

Proper electronic structure of near-infrared absorbing functional dyes discovered

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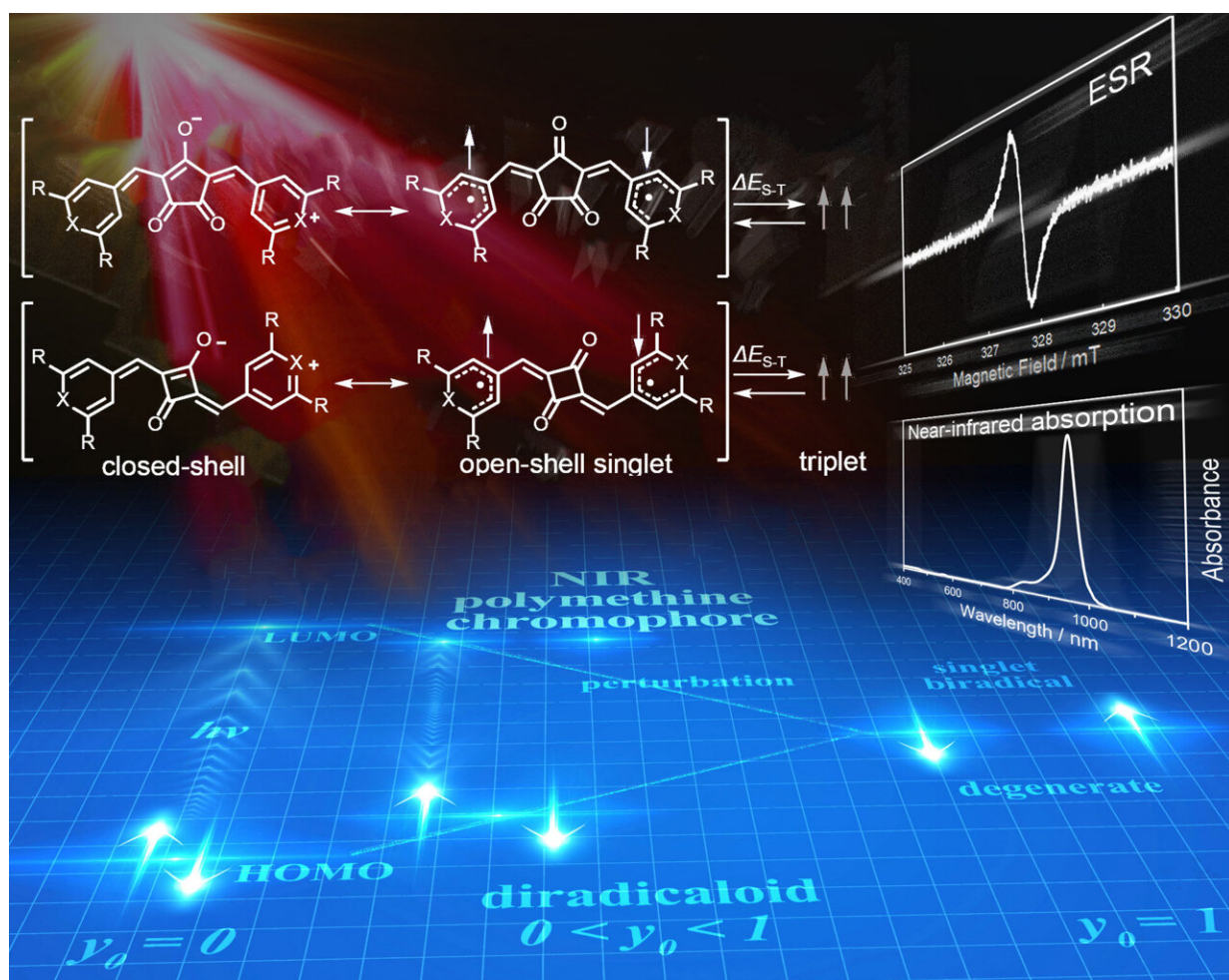


Illustration of properties and electronic structure of a near-infrared absorbing dye in an intermediate state between closed- and open-shell states. Credit: Takeshi Maeda, Osaka Metropolitan University

Near-infrared light, whose wavelength is longer than visible light, is invisible and can pass through many substances. Organic materials that efficiently absorb near-infrared light are essential for technological innovations that utilize near-infrared light, such as the dyes in the infrared blocking filters of smartphone cameras and security inks. These and many more technical applications make developing new dyes that can absorb longer wavelengths of near-infrared light desirable.

Previously, near-infrared absorbing organic materials were treated as closed-shell molecules without unpaired electrons. However, a joint research group led by Associate Professor Takeshi Maeda, Assistant Professor Daisuke Sakamaki, and Professor Hideki Fujiwara from Osaka Metropolitan University discovered that near-infrared absorbing oxocarbon-based dyes have an intermediate state between closed-shell and open-shell electronic configurations. They also found that as the wavelengths of [near-infrared light](#) absorbed increase, so does the contribution of open-shell forms in the dye.

Their research results were published in *Chemical Science* on January 16, 2023.

"We have clarified the proper electronic structure of near-infrared absorbing oxocarbon-based dyes that are regarded as pure closed-shell molecules. We hope that this will lead to advances in the molecular design, properties, functions, and applications of near-infrared absorbing [dyes](#) and to the development of new near-infrared absorbing organic materials that be used in society," Professor Takeshi Maeda said.

More information: Takeshi Maeda et al, Unveiling a new aspect of oxocarbons: open-shell character of 4- and 5-membered oxocarbon derivatives showing near-infrared absorption, *Chemical Science* (2023). [DOI: 10.1039/D2SC06612B](https://doi.org/10.1039/D2SC06612B)

Provided by Osaka Metropolitan University

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