

Up- and down-conversion in molecules and materials

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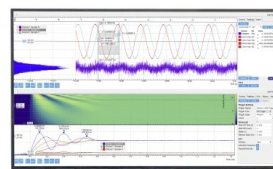
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I. INTRODUCTION

The conversion of energy within materials has many applications. If one could convert the energy of a blue photon into two lower-energy particles, or into two red photons, solar cells could be fabricated much more efficiently. On the other hand, if one could combine the energy of two particles to form higher-energy particles, it could be used to activate a chemical reaction, for example, releasing a drug or sensitizing a standard silicon camera for infrared light.

Many of these applications have seemed like science fiction in the past, but recent breakthroughs have brought them closer to reality. In molecules, the particles that carry energy are excitons, and the conversion of exciton energy between a spin-singlet exciton and two spin-triplet excitons can be used for upconversion (UC) or downconversion (DC). Molecular DC is termed singlet fission (SF), where one singlet exciton is converted into two triplet excitons,¹ and molecular UC is termed triplet fusion or triplet-triplet annihilation (TTA), where two spin-triplet excitons combine to form a singlet exciton.² The energy of these excitons can be accessed either by conversion to a photon (emission from the singlet exciton or via an intermediate to access the triplet excitons) or by transferring it to another material, exciting electronic transitions. A special case of UC is thermally activated delayed fluorescence, where thermal energy is used to convert between triplet and singlet exciton states.

In addition, inorganic materials are increasingly explored for UC and DC. The classic example concerns multiple exciton

generation (MEG), where one high-energy (hot) excitation in an inorganic semiconductor is converted into multiple band edge excitations.³ While inefficient in most bulk semiconductors, MEG can be efficient in nanomaterials. Rare-earth doping has also been used for DC, where energy can be stored in and emitted from well-defined atomic states. In a suitably designed system, these states can be used to split the energy from higher-energy excitations. More recently, when doped into metal-halide perovskites, these rare-earth ions, in particular ytterbium ions, have led to highly efficient DC due to quantum cutting.⁴ The rich f-electron configuration of lanthanide ions has also been actively used for UC. In particular, lanthanide-doped inorganic upconverting nanoparticles (UCNPs) have been used for a wide range of biological applications.⁵

While the material systems are diverse and often form the main focus of the research, many concepts and applications for UC and DC align. The article collection in the Journal of Chemical Physics termed *Up- and Down-Conversion in Molecules and Materials* aims to bring together the different ways to convert energy in materials, highlight the common concepts, and define the most promising directions and challenges for future research. In the following, we summarize the collection and put the contributions into context.

II. DOWNCONVERSION

DC describes the conversion of higher-energy particles into single or multiple lower-energy particles. Here, we highlight examples of singlet fission and lanthanide-based DC systems.

A. Singlet fission

Many of the contributions to this article collection focus on singlet fission. While already discovered in the 1960s,⁶ singlet fission has only gathered widespread attention following the realization that it could be useful for solar cell applications.⁷

Singlet fission is the conversion of one singlet exciton into two triplet excitons [Fig. 1(a)]. Most commonly, it is observed in molecular crystals, where the packing plays a significant role for the singlet fission rate because the singlet exciton is typically delocalized across several molecules, and the singlet fission process involves several states, some of which are also delocalized, such as the charge transfer states. By comparing a dimer and a trimer configuration of 2,5-bis(fluorene-9-ylidene)-2,5-dihydrothiophene (ThBF) using a combination of quantum mechanical calculations and molecular mechanics, Accomasso *et al.* showed that the increased delocalization in the trimer configuration leads to a fast singlet fission rate.⁸

The importance of the molecular crystal to the singlet fission rate was further corroborated by Nagami *et al.*,⁹ who calculated the vibronic coupling contribution to the singlet fission process in pentacene and its derivatives, where they explicitly included intermolecular interactions. They showed that the vibronic coupling in the intermolecular space is an important parameter for the predicted singlet fission rate in pentacene. Based on that knowledge, they designed halogenated pentacene derivatives with enhanced intermolecular vibronic coupling. Finally, they showed that the enhanced vibronic coupling does not always lead to an enhanced singlet fission rate.

An experimental study showing how the molecular packing affects the excited states and their dynamics was performed by Van Schenk *et al.*¹⁰ They also compared fluorinated anthradithiophene derivatives in three different packing motifs: “brickwork,” “twisted-columnar,” and “sandwich-herringbone,” to the same molecules in solutions. They found large differences in the delocalization of the Frenkel exciton, and the extent to which they observed the triplet pair state, relevant for singlet fission.

