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**Toward tunable molecular switches from organic compounds**

Newly synthesized organic molecules can be tuned to emit different colors depending on their molecular structures in crystal form

*Joint press release by Hokkaido University and Kyushu University.*

Molecular switches are chemicals with molecular structures that can be shifted between two or more stable configurations in response to changes in their environment. They are of great interest in the development of molecular computers, molecular machines, and drug delivery systems. Compounds with conformational isomers—identical molecular formulas but different molecular structures—can make very effective molecular switches.

Researchers at Hokkaido University and Kyushu University have developed a technique to synthesize potential molecular switches from anthraquinodimethanes (AQDs), a group of overcrowded organic molecules. The study, led by Associate Professor Yusuke Ishigaki at Hokkaido University and Associate Professor Toshikazu Ono at Kyushu University, was published in the journal *Materials Chemistry Frontiers*.

"AQDs are a type of overcrowded ethylene, molecules with carbon-carbon double bonds surrounded by large chemical groups," explains Ono. "They have two common isomers, the folded and twisted forms. They are especially interesting as molecular switches, as their sterically hindered double bond can provide isomers absorbing and emitting different wavelengths of light."

AQDs generally adopt the most stable folded or twisted form, making it difficult to isolate pure samples of any other isomer to study its properties. The researchers surmounted this obstacle by designing flexible AQD derivatives that can more easily and stably form different isomers.

The synthesized derivatives were not only able to stably form twisted and folded isomers, but also other isomeric forms, when recrystallized in different solvents. The researchers performed detailed analysis of the derivatives to fully understand their properties.

In a crystalline state, each of these isomers absorbs and emits distinct frequencies of light, which is due to the differences in the distribution of electrons in the isomer molecules. Interestingly, the light absorption and emission changed when the crystals were ground into amorphous solid, and following treatment with appropriate solvents can produce original or other crystals with a variety of colors.

"This work is the first report on the isolation of multiple isomeric forms of AQD," Ishigaki concluded. "Their absorption and emission of different light frequencies, and more importantly, the ability to modulate the absorption and emission by external stimuli, make these compounds excellent candidates for the development of molecular switches."

Original release from Hokkaido University

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For more information about this research, see "Exceptionally flexible quinodimethanes with multiple conformations: polymorph-dependent colour tone and emission of crystals," Kazuma Sugawara, Toshikazu Ono, Yoshio Yano, Takanori Suzuki, and Yusuke Ishigaki, *Materials Chemistry Frontiers,* https://doi.org/10.1039/D2QM01199A

**About Kyushu University**
Kyushu University is one of Japan's leading research-oriented institutes of higher education since its founding in 1911. Home to around 19,000 students and 8,000 faculty and staff, Kyushu U's world-class research centers cover a wide range of study areas and research fields, from the humanities and arts to engineering and medical sciences. Its multiple campuses—including one of the largest in Japan—are located around Fukuoka City, a coastal metropolis on the southwestern Japanese island of Kyushu 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.' Its synergistic application of knowledge will encompass all of academia and solve issues in society while innovating new systems for a better future.

Fig. 1. Crystals of the newly synthesized compounds, anthraquinodimethane derivatives, which have different colors depending on their molecular structure (Yusuke Ishigaki)

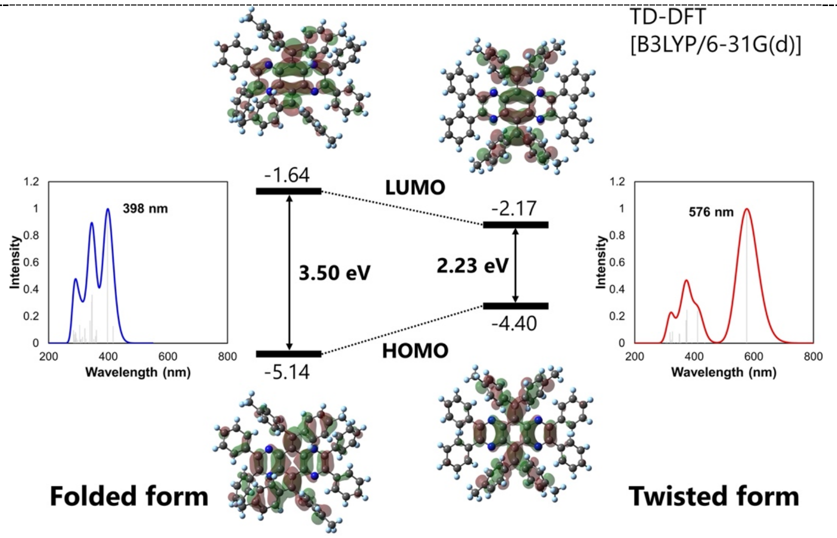


Fig. 2. The folded and twisted isomers absorb different wavelengths of light (Kazuma Sugawara, et al. Materials Chemistry Frontiers. February 8, 2023).

