Triplet sensitization of a near-infrared emissive Molybdenum complex via singlet fission

(*[1]Fac. Eng., Kyushu Univ., [2]Grad. Sch. Eng., Kyushu Univ., [3]Grad. Sch. Sci., Kyushu Univ., [4]CMS, Kyushu Univ., [5]JGU, [6]K-NETs, [7]JST-ACT-X*) ○Percy Gonzalo Sifuentes Samanamud[1] • Adrian Sauer[5] • Ilias Papadopoulos[2] • Ami Takada[3] • Aki Masaoka[2] • Yuta Sawada[2] • Yuya Watanabe[2] • Kiichi Mizukami[2] • Kiyoshi Miyata[3] • Ken Onda[3] • Katja Heinze[5] • Yoichi Sasaki[2,4,7] • Nobuo Kimizuka[2,4,6]

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Singlet fission (SF) is a multiple exciton generation process that multiplies one singlet exciton into two triplet excitons in specific organic molecules. This mechanism has attracted significant interest for its potential to enhance the efficiency of photovoltaic devices and light-emitting diodes.[1] However, practical applications beyond these applications remain undeveloped due to the scarcity of chromophores satisfying the energy alignments ($E(S_1) > 2E(T_1)$) and no practical means to demonstrate photon multiplication based on the SF process.

In this study, we developed a new methodology of SF-based photon multiplication that employs a near-infrared emissive molybdenum complex, *mer*-$MoCl_3$(ddpd),[2] whose energy levels can be precisely tuned via ligand design. As part of our approach, TIPS-tetracene dimers were synthesized as SF hosts capable of undergoing intramolecular SF, followed by efficient triplet energy transfer. Unlike precedent efforts, the proposed system demonstrates successful SF and subsequent triplet energy harvesting by the emissive chromophore in the solution state.

This presentation will explore the unique properties of this molybdenum complex and its role in optimizing SF-based sensitization efficiency in solution-phase systems, providing insights into its potential for advancing energy conversion technologies.

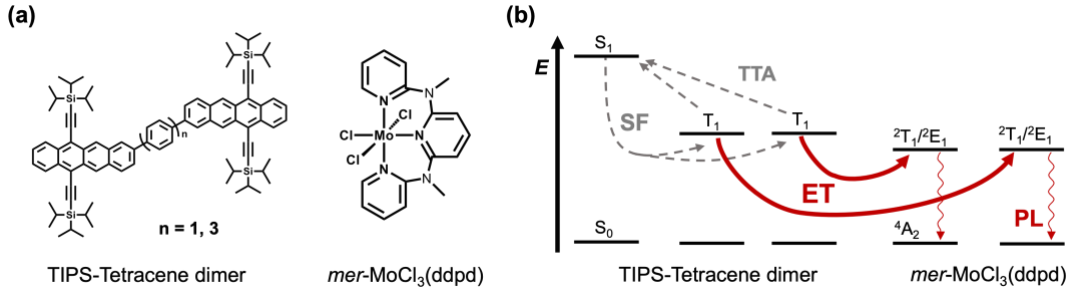

Fig. 1 (a) Chemical structure of TIPS-Tetracene dimers and *mer*-$MoCl_3$(ddpd) and (b) schematic diagram of triplet sensitization via SF.

1) M. B. Smith et al., *Chem. Rev.*, **2010**, 11, 6891–6936.
2) W. R. Kitzmann et al., *Inorg. Chem.*, **2023**, *62*, 15797–15808.