Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Development of functionally separated D-π-A fluorescent dye with pyrazyl group as electron-accepting group for dye-sensitized solar cell

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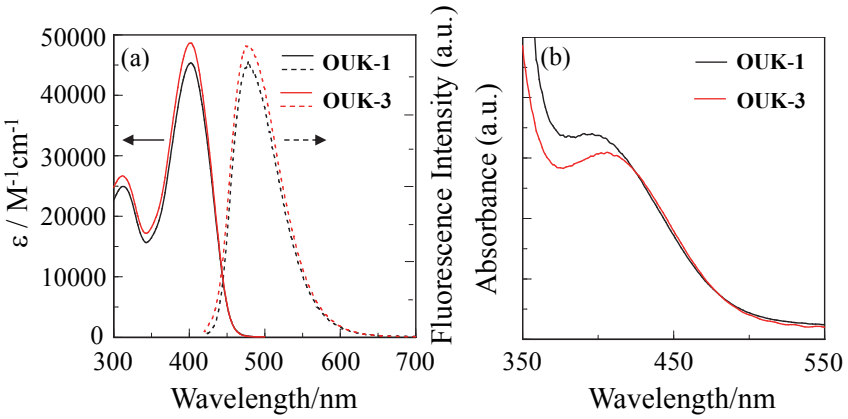

Fig. S1 Absorption (–) and fluorescence (···) spectra of **OUK-1** and **OUK-3** in 1,4-dioxane and (b) absorption spectra of **OUK-1** and **OUK-3** adsorbed on TiO_2 film.

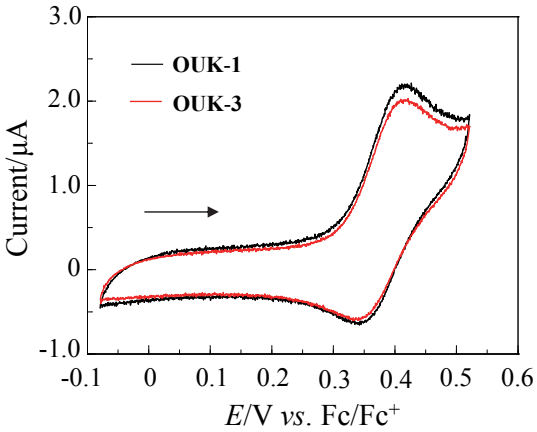

Fig. S2 Cyclic voltammograms of (a) **OUK-1** (0.1 mM) (black) and (b) **OUK-3** (0.1 mM) (red) in DMF containing 0.1 M Bu_4NClO_4 at a scan rate of 10 mV s^{-1}. The arrow denotes the direction of the potential scan.

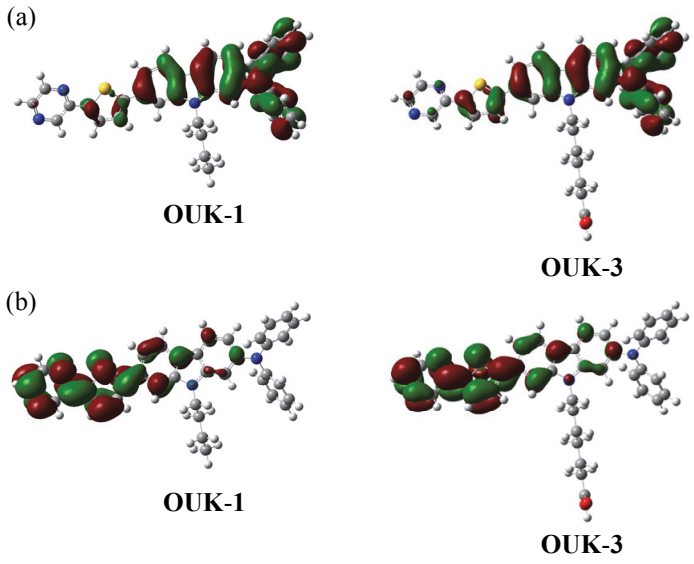

Fig. S3 (a) HOMO and (b) LUMO of **OUK-1** and **OUK-3** by the density functional theory (DFT) calculations at B3LYP/6-31G(d, p) level.