Hu *et al.* attempted to understand the optical properties of singlet fission molecule solutions and crystals from a theoretical

standpoint.¹¹ They used a multimode Brownian oscillator model to predict the absorption line shapes of the model system rubrene. They then used this result to show that the admixture of the S_1 and TT states is required to explain the fast initial singlet fission rate in rubrene.

Next to molecular crystals, recently, a new class of singlet fission molecules has appeared where fission of the initial singlet exciton happens on a single molecule. This intramolecular singlet fission (iSF) mechanism has the advantage that it does not depend on the crystal packing and that the rich toolbox of molecular engineering can be used to optimize this material class. Walwark and Grey simulated the time-resolved fluorescence yield of these molecules’ stochastic simulations under excitation from periodic light pulses.¹² They found that the fluorescence yield can sometimes behave in a non-monotonic fashion, with characteristic “dips” after excitation, resulting from the decay of a triplet exciton that would otherwise bleach the ground state. They proposed these characteristic dynamics as a new detection capability for iSF molecules.

For iSF materials, as well as for crystalline singlet fission materials, it is important to describe the multi-excitonic states and the charge transfer states correctly in order to understand the singlet fission process. Jiang and Zimmerman¹³ showed that restricted active space-spin flip methods can be used to describe charge transfer states, in addition to the multi-excitonic states they are typically employed for. Using an anthraquinone–quinoidal bithiophene system, they showed that the coupled (TT) state could directly lead to electron transfer into an acceptor, rather than triplet separation.

Given the importance of molecular arrangement for the singlet fission process, it is perhaps surprising that polymers can also undergo singlet fission. He *et al.* studied such a specific case of iSF by varying the solvent polarity of the polymer solution.¹⁴ They studied the dynamics of the singlet and triplet pair states by transient emission spectroscopy and found emission from both the singlet and (TT) states. Surprisingly, the (TT) state emission shows a strong dependence on the solvent polarity, indicating a strong charge-transfer component. They further showed that the dominant decay mechanism of the (TT) state on these polymers is a non-radiative decay, emphasizing the need to find polymers where the triplet excitons can dissociate on the polymer chain.

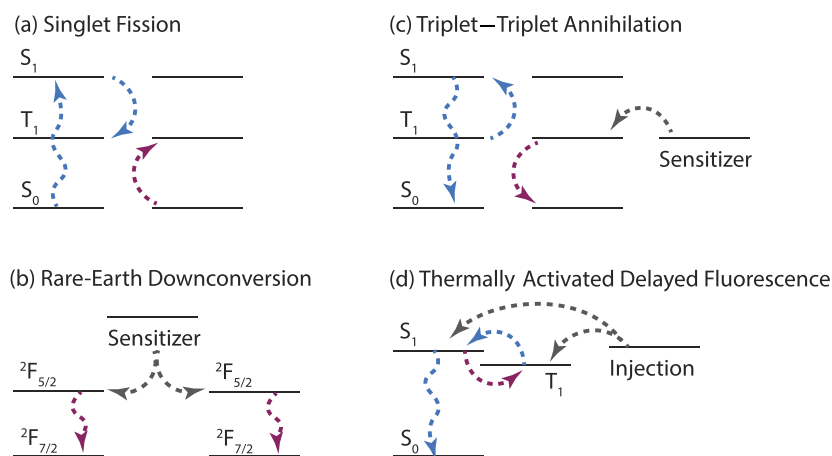


FIG. 1. Schematic representation of (a) singlet fission, where one excited singlet exciton is converted into two triplet excitons, (b) rare-earth downconversion, where a host material (sensitizer) excites two atomic transitions (depicted $^2F_{5/2}$ in Yb), which then emit light, and (c) triplet-triplet annihilation, the reverse process of singlet fission. (d) Thermally activated delayed fluorescence uses thermal energy to allow for reverse intersystem crossing from the triplet exciton to the emissive singlet exciton.

In addition to describing the CT states accurately, spin-orbit coupling is of relevance to singlet fission because it governs the spin mixing and, hence, the coupling of the spin-triplet exciton to the spin-singlet ground state. Carreras *et al.* expanded the restricted active space configuration interaction methods to include spin-orbit couplings using the Breit–Pauli Hamiltonian.¹⁵ They used this method to calculate the spin-orbit coupling in a range of molecular systems and explored the factors that govern the accuracy of the result.

