

The 817th

MANA Seminar



A collaborative experimental and computational approach for the discovery of enhanced organic phosphorescent molecules

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Friday, January 23rd 14:00 – 14:45

The strong afterglow emission from organic phosphorescence immediately after the excitation light is turned off is useful for high-resolution multicolor imaging independent of autofluorescence. Our group is developing conjugated molecules that enable high phosphorescence quantum yields in order to achieve the higher-resolution afterglow imaging. Measurements of triplet generation efficiency, including transient absorption, have clarified the photophysical rates from the triplet state. The photophysical rates from the triplet state was calculated using dynamic quantum chemical calculations that include molecular conformational distributions. This rapid collaboration between experiments and calculations confirmed that the proposed dynamic quantum chemical calculations are suitable for predicting the phosphorescence properties of many organic π -molecules. Using the dynamic quantum chemical calculations, we demonstrated that molecules with through-bond interactions or through-space interactions between the chalcogen atom and the π chromophore are favorable for enhancing long-wavelength organic phosphorescence. This improved yield of organic phosphorescence enables afterglow measurements from single nanocrystals, and these organic phosphorescent crystalline nanoparticles enable high-speed two-dimensional oxygen concentration imaging.

Venue: Auditorium, 1F, WPI-MANA Bldg., Namiki

Chair: Dr. Takashi Nakanishi (MANA Group Leader)

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