

# Understanding Correlation among Electron-Phonon-Spin Degree of Freedom in Advanced Molecular Optoelectronics

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Microscopic understanding of exciton and carrier physics in molecular materials for optoelectronics is a great challenge because of their complexity resulting from strong electron-phonon coupling and perhaps interaction to spin degree of freedom; e.g. superior optoelectronic properties of lead-halide perovskites materials likely originate from its unique electron-phonon coupled dielectric screening of carriers [1,2], electron spin-flip of intersystem crossing in molecular optoelectronic materials are strongly connected to molecular geometries in the excited states and vibronic coupling [3,4], and singlet fission, ultrafast generation of a correlated triplet pair state from a singlet excited state, is viewed as an extreme example of a concerted process of electron-phonon-spin degrees of freedom [5,6]. Here, I would like to discuss a few topics mainly focusing on thermally activated delayed fluorescence and singlet fission materials regarding the quest to understand the functions using various time-resolved spectroscopy.

## References

- [1] H. Zhu<sup>†</sup>, K. Miyata<sup>†</sup>, Y. Fu, J. Wang, P. P. Joshi, D. Niesner, K. W. Williams, S. Jin, X.-Y. Zhu\*, “Screening in crystalline liquids protects energetic carriers in hybrid perovskites”, *Science* 353, 1409-1413 (2016).
- [2] K. Miyata, D. Meggiolaro, M. T. Trinh, P. P. Joshi, E. Mosconi, S. C. Jones, F. D. Angelis, X.-Y. Zhu\*, “Large polarons in lead halide perovskites”, *Science Advances* 3, e1701217 (2017).
- [3] K. Miyata, Y. Kurashige, K. Watanabe, T. Sugimoto, S. Takahashi, S. Tanaka, J. Takeya, T. Yanai, Y. Matsumoto\*, “Coherent singlet fission activated by symmetry breaking”, *Nature Chem.* 9, 983-989 (2017).
- [4] K. Miyata, F. S. Conrad-Burton, F. L. Geyer, X.-Y. Zhu\*, “Triplet pair states in singlet fission”, *Chem. Rev.* 119, 4261-4292 (2019).
- [5] M. Saigo, K. Miyata\*, S. Tanaka, H. Nakanotani, C. Adachi, K. Onda\*, “Suppression of Structural Change upon S<sub>1</sub>-T<sub>1</sub> Conversion Assists the Thermally Activated Delayed Fluorescence Process in Carbazole-Benzonitrile Derivatives”, *J. Phys. Chem. Lett.* 10, 2475-2480 (2019).
- [6] Y. Shimoda, K. Miyata\*, M. Saigo, Y. Tsuchiya, C. Adachi, K. Onda, “Intramolecular-rotation driven triplet-to-singlet upconversion and fluctuation induced fluorescence activation in linearly connected donor-acceptor molecules”, *J. Chem. Phys.* 153, 204702 (2020).