B. Quantum cutting in lanthanide ions

Quantum cutting can be thought of as the all-inorganic counterpart to SF [Fig. 1(b)]. One of the great drawbacks of this approach of DC is the low absorption cross section of the lanthanide ions. To circumvent this, Ishii and Miyasaka took advantage of the high absorption of a quasi-2D CsPbCl₃ perovskite and created a layered structure where Yb³⁺ ions are sandwiched between perovskite layers.¹⁶ Upon absorption of the incident light at 300 nm, energy transfer from the perovskite to Yb³⁺ ions enables the quantum cutting process and emission is observed at 938 nm, with photoluminescent quantum yields exceeding 130%. Additional inclusion of Er³⁺ ions in the interlayer between the quasi-2D CsPbCl₃ perovskite layers allowed for the observation of Er³⁺ emission at 1540 nm with a quantum yield of 12.6%.

III. UPCONVERSION

UC is the conversion of multiple lower-energy particles into a single higher-energy particle. We highlight the contributions to triplet-triplet annihilation (TTA), sensitized by both molecules and inorganic nanostructures. We then show examples of thermally activated delayed fluorescence, an UC process that does not involve particle interconversion but thermal energy instead. We also highlight the contributions to the inorganic UC counterpart, lanthanide-based UC, and non-linear UC.

A. Triplet-triplet annihilation: Molecular triplet sensitizers

TTA-based UC, the inverse process of singlet fission, has a similar history to singlet fission. TTA-UC was first discovered in the 1960s¹⁷ but began to attract renewed attention in the 2000s.¹⁸ TTA-UC can convert low-energy light of long wavelengths into higher-energy light of shorter wavelengths and is characterized by its ability to efficiently convert even low-intensity excitation light such as sunlight [Fig. 1(c)]. TTA-UC is expected to improve the efficiency of solar energy utilization technologies, such as solar cells and photocatalysts, and to be applied to biotechnologies, such as bio-imaging and optogenetics.

A typical TTA-UC system consists of a triplet donor (sensitizer) and a triplet acceptor (emitter). The donor sensitizes the excited triplet of the acceptor, and the two acceptor molecules in the excited triplet state generate a fluorescent singlet excited state by TTA. Although metal complexes containing heavy metal ions such as Pt and Ir are often used as sensitizers because of their high intersystem crossing (ISC) efficiency due to the heavy atom effect, there is a need to develop sensitizers that do not contain heavy metals from the viewpoint of biocompatibility. Hu *et al.* systematically synthesized

spin-orbit charge transfer intersystem crossing (SOCT-ISC) molecules as sensitizers without heavy metals and clarified the correlation between molecular structure and sensitizing ability.¹⁹

In order to increase the energy gain, which is the difference between the absorption and emission wavelengths in TTA-UC, it is desirable that the triplet energy of the sensitizer and the emitter be close to each other so that the energy loss due to sensitization is small. However, if the triplet energy difference between the sensitizer and the emitter is too small, the back energy transfer from the emitter to the sensitizer becomes a serious problem. Meroni *et al.* studied the energy transfer and back energy transfer processes in detail in a model system where the triplet energy difference is less than the thermal energy at room temperature and clarified the strategy to maximize the TTA-UC efficiency by suppressing the back energy transfer.²⁰

Although fast molecular diffusion in solution can be used for efficient energy transfer from the sensitizer to emitter and TTA between emitters, it is important to use energy migration in solids where chromophore molecules are densely assembled for device applications.²¹ Barbosa de Mattos *et al.* constructed a quasi-solid TTA-UC system by covalently incorporating an emitter moiety into an oxotriphenylhexanoate (OTHO) gelator and introducing a sensitizer into the resulting organogel. By systematically introducing the emitter moiety at different positions in OTHO and investigating its photophysical properties, they have provided mechanistic insights into the design guidelines of energy migration-based TTA-UC.²²

Since TTA is a density-dependent bimolecular reaction, increasing the triplet density is important for making efficient solid-state TTA-UC materials. Sakamoto *et al.* used a copolymer of fluorene and anthracene as a host emitter and added not only a sensitizer but also an annihilator (9, 9'-bianthracene), which has a lower triplet energy than the host polymer, into the host polymer.²³ The triplet energy transferred from the sensitizer to the host polymer was collected by the annihilator bis-An, and the singlet energy obtained by TTA between the annihilators was transferred back to the host polymer, resulting in upconverted emission. By collecting the triplet energy in the aggregates of annihilators in the host polymer, they succeeded in improving the effective TTA rate constant.

