Supporting Information

Bioinspired Study of Energy and Electron Transfer in Photovoltaic System

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The surface morphology of the obtained nanostructures was characterized on a field-emission scanning electron microscope (FESEM MIRA-3, Tescan). The luminescence spectrum of ZnO nanostructures was measured on a highly sensitive, fiber-optic spectrophotometer AvaSpec-2048 at room temperature; photoexcitation of samples was performed by the third harmonic of a neodymium laser LCS-DTL-374QT (\(\lambda = 355\) nm, \(\tau = 7\) ns, \(E = 5\) mJ). The absorption spectrum was measured by the spectrophotometer (AvaSpec-2048) at room temperature after the dye molecules were desorbed from ZnO nanostructures in 0.1 mol/L NaOH solution of water and ethanol (50:50, v/v). The photocurrent-voltage characteristics were measured using a Source Meter instrument (Keithley 2400) by irradiating with simulated solar light; that is, AM 1.5 100 mW/cm\(^2\) (PET PHOTO Emission TECH., INC). The cell active area was 0.2 cm\(^2\). The impedance of the cells was measured by using an impedance meter (Z-500PRO, Elins). All impedance measurements were performed under a bias light illumination of 100 mW/cm\(^2\) from a simulated solar light (PET PHOTO Emission TECH., INC) at open circuit condition. Impedance
measurement of cells was recorded in a frequency range from 0.05 Hz to 200 kHz with an AC amplitude of 10 mV.

SQ dye was chosen as the energy acceptor and the main sensitizer of the solar cell because of its optimal arrangement of HOMO-LUMO orbitals with respect to the conduction band of TiO₂. The results of the calculation performed by the INDO method has shown that the HOMO orbital of the dye has an energy of about -6.22 eV and the LUMO orbital energy is equal to -0.80 eV. It is evident that the polymethine dye may act as an electron donor with respect to TiO₂.

The excited-state lifetime of the donor and acceptor were measured using a pulsed spectrofluorimeter with picosecond resolution with registration in time-correlated photon counting mode (Becker & Hickl, Germany).

The current-voltage characteristics of the dye-sensitized solar cells were measured with a Solar Cell Tester CT50AAA (Photo Emission Tech. Inc., USA). The fill factor (FF) and energy conversion efficiency (η) were calculated according to the following equations:

\[
FF = \frac{I_{\text{max}} \times U_{\text{max}}}{I_{\text{sc}} \times U_{\text{oc}}} 
\]

(1)

\[
\eta = \frac{FF \times I_{\text{sc}} \times V_{\text{oc}}}{P_{\text{in}}} \times 100\% 
\]

(2)

where: \( I_{\text{max}}, U_{\text{max}} \) – values of maximal current and voltage, respectively; \( I_{\text{sc}}, V_{\text{oc}} \) – values of short-circuit current and open-circuit voltage; \( P_{\text{in}} \) – power of the incident light.

\[
E_{ET} = 1 - \frac{\tau_D}{\tau_{0D}} 
\]

(3)

Table 1. Calculated values of critical parameters of energy transfer
| Solution          | Overlap integral, $M^{-1} cm^3$ | $R_0$, Å  | $C_0$, mol/L |
|-------------------|---------------------------------|--------|-------------|
| Donor-acceptor    | $8.1 \times 10^{-13}$           | 31     | $1 \times 10^{-2}$ |

Supporting Figure 1. Structure formulae of the donor (at the left) and acceptor of energy (at the right).

Supporting Figure 2. Spectral photosensitivity of the solar cell based on acceptor (Curve 1) and donor-acceptor compound (Curve 2).
Supporting Figure 3. UV-vis absorption spectra of dyes desorbed from ZnO nanostructures