Supplementary Information

Rational Modifications on Ruthenium Terpyridine Sensitizers with large Jsc for Dye-Sensitized Solar Cells: A Combined DFT and Relativistic TDDFT Studies

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Fig. S1 The fully optimized structures of DX1-DX5 in gas phase by PBE0. (The basis set for Ru is SDD and for non-metal atoms is 6-31G*)

Fig. S2 The calculated absorption spectrum (the black line) and experimental one (the red line) of DX1.

Fig. S3 Optimized configuration of DX5/TiO2 complex (binding patterns with respect to the triazine ring).

Table S1 The O1-Ti1 and O2-Ti2 distances of the DX4/TiO2 and DX5/TiO2 complexes (binding patterns with respect to the pyrimidine and triazine ring, respectively)

Fig. S4 Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX2 in DMF. (The black line represents (TiO2)38 cluster DOS. The blue line represents (TiO2)38 cluster contribution to the total DOS.)

Fig. S5 Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX3 in DMF. (The black line represents (TiO2)38 cluster DOS. The blue line represents (TiO2)38 cluster contribution to the total DOS.)

Fig. S6 Schematic representation of the model used to evaluate the CB shift caused by
the sensitizer adsorption for DX4 in DMF. (The black line represents (TiO$_2$)$_{38}$ cluster DOS. The blue line represents (TiO$_2$)$_{38}$ cluster contribution to the total DOS.)

**Fig.S7** Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX5 in DMF. (The black line represents (TiO$_2$)$_{38}$ cluster DOS. The blue line represents (TiO$_2$)$_{38}$ cluster contribution to the total DOS.)

**Fig.S1** The fully optimized structures of DX1-5 in gas phase by PBE0. (The basis set for Ru is SDD and for non-metal atoms is 6-31G*)
Fig. S2 The calculated absorption spectrum (the black line) and experimental one (the red line) of DX1.

Fig. S3 Optimized configuration of DX5/TiO₂ complex (binding patterns with respect to the triazine ring). The left structure represents a magnified image of the selected part of DX5/TiO₂ (dashed circle). The distances between O atoms of DX5 and Ti atoms of the TiO₂ are also shown.

Table S1 The O1-Ti1 and O2-Ti2 distances of the DX4/TiO₂ and DX5/TiO₂ complexes (binding patterns with respect to the pyrimidine and triazine ring, respectively) (the unit is Å).
Fig. S3  Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX2 in DMF. (The black line represents (TiO$_2$)$_{38}$ cluster DOS. The blue line represents (TiO$_2$)$_{38}$ cluster contribution to the total DOS.)
**Fig.S4** Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX3 in DMF. (The black line represents (TiO$_2$)$_{38}$ cluster DOS. The blue line represents (TiO$_2$)$_{38}$ cluster contribution to the total DOS.)

**Fig.S5** Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX4 in DMF. (The black line represents (TiO$_2$)$_{38}$ cluster DOS. The blue line represents (TiO$_2$)$_{38}$ cluster contribution to the total DOS.)

**Fig.S6** Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for DX5 in DMF. (The black line represents (TiO$_2$)$_{38}$ cluster DOS. The blue line represents (TiO$_2$)$_{38}$ cluster contribution to the total DOS.)