

Dye absorption structure of dye-sensitized solar cells elucidated on molecular level

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NIMS researchers elucidated the relationship between the photocurrent and the peculiar changes in the absorption structure occurring in the vicinity of the molecular-electrode interface in dye-sensitized solar cells

The Organic/Inorganic Hybrid Photovoltaics Group of the NIMS, Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), elucidated the relationship between the photocurrent and the peculiar changes in the absorption structure occurring in the vicinity of the molecular-electrode interface in [dye-sensitized solar cells](#), by conducting a soft X-ray radiation experiment at the High Energy Accelerator Research Organization (KEK).

A research group led by Dr. Mitsunori Honda (post-doctoral researcher; currently a fixed-term researcher at the Quantum Beam Science Directorate R&D Directory of the Japan Atomic Agency (JAEA)) and Dr. Masatoshi Yanagida (Group Leader) of the Organic/Inorganic Hybrid Photovoltaics Group of the Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN; headed by Director-General Kohei Uosaki) of the National Institute for Materials Science (NIMS; headed by President Sukekatsu Ushioda) elucidated the relationship between the photocurrent and the peculiar changes in the absorption structure occurring in the vicinity of the molecular-electrode interface in dye-sensitized solar cells, by conducting a soft X-ray radiation experiment at the High Energy Accelerator Research Organization (KEK).

Dye-sensitized solar cells attract attention as a low-cost and high-flexibility type of next-generation solar cells. However, for their commercial application, it is necessary to achieve higher photoelectric conversion efficiency (especially in terms of the photocurrent) beyond the presently available level. In dye-sensitized solar cells, since dyes absorb light and separate charges, the photocurrent is thought to be dependent on the dye absorption structure, and therefore elucidation and control of the absorption structure on real devices are indispensable for increasing the conversion efficiency.

The research group analyzed the absorption structure of N719, a ruthenium metal complex dye, using X-ray photoelectron spectroscopy and X-ray absorption near edge structure analysis for investigating the electronic structure of dye molecules. Normally, N719 dye is absorbed on the TiO₂ surface via a carboxyl (COOH) group. However, the experiment result showed that there was a strong interaction between NCS- (thiocyanate ligand) and TiO₂. Such an absorption structure had not been taken into consideration in the previous model but might have impeded the photocurrent.

The experiment also revealed that the strong interaction between NCS- and TiO₂ would disappear upon simultaneous absorption of D131 dye (a dye that demonstrates strong light absorption properties within the short wavelength range and is widely used as a co-absorption agent). The research team controlled the optimal absorption structure based on this experiment result and found that the external quantum efficiency would increase in the visible light range of solar cells (about a 0.3% increase in the photoelectric conversion efficiency under sunlight.)

More information: The research results were published on August 22 in a journal of the American Chemical Society, the *Journal of Physical Chemistry C* (2013, Vol. 117, 17033-17038 [DOI: 10.1021/jp404572y](https://doi.org/10.1021/jp404572y)), as the achievement made by GREEN under the MEXT Program for

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