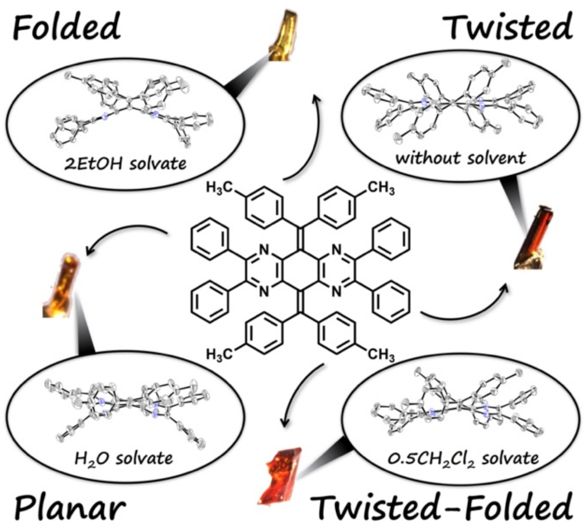


Fig. 3. The methyl derivative of the new compound has four different isomers, with different crystal structures each (Kazuma Sugawara, et al. Materials Chemistry Frontiers. February 8, 2023).

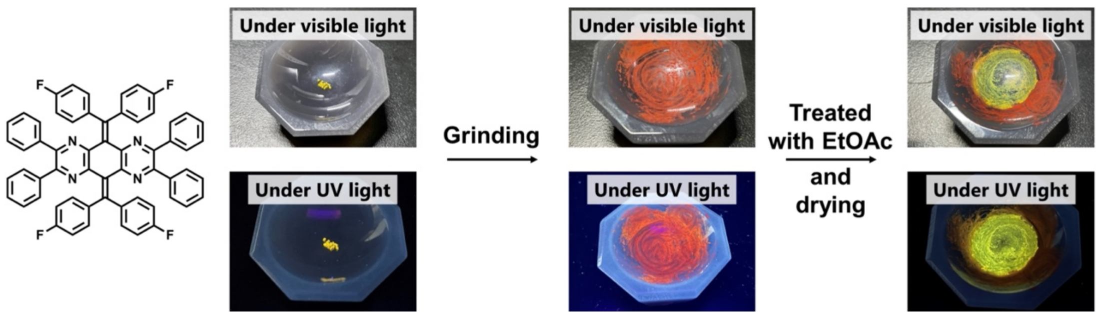


Fig. 4. When ground into amorphous solid and treated with appropriate solvents the light absorption and emission changes (Kazuma Sugawara, et al. Materials Chemistry Frontiers. February 8, 2023).

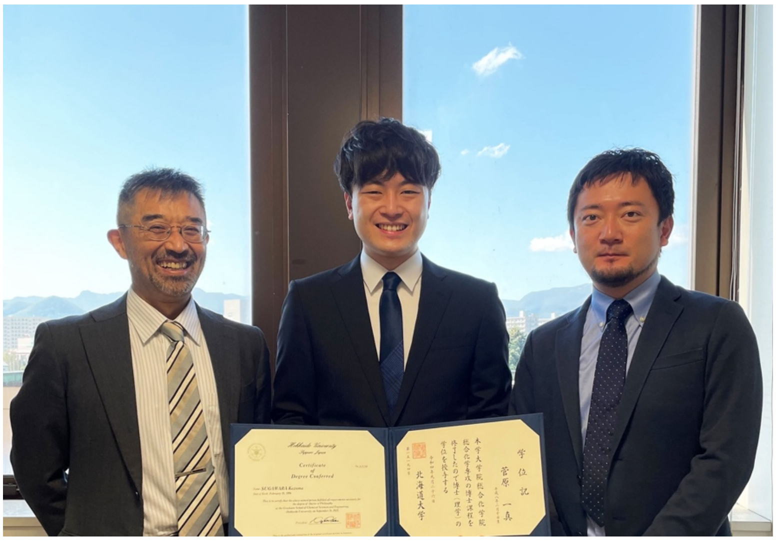

Fig. 5. Takanori Suzuki (left) Kazuma Sugawara (center) and Yusuke Ishigaki (right), authors from Hokkaido University (Photo: Yusuke Ishigaki).

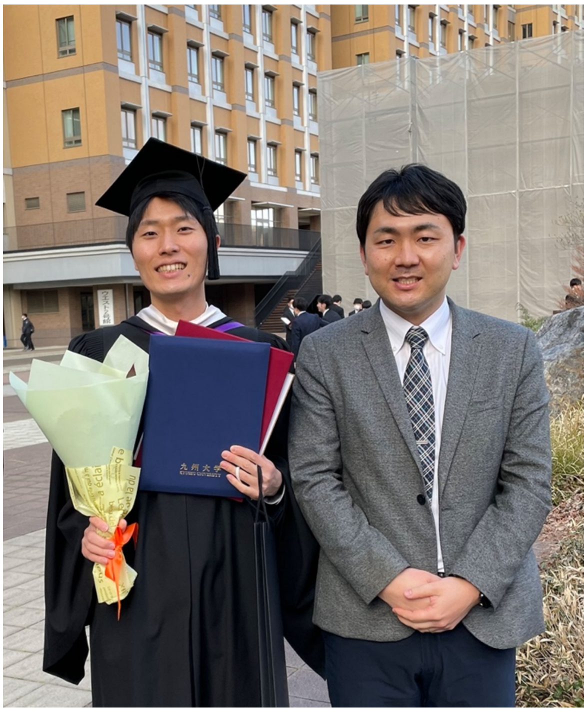

Fig. 6. Yoshio Yano (left) and Toshikazu Ono (right), authors from Kyushu University (Photo: Toshikazu Ono).

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