Photovoltaic characterization of di-branched organic sensitizers for DSSCs

Norberto Manfredi a,*, Vanira Trifiletti a, Fabio Melchiorre b, Giorgio Giannotta b, Paolo Biagini b,**, Alessandro Abbotto a,***

a Department of Materials Science, Milano – Bicocca Solar Energy Research Center – MIB-Solar, University of Milano – Bicocca, Via Cozzi 55, I-20125, Milano, Italy
b Research Center for Renewable Energy & Environmental Istituto Donegani, Eni S.p.A., via Fauser 4, I-28100, Novara, Italy

Article info
Article history:
Received 24 April 2019
Received in revised form 27 May 2019
Accepted 13 June 2019
Available online 4 July 2019

Keywords:
Photovoltaics
Renewable energies
Dye sensitized solar cells
Organic dyes

Abstract
In this work, the data on the effect of peripheral functionalization of a series of triphenylamine based di-branched dyes used as sensitizers in dye-sensitized solar cells are presented. The effect of different alkyl functionalities on the donor moiety upon the optical and photovoltaics parameters have been investigated in dye-sensitized solar cells (DSSCs) using a 10-μm TiO2 active layer. The absorption spectra, output efficiency, and incident photon to conversion efficiency of the DSSCs have been collected. The data can be exploited for properly designing efficient, stable, and industrially viable dyes for third generation solar devices.

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1. Data

The dataset presented in this article show pertinent properties about a series of di-branched dyes, depicted in Fig. 1, which have been previously included in a patent application [2]. This dataset is mainly addressed to researchers and practitioners in the field of hybrid and organic solar cells.

Fig. 2 shows the UV-Vis absorption spectra of dye-sensitized TiO2 films. Table 1 and Fig. 3 describe the photovoltaic performances of DSSCs sensitized by the investigated dyes, in presence of chenodeoxycholic acid (CDCA) as a co-adsorbent agent. Fig. 4 shows the corresponding IPCE plots.

2. Experimental design, materials, and methods

The following materials were purchased from commercial suppliers: FTO-coated glass plates (2.2 mm thick; sheet resistance ~7 Ω per square; Solaronix); Dyesol 18NR-T transparent TiO2 blend of active 20 nm anatase particles; N719 (Sigma-Aldrich). UV-O3 treatment was performed using Novascan PSD Pro Series — Digital UV Ozone System. Details on materials and instruments are reported in Table 2.

The thickness of the layers was measured by means of a VEECO Dektak 8 Stylus Profiler. PV measurements of DSSCs were carried out with an antireflective layer and with black metal mask on top of the photoanode of 0.28 cm² surface area under a 500 W Xenon light source (ABET Technologies Sun 2000 class ABA Solar Simulator). The power of the simulated light was calibrated to AM 1.5 (100 mW cm⁻²) using a reference Si cell photodiode equipped with an IR-cutoff filter (KG-5, Schott) to reduce the mismatch in the region of 350–750 nm between the simulated light and the AM 1.5 spectrum. Values were recorded after 3 and 24 h, and 7 days of ageing in the dark. I–V curves were
obtained by applying an external bias to the cell and measuring the generated photocurrent with a Keithley digital source meter. Incident photon-to-current conversion efficiencies (IPCE) were recorded as a function of excitation wavelength by using a monochromator (Omni 300 LOT ORIEL) with single grating in Czerny-Turner optical design, in AC mode with a chopping frequency of 1 Hz and a bias of blue light (0.3 sun). Absorption spectra were recorded on a V-570 Jasco spectrophotomer.

3. Preparation of DSSCs

DSSCs have been prepared to adapt a procedure reported in the literature [3]. In order to exclude metal contamination all of the containers were in glass or Teflon and were treated with EtOH and 10% HCl prior to use. Plastic spatulas and tweezers have been used throughout the procedure.

- FTO glass plates were cleaned in a detergent solution for 15 min using an ultrasonic bath, rinsed with pure water and EtOH.

![Fig. 1. TT-a dyes investigated in this work.](image)

![Fig. 2. UV–Vis spectra of the 10-μm thick transparent TiO₂ (Dyesol 18NR-T) photoanodes sensitized by TT-a-00 – TT-a-04 dyes with an equimolar amount of CDCA.](image)
After treatment in a UV-O₃ system for 18 min, the FTO plates were treated with a freshly prepared 40 mM aqueous solution of TiCl₄ for 30 min at 70 °C and then rinsed with water and EtOH.

