Department of Applied Chemistry and Food Science

Key words: Photocatalysis, Titanium dioxide, Self-assembled monolayers, Silane coupling agents, Dye-sensitized solar cell

Doctor(Engineering) / Senior Lecturer

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Education

Department of Environmental and Biological Chemistry, Fukui University of Technology, Department of Applied Science and Engineering, Environmental and Biological Chemistry Course, Fukui University of Technology (Master/Doctor Course; skip the master 2nd-grade)

Professional Background

WORLD INTEC CO., LTD. R&D (Assigned to chemical manufacturers)

Consultations, Lectures, and Collaborative Research Themes

Fabrication and characterization of dye-sensitized solar cell,
Quantum chemical calculation by using Gaussian

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Main research themes and their characteristics

「A study of dye-sensitized solar cell containing a photosensitizing dye covalently attached to silane coupling agents」

Surface modifiers (silane coupling agents (SCAs), phosphonic acids, alkanethiols, and so on) are added the functions such as adhesiveness and hydrophobicity to the surface of materials. In our group, the enhancement of photocatalytic activity and the addition of functions for the titanium dioxide (TiO_2) by surface modification are investigating. This poster reports the study of TiO_2 based dye-sensitized solar cell (DSSC) containing SCAs (Fig.1). This study carries out the modification of TiO_2 surface deposited on the substrate by SCAs based self-assembles monolayers (SAMs), and binding between the terminal functional group of SCAs and photosensitizing dye. The aim of this study is controlling the orientation and/or arrangement of photosensitizing dye adsorbed on TiO_2, and enhancement the photovoltaic conversion efficiency of DSSC. In addition to the fabrication and characterization of DSSC, our group also performs the quantum chemical calculations to confirm the organic dyes covalently attached to SCAs acts as a photosensitizer for DSSC. Fig. 2(left) illustrates the frontier molecular orbitals of photosensitizing dye covalently attached to SCAs calculated by Gaussian 09W and the energy diagram. Here, neutral cresyl violet (CV_0), which is selected in the previous report, shows as a photosensitizing dye. Lowest unoccupied molecular orbital (LUMO) level was higher than the conduction band of TiO_2 (-4.0 eV). Additionally, highest occupied molecular orbital (HOMO) level was lower than the redox potential of iodide/triiodide ion (-4.8 eV), which is a common redox couple in the electrolyte solution in DSSCs. These results indicate the occurrence of electron injection from CV_0 to TiO_2 and oxidized CV_0 can be regenerated in the electrolyte. Fig. 2(right) illustrated the simulated UV-visible absorption spectra of CV_0 and CV_0 covalently attached to SCAs (black and red lines, respectively). The maximum absorption peak (λ_{max}) of CV_0 was observed ~520 nm, and light harvesting efficiency (LHE) was calculated the 0.83 by using oscillator strength value at λ_{max}. Red-shift of λ_{max} and increase of LHE were observed in the case of CV_0 covalently attached to SCAs. From this result, it was revealed that the SCAs was resulted in improving the optical properties of CV_0. More detail calculation related to the photosensitizing dye attached to SCAs is continuing in our group. Additionally, the fabrication and characterization of DSSC containing above dyes are investigating to achieve the target 7 for SDGs.

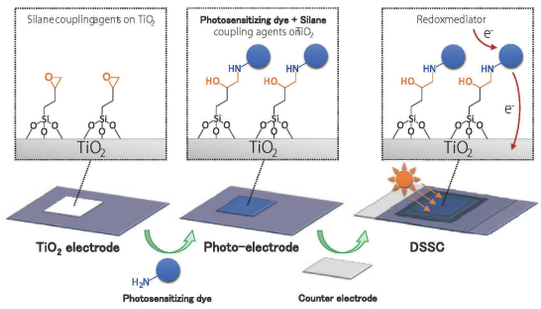

Fig.1 Fabrication of DSSC containing a photosensitizing dye combined with SCA. Here, SCA with epoxy group and photosensitizing dye with amino group were illustrated.

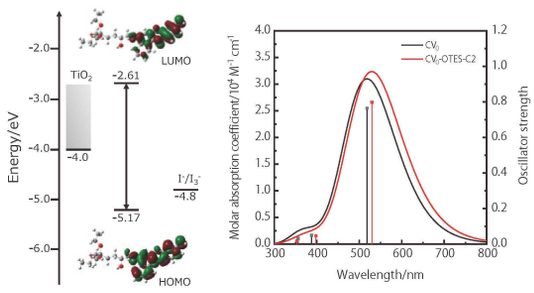

Fig.2 (left) Frontier molecular orbitals and energy diagram of CV_0 combined with SCA calculated by using CPCM-B3LYP/6-31G*level. (right) Simulated UV-visible absorption spectra of CV_0 and CV_0 combined with SCA calculated by using CPCM-TD-B3LYP/6-31+G* level. Vertical lines indicate the oscillator strength.

Major academic publications

T. Takeshita
"Computational Study of Cresyl Violet Covalently Attached to the Silane Coupling Agents: Application to TiO_2-Based Photocatalysts and Dye-Sensitized Solar Cells" Nanomaterials, 10 (2020) 1958.

T. Takeshita
"DFT and TD-DFT Study on Azobenzene-Based Dye Covalently Attached to Silane Coupling Agents: Toward Dye-Sensitized TiO_2 Catalyst and Dye-Sensitized Solar Cell Applications" ChemistrySelect, 6 (2021) 6011-6018.

T. Takeshita
"Effect of the TiO_2 surface modification with 3-glycidyloxypropyltrimethoxysilane on the aggregation of cresyl violet: Application to a dye-sensitized solar cell" Materials Chemistry and Physics, 286 (2022) 126196.

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"Study on dye molecules immobilised on the surface of titanium dioxide by a silane coupling agent" Impact, 2022 (2022) 54-56.