Department of Applied Chemistry and Food Science

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Doctor(Engineering) / Senior Lecturer

Tatsuya Takeshita

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

e-mail address

takeshita@fukui-ut.ac.jp

Main research themes and their characteristics

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

Dye-sensitized solar cells (DSSCs) have the potential to play an important role in next-generation solar cells. It is well known that the photovoltaic conversion in DSSCs is based on the electron injection from the photoexcited dye to the conduction band (CB) of titanium dioxide (TiO_2) and the regeneration of the oxidized dye by an electrolyte. The efficiency of the electron injection process (Φ_{inject}) is affected by a number of factors, such as the dye aggregation on the TiO_2 surface. Generally, dye aggregation in DSSCs induces a decrease in Φ_{inject} with quenching of the excited state; therefore, this phenomenon deserves to be further studied. Our group is currently interested in self-assembled monolayers (SAMs) based on silane coupling agents (SCAs) which have the potential to prevent dye aggregation on the TiO_2 surface. It is known that SCAs adsorbed onto inorganic materials form highly oriented SAMs via a siloxane network. Hence, it is expected that the orientation of the photosensitizing dye can be controlled by binding the photosensitizing dye to specific SAMs onto the TiO_2 surface. Control of the orientation using SAM based on SCAs is therefore a powerful tool to prevent dye aggregation and enhance Φ_{inject}. Here, we indicate the results of a DSSC involving a TiO_2 electrode chemically modified by a cresyl violet (CV^+) covalently attached to a 3-glycidyloxypropyltrimethoxysilane (GPTMS).

CV^+ forms H-dimers and/or H-aggregated species. The dye-adsorbed TiO_2 thin film was prepared on a glass slide with the aim of understanding the influence of GPTMS on aggregation of CV^+ (Fig. 1). The surface of the TiO_2 thin film turned from white to purple after dipping CV^+ solution (CV^+/TiO_2). Colorization of the TiO_2 surface was also observed in the case of the GPTMS/TiO_2 electrode. However, the surface color was clearly lighter than for the above-mentioned electrodes (CV^+-GPTMS/TiO_2). We believe the species CV^+ become covalently attached to the TiO_2 surface via the epoxy-ring opening reaction between the epoxy group of GPTMS and the amino group of CV^+, preventing dye aggregation. Subsequently, the total transmittance spectra of the thin films deposited on a glass slide were measured to obtain information about the aggregation of CV^+ on the TiO_2 surface. For CV^+/TiO_2, a broad spectrum was observed, whereas a relatively narrow band appeared in the case of CV^+-GPTMS/TiO_2. According to the absorption spectra measurement of CV^+ in solution and literatures, the broad absorption band in the region 400–570 nm and 620–800 nm for CV^+/TiO_2 suggests the formation of H- and J-aggregated species, respectively. By contrast, the presence of the monomer is considered dominant in the case of CV^+-GPTMS/TiO_2 because the broad H- and J-bands were not observed. Therefore, we concluded that GPTMS prevents the aggregation of CV^+ on the TiO_2 surface. Finally, an open sandwich-type DSSC was assembled by using a dye-adsorbed TiO_2 electrode, counter electrode, and electrolyte solution. The photovoltaic conversion efficiency of the DSSC with the CV^+/TiO_2 photoelectrode was quite low (0.0020%), whereas the photovoltaic conversion efficiency for the CV^+-GPTMS/TiO_2 photoelectrode showed a 7-fold increase (0.014%). Based on the results obtained so far, this can be clearly attributed to the increase in current density and applied voltage due to the scarce presence of H-dimers and/or H-aggregated species (Fig. 2). Therefore, it was concluded that the GPTMS treated onto the TiO_2 surface prevents the aggregation of CV^+, resulting in the enhancement of the photovoltaic conversion efficiency of the DSSC.

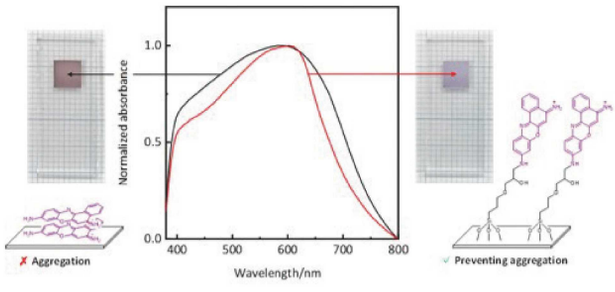

Fig.1 Total transmittance spectra of the CV^+/TiO_2 (left) and CV^+-GPTMS/TiO_2 (right).

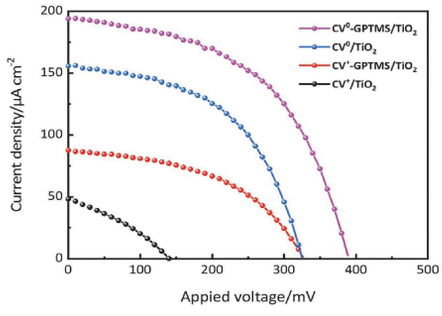

Fig.2 The current density-applied voltage profiles of the DSSCs containing a CV^+/TiO_2 (black) and CV^+-GPTMS/TiO_2 (red) photoelectrodes (blue and purple are data when sensitized by deprotonated species).

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
"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.