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A new model to accurately develop better OLEDs

Researchers develop a new analytical model detailing the kinetics of the exciton dynamics in TADF materials, the primary component in OLEDs

Fukuoka, Japan—Organic light emitting diodes, or OLEDs, are a type of photoluminescence device that utilizes organic compounds to produce light. Compared to traditional LEDs, OLEDs have shown to be more efficient, can be built into super-thin and flexible materials, and have higher dynamic range in image quality. To further develop better OLEDs, researchers around the world work to understand the fundamental chemistry and physics behind the technology.

Now, researchers at Kyushu University have developed a new analytical model that details the kinetics of the exciton dynamics in OLED materials. The findings, published in *Nature Communications*, has the potential to enhance the lifetime of OLED devices, and accelerate the development of more advanced and efficient materials.

Fluorescence devices like OLEDs light up because of excited electrons, or excitons. When you add energy into atoms, their electrons get excited and jumps to a higher energy state. When they come back down to their regular energy state they produce fluorescence. Excitons also can go into different states, namely a singlet state, denoted as S_1, or a triplet state, denoted as T_1. Fluorescence can only happen when excitons drop from the singlet state.

"Thankfully, excitons can transfer between the triplet and singlet state. Therefore, if we can convert triplet excitons into singlets, the efficiency of fluorescence drastically improves," explains Professor Chihaya Adachi of Kyushu University's Center for Organic Photonics and Electronics Research (OPERA), who led the study. "One of the major breakthroughs of OLED research was in the development of thermally activated delayed fluorescence, or TADF, materials. These materials would close the 'gap' between S_1 and T_1, so that T_1 excitons more easily transfer to S_1, thus producing more fluorescence."

Understanding the gap between S_1 and T_1 in TADF materials is fundamental in both evaluating the efficiency of OLED materials and in testing the efficacy of new materials. However, the standard method of testing this gap has been occasionally unreliable due to its inherent subjectivity and conditional assumptions.

"When developing new TADF materials we employ quantum calculations to forecast this gap, denoted as ΔE_{st}. However, it's not feasible to theoretically calculate the behavior of all electrons to determine the accurate excitation state configuration. So, to reduce computation costs we usually work with certain assumptions. But this results in different values between experimental and estimated data," explains first author of the study, Research Associate Professor Youichi Tsuchiya.

"To close the gap between theoretical and experimental methods our team worked to developed a model that can more accurately estimate ΔE_{st}. Our new analytical method employed several fundamental theories of physical chemistry and put into account the exciton transfer between the triplet energy states."

Accurately describing the excited-state structures of organic molecules was something that had been difficult to explore in detail until now. The team hopes their work will not only contribute to the research and development of high-performance luminescent materials but also pave the way for further advances in photochemistry.

"This new analytical method will be utilized on other types of TADF materials as well, helping us to clarify exciton dynamics in future OLED research," concludes Adachi. "We also want to explore the use of AI to accurately predict the properties of new materials."

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For more information about this research, see "Temperature dependency of energy shift of excitonic states in a donor–acceptor type TADF molecule," Youichi Tsuchiya, Keito Mizukoshi, Masaki Saigo, Tomohiro Ryu, Keiko Kusuhara, Kiyoshi Miyata, Ken Onda, and Chihaya Adachi, *Nature Communications* https://doi.org/10.1038/s41467-025-59910-z

About Kyushu University

Founded in 1911, Kyushu University is one of Japan's leading research-oriented institutes of higher education, consistently ranking as one of the top ten Japanese universities in the Times Higher Education World University Rankings and the QS World Rankings. The university is one of the seven national universities in Japan, located in Fukuoka, on the island of Kyushu—the most southwestern of Japan's four main islands with a population and land size slightly larger than Belgium. Kyushu U's multiple campuses—home to around 19,000 students and 8000 faculty and staff—are located around Fukuoka City, a coastal metropolis that is frequently ranked among the world's most livable cities and historically known as Japan's gateway to Asia. Through its VISION 2030, Kyushu U will "drive social change with integrative knowledge." By fusing the spectrum of knowledge, from the humanities and arts to engineering and medical sciences, Kyushu U will strengthen its research in the key areas of decarbonization, medicine and health, and environment and food, to tackle society's most pressing issues.

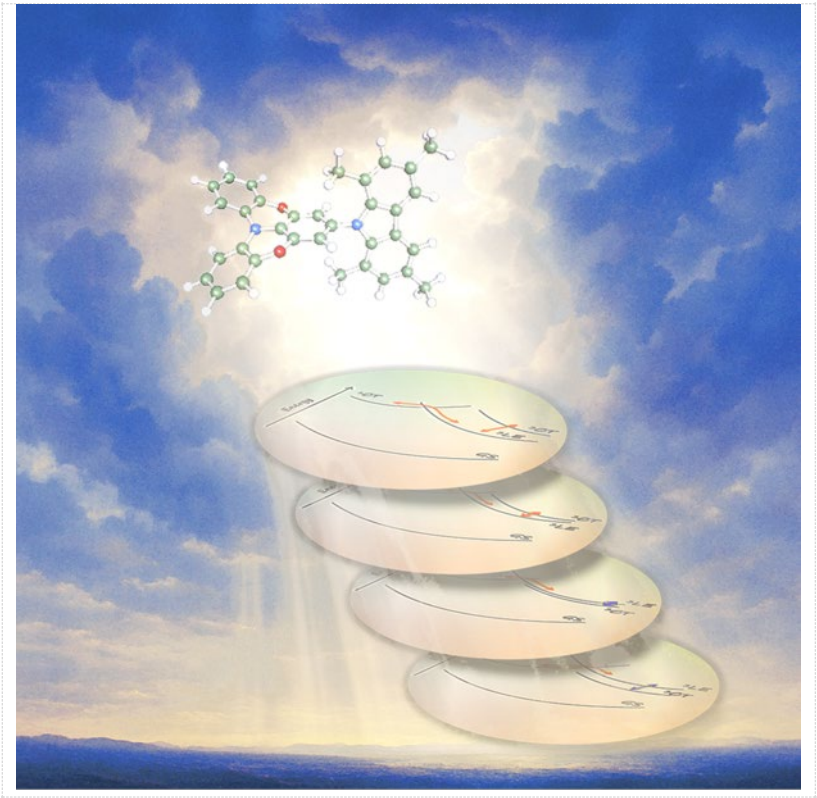

Fig. 1. Excitonic energy configuration changes of a TADF material. Excitonic state alignment is affected by temperature and the solvent the material is in. This leads the peculiar exciton kinetics when the energy gap between S_1 and T_1 approaches to zero. (Chihaya Adachi, Youichi Tsuchiya/Kyushu University)

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