0$  spin-orbit coupling or have large reorganization energies.<sup>177,178</sup> Rational design of annihilators where such modes are suppressed will require collaboration between computational and experimental researchers. This requires accurate calculations of the triplet energy surface, which is traditionally challenging and resource intensive, however recent advances in incorporating machine learning into the computational pipeline are encouraging.<sup>179–181</sup>

Naturally, the triplet exciton decay may be bimolecular, TTA being the desirable pathway. However, as was the case with singlet excitons, triplet states may also succumb to excimer formation.<sup>182</sup> Triplet excimers (Fig. 7) have been thoroughly investigated in naphthalenes, however their presence has been shown in other TTA-relevant chromophores such as anthracene, tetracene and pyrene.<sup>183–186</sup> Additionally, exciplex (excited state complex) formation between triplet excited DPA and ground state PtOEP has been identified,<sup>187</sup> which further highlights the importance of deciphering this decay channel. As triplet states are ‘dark’ excitons, the stabilization in a triplet excimer is presumably of purely CT character. Expectedly, triplet excimer is most stable in naphthalene dimers with face-to-face stacking,<sup>188,189</sup> however other stacking motifs can also lead to triplet delocalization.

Triplet excimers are challenging to detect due to their inherent dark nature and transient absorption spectra that may be convoluted by monomeric triplets or impurities.<sup>183,190–192</sup>



Fig. 7 Triplet excimer ( $T_{ex}$ ) formation delocalizes the triplet state and serves as a trap state that may prevent TTA from occurring.

Typical method for enhancing phosphorescence, *i.e.*, cooling to cryogenic temperatures, may prevent the intermolecular reorganization that is required for excimer formation and would be accessible at ambient temperature.<sup>193</sup> Therefore, we conclude that excimer formation may be a significantly underestimated triplet decay pathway in TTA-UC systems and warrants more extensive investigation in different annihilator classes, especially in the solid state.

Long-lived triplets still need to diffuse to achieve efficient TTA-UC. Rapid diffusion will naturally enhance TET between the sensitizer and the annihilator, at least by maximizing the mixing entropy associated with TET by expanding the number of annihilator sites accessible within the triplet lifetime.<sup>194</sup> For interfacial sensitizer–annihilator systems triplet diffusion can act as the rate limiting step for TTA-UC, further highlighting the need for highly mobile triplets.<sup>195,196</sup> Factors that influence triplet diffusion are rather well-known, thanks to the abundance of research in the organic electronics and photovoltaics community. As triplet transfer requires orbital overlap,<sup>197</sup> or more particularly HOMO–HOMO and LUMO–LUMO overlap, TET coupling is maximized in symmetric face-to-face stacking.<sup>198,199</sup> However, as we have discussed, such assembly motifs can induce other undesirable effects such as excimer formation. Therefore, finding annihilator systems where triplet diffusion is rapid without trading off other performance parameters, such as efficient TTA, is paramount.<sup>200,201</sup> For example, achieving significant SF/TTA coupling typically requires that the molecules are slipped along both  $x$  and  $y$  coordinates.<sup>202</sup> Naturally, a molecular aggregate or crystal is not static, and thermal effects can induce significant changes in the intermolecular couplings relevant to TTA-UC. Again, using rubrene as a prototypical annihilator, Diaz-Andres *et al.*<sup>203</sup> showed *in silico* that TET coupling was considerable between stacked rubrene molecules at 0 K but SF/TTA coupling was negligible. Notably, at 298 K TET coupling decreased minimally, whereas SF/TTA coupling increased greatly. Similarly, Volek *et al.* have demonstrated that SF occurs faster at the edge than in the bulk of rubrene crystal due to disordered packing.<sup>204</sup> These results indicate that rational design of solid-state annihilators requires taking such perturbations, whether thermal (vibrational) or packing-related, into account.

Not surprisingly, such holistic phonon engineering efforts have been carried out by the organic electronics and more recently by the singlet fission community to optimize exciton and charge carrier transport. Rather frustratingly, phonons can either make or break transport and dissecting the factors that play a part are still somewhat debated and warrant their own reviews.<sup>84,205–211</sup> However, we are happy to provide some examples here that highlight the importance of understanding the dynamic nature of exciton/charge transfer: the seminal work of Schweicher *et al.*<sup>212</sup> coined the term ‘killer phonon mode’ that contributes strongly to the electron–phonon coupling and thus magnifies disorder and effectively hampers charge mobility. On a more positive note, Lynch *et al.*<sup>213</sup> were able to identify ‘spectator’ and ‘driving’ phonon modes of exciton transport following SF in pentacene crystals. These two instances



highlight that it is possible, at least in theory, to phonon engineer materials with very mobile triplets.