A transparent layer of 0.20 cm² was screen-printed using Dyesol 18NR-T TiO₂ paste described above. The coated films were thermally treated at 125 °C for 6 min, 325 °C for 10 min, 450 °C for 15 min, and 500 °C for 15 min. The heating ramp rate was 5–10 °C/min.

The sintered layer was treated again with 40 mM aqueous TiCl₄ (70 °C for 30 min), rinsed with EtOH and heated at 500 °C for 30 min.

After cooling down to 80 °C the TiO₂ coated plate was immersed into a solution of the dye for 5 h at room temperature in the dark. Counter electrodes were prepared according to the following procedure.

1-mm hole was made in a FTO plate, using diamond drill bits.

The electrodes were then cleaned with a detergent solution for 15 min using an ultrasonic bath, 10% HCl, and finally acetone for 15 min using an ultrasonic bath.

After thermal treatment at 500 °C for 30 min, a drop of 5 × 10⁻³ M solution of H₂PtCl₆ in EtOH was added on the cold FTO and the thermal treatment at 500 °C for 30 min repeated. Cells assembly procedure.

### Table 1
Main PV parameters of DSSCs based on the di-branched sensitizers TT-a-00 – TT-a-04 in comparison with the benchmark N719.

| Dyes⁻¹ | Jsc [mA cm⁻²] | V_{oc} [mV] | FF [%] | PCE [%] |
|--------|---------------|-------------|--------|---------|
| TT-a-00ᵇ | 12.5          | 636         | 63     | 5.0     |
| TT-a-01ᵇ | 14.8          | 604         | 62     | 5.6     |
| TT-a-02ᵇ | 14.2          | 642         | 64     | 5.9     |
| TT-a-03ᵇ | 14.9          | 643         | 62     | 5.9     |
| TT-a-04ᵇ | 12.9          | 625         | 58     | 4.7     |
| N719ᶜ   | 14.8          | 724         | 68     | 7.3     |

⁻¹ Active layer 10-µm TiO₂ Dyesol 18NR-AO; electrolyte: Z960 (1.0 M 1,3-dimethylimidazolium iodide, 0.03 M I₂, 0.05 M LiI, 0.10 M guanidinium thiocyanate, and 0.50 M 4-t-butylpyridine in acetonitrile/valeronitrile 85:15).

ᵇ 2 × 10⁻⁴ M dye solution in EtOH with an equimolar amount of CDCA.

ᶜ 5 × 10⁻⁴ M dye solution in EtOH with an equimolar amount of CDCA.

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**Fig. 3.** Current–voltage characteristics of DSSCs sensitized by TT-a-00 – TT-a-04 in comparison with the control cell sensitized by benchmark N719.
Table 2
Detailed description of materials and instruments.

| Materials/Instrument | Physical form                  | Market price         | Note                                      |
|----------------------|--------------------------------|----------------------|-------------------------------------------|
| FTO-coated glass plates | Transparent glass            | Solaronix, TCO30-8, 10.00 CHF each |
| Dyesol 18NR-T        | Titanium dioxide paste (gel)  | Greatcell Solar's 18NR-T, 476.78 AUD$ 100 g |
| N719                 | Dark purple powder           | Sigma Aldrich, CAS Number: 207347-46-4 703214-1G, 437.00 € 1 g |
| Novascan PSD Pro Series – Digital UV Ozone System | Instrument | Contact suppliers | http://www.novascans.com/products/uv_ozone_cleaners_silicon_glass_wafers.php |

Fig. 4. IPCE of DSSCs sensitized by TT-a-00 – TT-a-04.
• The dye adsorbed TiO₂ electrode and Pt-counter electrode were assembled into a sealed sandwich-type cell by heating with a hot-melt ionomer-class resin (Surlyn 30-μm thickness) as a spacer between the electrodes.
• A drop of the electrolyte solution was added to the hole and introduced inside the cell by vacuum backfilling.
• Finally, the hole was sealed with a sheet of Surlyn and a cover glass. A reflective foil at the back side of the counter electrode was taped to reflect unabsorbed light back to the photoanode.

Acknowledgments

This work has been performed under research contract No. 3500010866 between Milano-Bicocca Solar Energy Research Center — MIB-Solar - University of Milano-Bicocca and Eni S.p.A., Rome, Italy.

Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104167.

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