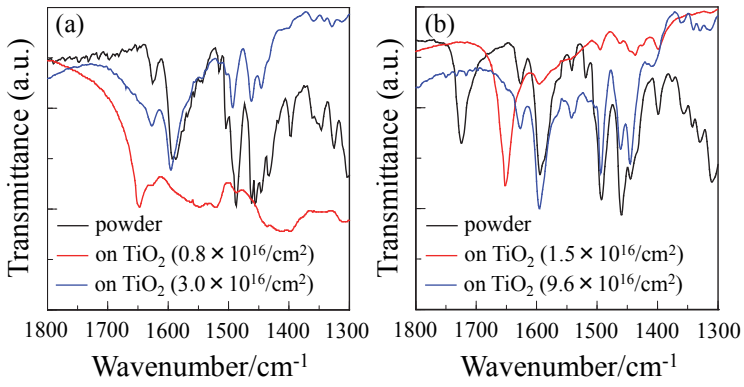

Fig. S4 FTIR spectra of the dye powders and the dyes (0.8×10^{16} and 3.0×10^{16} molecules per cm^2 for **OUK-1** and 1.5×10^{16} and 9.6×10^{16} molecules per cm^2 for **OUK-3**) adsorbed on TiO_2 nanoparticles for (a) **OUK-1** and (b) **OUK-3**.

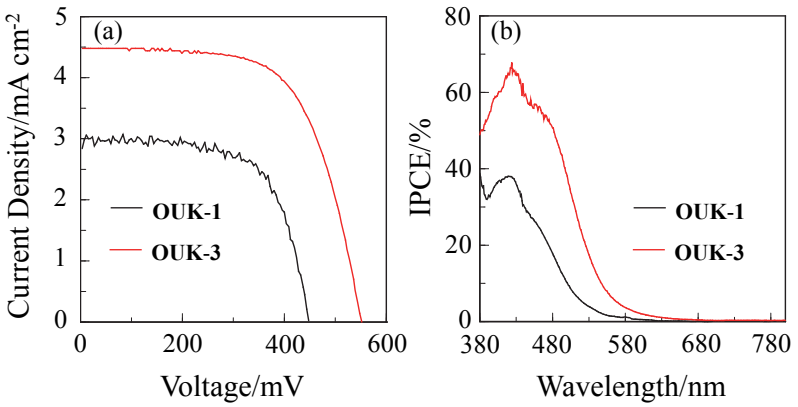

Fig. S5 (a) *I–V* curves and (b) IPCE spectra of DSSCs based on **OUK-1** and **OUK-3**.

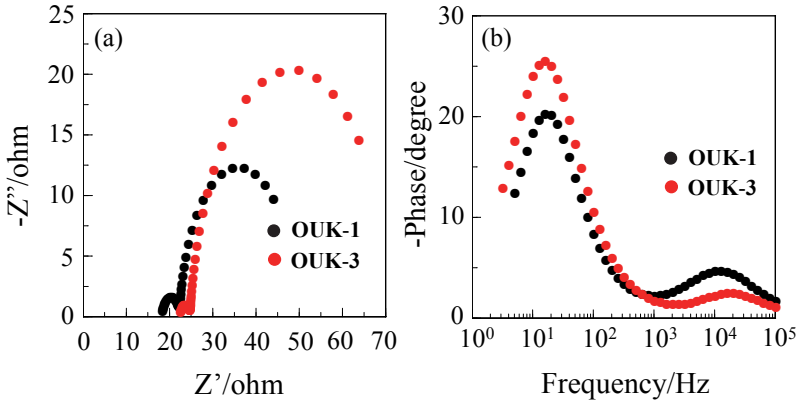

Fig. S6 (a) Nyquist plots and (b) Bode phase plots of DSSCs based on **OUK-1** and **OUK-3**.