Finally, we would like to summarize that designing annihilators that exhibit long-lived and mobile triplets requires holistic understanding of both intramolecular and intermolecular vibrational modes that may contribute to triplet decay or transport as well as balancing the packing to facilitate both triplet transport, TTA and emissive singlets as outlined in the previous section. A possible solution, albeit beyond the strict scope of this Perspective, is to include a triplet mediator that facilitates triplet diffusion without interfering with TTA.<sup>214</sup> Further, as we will discuss in the next section, rapidly diffusing triplets may rather controversially reduce the TTA-UC yield (in addition to facilitating trapping),<sup>215</sup> which is why we especially encourage efforts to find annihilators with long-lived triplets.

## 5. Decoupling singlet fission

As already highlighted with eqn (2), SF and TTA always represent the two sides of the same coin. In this last section we will investigate different methods to bias that coin to show the obverse heads (TTA) rather than the reverse tails (SF) side.

By a first glance, differentiating between these two processes seems rather facile by their different energetic requirements. However, as already discussed above, SF can occur in systems where the triplet pair has significantly higher energy than the singlet. Typical examples of such systems are anthracene and tetracene,<sup>216,217</sup> where an energy barrier of more than 200 meV needs to be overcome, yet SF is still fast. These energetic assignments are often based on optical transitions, which reflect more the enthalpy of excitation rather than the total free energy. As such, entropic contributions are often cited as the driving force in such endothermic systems SF, as multiexciton generation, or more precisely the triplet pair dissociation, increases the multiplicity or statistical weight of the excitation.<sup>12,13,218</sup> As annihilators are often chosen based on (spectroscopic) energies that indicate exothermic TTA, endothermic SF systems are especially useful models for discerning factors that bias TTA over SF.

The dissociation of <sup>1</sup>(TT) to free triplets (Fig. 8) must overcome an energy barrier. As expected, this step has been shown to be thermally activated in endothermic SF.<sup>219</sup> Naturally, this energy barrier is sensitive to the interchromophore coupling<sup>220–223</sup> and the binding energy of the triplet pair. Besides energetic contributions, intramolecular vibrational modes may promote the dissociation step.<sup>224</sup> Thus, tuning these inter and intramolecular handles can hinder SF by, for example, making the binding energy of the triplet pair higher.<sup>225,226</sup> More relevantly, SF has been shown to be strongly driven by the triplet separation following dissociation in both exothermic and endothermic SF, *i.e.*, rapid triplet transport increases the yield of free triplets.<sup>212,221,227–231</sup>

The fact that the dissociation step requires triplet diffusion makes the SF/TTA-UC dynamics both morphology and size-dependent. As an example, BPEA can undergo both SF and TTA shows higher triplet yields in larger particle sizes, and a crystal-structure dependent SF yield.<sup>50,232,233</sup> Volek *et al.*

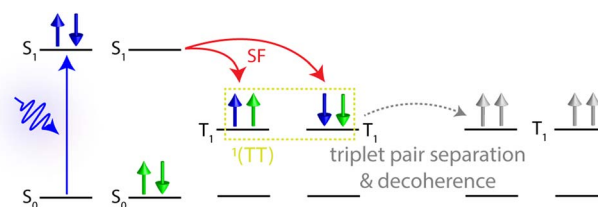


Fig. 8 Singlet fission (SF) proceeds by initially forming a triplet pair state that separates into free triplets. The triplet pair separation needs to overcome an energy barrier. SF is entropy-driven and fast triplet diffusion increases the yield of free triplets.

demonstrated that the SF/TTA balance in *N,N'*-bis(2-phenylethyl)-3,4,9,10-perylenedicarboximide can be tuned by crystal size.<sup>234</sup> In terms of morphology, Wiegold *et al.* have shown that rubrene can be biased towards TTA over SF by rendering it amorphous instead of (poly)crystalline.<sup>235</sup> These results highlight the importance of sample and device preparation processes, while we are mainly concerned with molecular design in this Perspective.

