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PRESS RELEASE (2025/11/04)

Controlling next-generation energy conversion materials with simple pressure

New study provides guidelines on creating photoreactive molecules that are sensitive to mechanical stimuli using flexible linkers

Fukuoka, Japan—Researchers at Kyushu University have designed a class of molecules whose ability to amplify light energy can be actively controlled by simply applying pressure. The findings, published in the journal *Chemical Science*, may open new possibilities for highly efficient energy conversion devices and advanced medical therapies.

The study is centered on a physical process called singlet fission (SF). SF is a mechanism where, when a molecule is struck by a single high-energy photon, it splits that energy to create two lower-energy excited states instead of just one. In effect, it acts like an energy amplifier, potentially doubling the yield of useful excited molecules.

However, designing materials that reliably perform SF is challenging because the core molecules must meet a strict energy balance, driving chemists to look beyond merely modifying functional molecular groups. To overcome this limitation, researchers work to develop 'smart' molecules whose function can be actively controlled by external stimuli, such as temperature or mechanical pressure.

In this study, a research team led by <u>Professor Gaku Fukuhara</u> from the <u>Institute for Materials Chemistry and Engineering</u> at Kyushu University, in collaboration with Professor Taku Hasobe from Keio University, worked on developing a molecule that can be controlled through hydrostatic pressure.

The researchers synthesized a series of SF-active molecules composed of two pentacene (a compound made of 5 fused benzene rings) units connected by flexible polar linkers—molecular chains that act like adjustable bridges between the units. They then examined how these molecules behave under different pressure conditions and solvent environments.

Through simulations and experiments, they determined that the flexibility of the linkers was a major factor in determining the SF properties of the molecule. Unlike previous, more rigid designs, the flexible linkers gave way to a phenomenon known as SF dynamics inversion. In moderately polar solvents, like toluene, the linkers were found to undergo spontaneous solvation (attracting solvent molecules) when under pressure, which suppressed the SF reaction rate. However, switching to a more polar solvent like dichloromethane inverted the pressure-induced effect, leading to an acceleration of the SF reaction.

"These results present a new concept for controlling excited-state reactions through external mechanical stimuli and establish the foundation for designing pressure-responsive photoactive materials," states Fukuhara.

Beyond simply controlling the SF reaction rate, the team made important discoveries about the resulting triplet excitons, which are useful energy carriers. They found that the lifetime of these states was linked to pressure, an effect caused by the changes in viscosity of the surrounding solvent. Moreover, the triplet quantum yield, which determines the efficiency of triplet production, did not decrease under pressure.

"The results obtained and concepts proposed in our work will enable us to construct actively controllable SF materials, based on molecular design guidelines established by us. Applying these principles may lead to phototherapeutic materials that function in biological environments, or pressure-responsive energy conversion devices," concludes Fukuhara.

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For more information about this research, see "Critical molecular design that can actively control intramolecular singlet fission by hydrostatic pressure," Rintaro Ogawa, Tomokazu Kinoshita, Tomoya Kuwabara, Hayato Sakai, Makoto Harada, Taku Hasobe, and Gaku Fukuhara, *Chemical Science*, https://doi.org/10.1039/D5SC04791A.

About Kyushu University

Founded in 1911, <u>Kyushu University</u> is one of Japan's leading research-oriented institutions 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. Located in Fukuoka, on the island of Kyushu—the most southwestern of Japan's four main islands—Kyushu U sits in a coastal metropolis frequently ranked among the world's most livable cities and historically known as Japan's gateway to Asia. Its multiple campuses are home to around 19,000 students and 8,000 faculty and staff. Through its <u>VISION 2030</u>, 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.

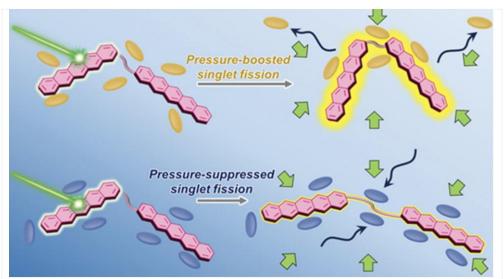


Fig. 1. Graphical abstract of the research. The image shows the active control of SF photoreaction processes via hydrostatic pressure depending on the solvent used. (Gaku Fukuhara/Kyushu University)

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