2-6-5. Room-Temperature Phosphorescent Materials

Overview

Light emission in which the electron spin multiplicity changes during the transition process is defined as phosphorescence. Short-lived phosphorescent materials derived from heavy metal complexes that have increased the phosphorescence emission rate have been applied to organic electroluminescent devices and have been introduced into the large-scale market for thin-film and flexible displays and lighting. Recently, research has progressed to increase the room-temperature phosphorescence yield to the long-wavelength region in long-lived phosphorescence from organic materials that do not contain heavy metals, and to apply it to time-resolved imaging.

Current Status and Frontiers

In 1998, the application of heavy metal complexes, which had increased phosphorescence emission rates, to organic electroluminescence triggered a great deal of phosphorescence research, leading to practical applications in displays and lighting (Fig. 1). Meanwhile, over the past 15 years, organic materials that do not use heavy atoms have also been reported to have improved phosphorescence performance and applications in the imaging field (Fig. 1).

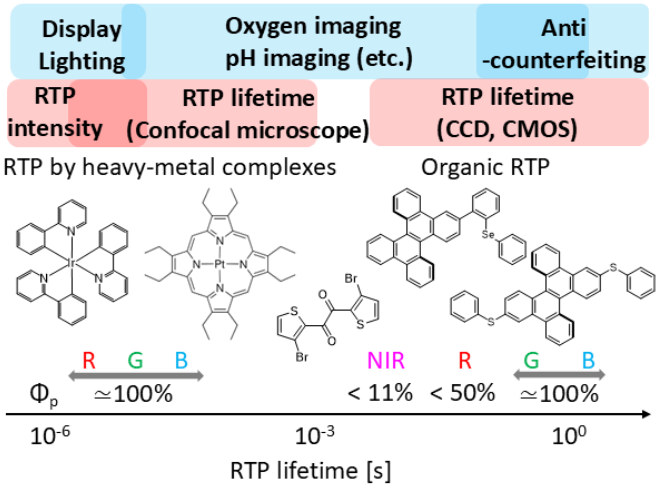

Figure 1. Relationship between phosphorescence lifetime and application area.

1. The solid host environment around organic molecules to allow RTP

The use of a host with a T_1 energy sufficiently higher than that of the guest (Fig. 2 (i)) and an excellent oxygen barrier to avoid oxygen quenching allows for significant suppression of T_1 deactivation caused by intermolecular electron exchanges of the guest molecule (Hirata, Watanabe, Adachi et al.). This significant suppression of T_1 deactivation allows for the generation of slow phosphorescence from organic guests.

2. Phosphorescence prediction through collaboration of experiments and calculations

With the development of transient absorption spectroscopy (Nakagawa et al.), it has

become possible to accurately optically quantify the radiative rate constant (k_r^T) and non-radiative rate constant (k_{nr}^T) from T_1. Based on the theoretical formulas for k_r^T and k_{nr}^T (El-Sayed et al.), k_r^T and k_{nr}^T have been calculated, and it has become possible to discuss the factors behind the improvement of Φ_p by examining the correlation between experimental and calculated values for k_r^T and k_{nr}^T (Fig. 2 (ii)) (Hirata et al.).

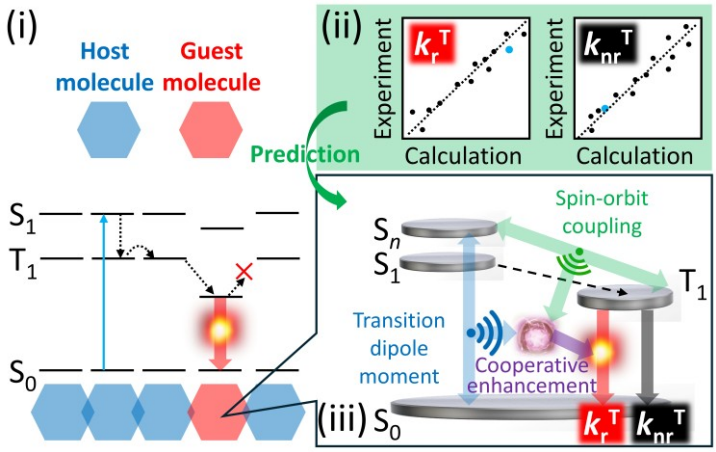

Figure 2. Material elements related to improving RTP yield.

3. Searching for key elements for strategic organic phosphorescence enhancement

Since 2018, a combination of experiments and calculations has confirmed that an increase in the product of the transition dipole moment and spin-orbit coupling involving a higher-order singlet excited state (S_n) contributes to a selective increase in k_r^T (Fig. 2 (iii)) (Hirata et al.). This concept has also been confirmed to apply to the fast phosphorescence of organic molecules containing heavy atoms (Tani, Miyata et al.). Furthermore, through-bond and through-space interactions between main group elements and π chromophores also contribute to the selective k_r^T enhancement (Hirata et al.).

4. Application development to high-resolution lifetime imaging and multi-tone imaging

High-resolution RTP lifetime imaging using confocal microscopes and two-dimensional photodetectors have been developed (Hirata et al.).

References

1. S. Hirata, et al., *Adv. Funct. Mater.*, **23**, 3386–3397 (2013).
2. I. Bhattacharjee, S. Hirata, *Adv. Mater.*, **32**, 2001348 (2020).
3. Y. Tani, et al., *Chem. Sci.*, **15**, 10784–10793 (2024).
4. R. K. Mulimani, et al., *Adv. Mater.*, **37**, 2502611 (2025).

Future Perspectives and Directions

Issues that are expected to be realized within the next 10 years: Achieving efficient RTP yield in the near-infrared wavelength, establishing molecular design for organic RTP, and establishing high-resolution, high-speed lifetime and multi-tone imaging technology.

(Author：Shuzo Hirata)