B. Triplet-triplet annihilation: Quantum-confined and bulk triplet sensitizers

One of the main drawbacks of the previously discussed molecular triplet sensitizers is a large exchange energy loss when converting between the singlet and triplet states. Therefore, recently, both quantum-confined and bulk semiconductors have been explored as triplet sensitizers to minimize energy losses and maximize UC efficiencies. However, as the triplet sensitization mechanism is not yet fully understood, an additional insight is required to boost the UC efficiencies beyond the state of the art. Quantum dot (QD)-based UC systems are commonly ternary systems: the QD functions as the triplet sensitizer, a transmitter ligand is coupled directly to the QD, enabling rapid harvesting of the excited state, and the annihilator that undergoes TTA.

Rigsby *et al.* systematically investigated the UC efficiency as a function of the CdSe QD size. The authors were able to show that the UC quantum yield decreases with an increasing size or decreasing bandgap of the CdSe QD. This behavior was linked to a decrease

in the triplet exciton transfer (TET) rate from the QD to the bound anthracene-based transmitter ligand (9-anthracene carboxylic acid, 9-ACA), which is a result of the decrease in the driving force for triplet transfer with an increasing QD size.²⁴

In addition to a reduced driving force for TET, the interplay of trap state filling and triplet sensitization becomes increasingly important for larger CdSe QDs, which commonly exhibit lower quantum yields due to increased trap densities. Jin and Lian explored the effect of trapped excitons on the TET mechanism between CdSe QDs and the anthracene-based transmitter ligand 9-ACA. The authors found that both band edge and trap-state emissions are efficiently quenched by the bound transmitter ligand. However, the band edge exciton is quenched much more rapidly than the trap emission, leading to near-unity quenching. Despite the slower TET from the trap state, the longer intrinsic trap exciton lifetime also yields high TET efficiencies. The authors of Ref. 25 found rapid trapping to play a crucial role for the overall TET mechanism between CdSe and 9-ACA, the state-of-the-art model system for QD-based UC.

A common strategy to mitigate the effect of such trap states is to use core-shell QD structures. However, the added passivating shells introduce an additional tunneling barrier for the TET process, and thick shells have previously been shown to be detrimental to the short-range TET process. However, recent work by Lai and Wu showed that the interfacial TET process from CdSe QDs to surface-bound Rhodamine B transmitter ligands is activated by a thin ZnS shell, which suppresses ultrafast hole trapping. As a result, the TET pathway is enabled, and the authors of Ref. 26 found a red-to-blue UC efficiency of 2.8%.

The TET mechanism in QD-sensitized TTA has often been attributed to a direct concerted Dexter-type triplet energy transfer. Jin *et al.* investigated the role of the competing Förster resonance energy transfer (FRET) and charge transfer processes in CdSe-sensitized triplet generation in boron dipyrromethene (BODIPY). By transient absorption spectroscopy, they found that the triplet state in BODIPY is populated via a charge-separated intermediate state, where BODIPY is oxidized and the QD is left with a conduction band electron. No contribution of a direct Dexter energy transfer was found, rather the authors of Ref. 27 found that the FRET and charge transfer pathways are the competitive pathways.

In addition to the QD-sensitized UC schemes previously discussed, recently, bulk lead halide perovskites have emerged as efficient triplet sensitizers for solid-state NIR-to-visible UC. The triplet sensitization mechanism here is based on a charge transfer of the photoexcited carriers created in the perovskite to the triplet state of the annihilator rubrene. Commonly fabricated in a two-step spin-coating process, the interface between the lead halide perovskite sensitizer and the rubrene annihilator is crucial for the overall device efficiency, as this is where the charge transfer occurs. Prashanthan *et al.* investigated the effect of the device fabrication conditions on the UC intensity.²⁸ In particular, they investigated the effect of the chosen antisolvent (chlorobenzene vs anisole) and the dripping time on the performance of the methylammonium lead iodide perovskite and the resulting UC in rubrene. They found a distinct correlation between the carrier lifetime in the perovskite film and the device performance. As a result, they concluded that the defect density at the interface, which correlates with the antisolvent used, is vital for the observed UC. Similarly, Bieber *et al.* investigated the influence

of a wide variety of parameters on the UC mechanism: stoichiometry, composition, solvent used for the rubrene deposition, and post-fabrication annealing. In this game of UC bingo, it was found that in contrast to perovskites used in photovoltaics, the stoichiometry with respect to excess lead iodide does not play a deciding role. Rather, the composition (methylammonium or formamidinium-rich) influences the charge extraction, the solvent (toluene vs chlorobenzene) plays a role in the UC efficiency as it influences the packing of the organic layer, and the post-fabrication annealing step is vital to further increase the device performance as it “heals” the interface affected by the second solution-processing step.²⁹ Overall, it was shown that the interface is the most crucial aspect of these solid-state UC devices.