Chemically modifying rubrene by inserting sterically bulky groups has been shown to effectively decouple SF.<sup>236,237</sup> Baronas *et al.*<sup>236</sup> attributed the suppression of SF to hindered triplet diffusion in the substituted rubrene. Naimovicus *et al.*<sup>47</sup> furthered this strategy beyond the well-worn rubrene scaffold by boosting the  $\Phi_{UC}$  of DPPs and dipyrrolonaphthyridinediones (DPNPs, Fig. 2) through the insertion of bulky sidegroups. As such, 'bulking up' annihilators appears to be a straightforward blueprint for improving solid-state annihilators, where SF is an active and undesired loss channel.

Overall, this leads us to postulate that fast triplet transport may hinder solid state TTA-UC by tilting the balance towards SF. This relaxes the design parameters of annihilators compared to singlet fission materials to some extent, since efficient SF needs to strike a balance between triplet pair formation and triplet



Fig. 9 The conversion between  $S_1$  and <sup>1</sup>(TT) occurs through an intermediate charge transfer (CT) state. Depending on the relative energies of these states, the CT state may act as a trap state that competes with SF. We suggest that, if its energy can be controlled, the CT state may be used to bias TTA over SF.



transport, two processes that inherently require different interactions from orbital overlap perspective.

In this section we have so far discussed controlling the triplet dissociation as a way of biasing TTA over SF. However, SF and TTA share another intermediate,  $^1(\text{TT})$ . Although still somewhat debated, the coupling between  $S_1$  and  $^1(\text{TT})$  is CT mediated (Fig. 9).<sup>238</sup> This raises the question whether this coupling can be tuned to steer the triplet pair into forming singlets rather than dissociate into triplets. By lowering the energy of the CT state below  $S_1$  and  $^1(\text{TT})$ , SF can be effectively quenched as a relaxation pathway.<sup>239</sup> Similarly, excimer formation has been shown to hinder singlet fission.<sup>146</sup> As such, careful balance between excitonic and charge transfer character, as already discussed in Section 3, or fully leaning into excimer formation can aid in distinguishing TTA from SF. This is further supported by the fact that the recombination of non-geminate triplets produces relatively more excimers than geminate triplet pairs, *i.e.*, chromophore assemblies that participate in SF are comparatively less likely to generate excimers.<sup>240</sup> This finding is also consistent with the results that emissive states formed in solution-based TTA rather than direct excitation are more predisposed to excimer formation.<sup>147,241</sup>

## 6. Conclusions and outlook

In summary, the realization of efficient solid-state photon upconversion depends on the sophisticated control of energetics, spin-character, and molecular packing within the annihilator layer which ultimately dictate the fate of the singlet and triplet state. While the basic energy conservation requirement of  $E(S_n) \lesssim 2 \times E(T_1)$  remains a good starting point for determination of viable annihilators, achieving a high singlet formation yield requires a deeper understanding of pathways such as HL-RISC and the role of orbital overlap in determining triplet-triplet coupling. Furthermore, managing triplet diffusion is a critical challenge; although high mobility is necessary to lower the intensity threshold  $I_{\text{th}}$ , it can also facilitate loss channels like SF or the formation of “dark” triplet excimers. Looking forward, the development of solid-state annihilators must transition from empirical “solution-first” approaches to predictive, data-driven design. The integration of machine learning and computational pipelines to model complex chromophore–chromophore interactions and crystal properties will be essential for identifying next-generation materials. We anticipate that future research will increasingly leverage phonon engineering to suppress non-radiative decay modes and optimize exciton transport, moving toward materials characterized as solids on excitonic timescales, such as liquid crystals. As TTA-UC moves toward specific applications like photocatalysis, the fundamental aspects of annihilator design remain paramount while more practical device development will likely shift focus from achieving, for example, the lowest possible  $I_{\text{th}}$  to maximizing absolute brightness or reaction rates. Moreover, as the underlying science becomes better understood and more mature, device engineering considerations, including light outcoupling strategies, optimized device architectures, and the mitigation of challenges such as scattering and inner

filter effects, will play an increasingly critical role. Ultimately, the continued synergy between the TTA-UC, OLED, and singlet fission communities will be the primary driver for mastering the fate of triplet states in the solid state.

## Author contributions

J. I. – conceptualization, writing – original draft, writing – review & editing. L. N. conceptualization, writing – original draft, writing – review & editing, funding acquisition.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

No primary research results, software or code have been included and no new data were generated or analysed as part of this review.

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