C. Thermally activated delayed fluorescence

Unlike singlet fission and TTA-UC, which use molecules with large singlet-triplet energy gap, an UC process called thermally activated delayed fluorescence (TADF) occurs when the singlet-triplet energy gap becomes small enough to be overcome by thermal energy [Fig. 1(d)]. TADF is a reverse intersystem crossing (RISC) process that converts the dark triplet produced by charge recombination in organic light-emitting diodes (OLEDs) into a luminescent singlet. Identifying design guidelines for maximizing the RISC rate is very important for obtaining highly efficient OLEDs based on TADF. Cho *et al.* performed a long-range corrected density functional theory calculation of TADF molecules with multiple electron donor sites and proposed that the smaller adiabatic singlet-triplet energy gap and intramolecular reorganization energy play a more important role in the RISC rate than the previously proposed change in spin-orbit coupling by introducing secondary donors.³⁰ Shimoda *et al.* investigated the molecular structure of linearly linked donor-acceptor TADF molecules in the ground and excited states by time-resolved infrared spectroscopy and quantum chemical calculations and proposed that the molecular rotation fluctuation plays an important role in the expression of TADF by mixing between the locally excited state with large oscillator strength and the charge-transfer state with a small singlet-triplet gap.³¹

D. Lanthanide-based upconversion

Inorganic upconverting nanoparticles (UCNPs) have also been actively studied in recent years as wavelength conversion materials from near-infrared to visible light. NaYF₄:Yb/Er, a typical UCNP, has been employed for biological applications such as imaging, sensing, photodynamic therapy, and optogenetics. NaYF₄:Yb/Er takes a cubic phase (α -phase) and a hexagonal phase (β -phase), and the β -phase has a better UC efficiency. However, the synthesis of β -phase UCNPs with high water dispersibility and routes that are free of toxic side products remains a challenging task. Dinic *et al.* synthesized hexagonal NaY_{0.5}Gd_{0.3}F₄:Yb,Er UCNPs by the solvothermal method using hydroxyl-carboxyl type chelators (citric acid and sodium citrate) and different fluoride sources (NaF, NH₄F, and NH₄HF₂).³² It was found that the phase, size, and shape of the obtained particles were affected by the type of the chelating agent and fluoride source. Calabro *et al.* found a method to convert bulk NaYF₄:Yb/Er into UCNPs by laser ablation in liquid (LAL).³³ The UCNPs synthesized by this LAL method can be coated with water-soluble ligands during

synthesis and can be stably dispersed in water. It was also found that UCNPs with more uniform morphology and closer composition to the original bulk material could be obtained by using high laser fluences than by using low laser fluence due to the explosive ejection mechanism.

E. Non-linear upconversion via second-harmonic generation

Another UC approach is generating higher harmonic frequencies via non-linear optical processes, a method commonly used in laser optics to frequency double or triple the incident wavelength. Vorontsov *et al.* achieved IR-to-visible UC by second-harmonic generation (SHG) in KH_2PO_4 single crystals, which are coupled with CdTe/CdS core-shell QDs. Upon irradiation of the crystal at 1064 nm, SHG generates upconverted light with a wavelength of 532 nm. This upconverted light is then re-absorbed by the embedded QDs, resulting in subsequent photoluminescence, enabling broadband-tunable UC with a fast response time.³⁴

IV. CONCLUSIONS

The article collection on *Up- and Down-Conversion in Molecules and Materials* demonstrates the breadth and depth of this emergent field. Both UC and DC need the concerted effort of material synthesis, spectroscopic characterization, and theoretical investigation. The collection includes contributions touching on all these aspects and also highlights the common themes for both UC and DC and both organic and inorganic systems. In all these systems, the material structure, energy transfer mechanisms, and the electronic and excitonic levels are key considerations in designing materials and devices. We hope that the article collection will form a valuable resource and help to further develop the field.

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