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/TiO_2** complex (binding patterns with respect to the triazine ring).

Table S1 The O1-Ti1 and O2-Ti2 distances of the **DX4/TiO_2** and **DX5/TiO_2** 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 $(TiO_2)_{38}$ 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 **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.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.)

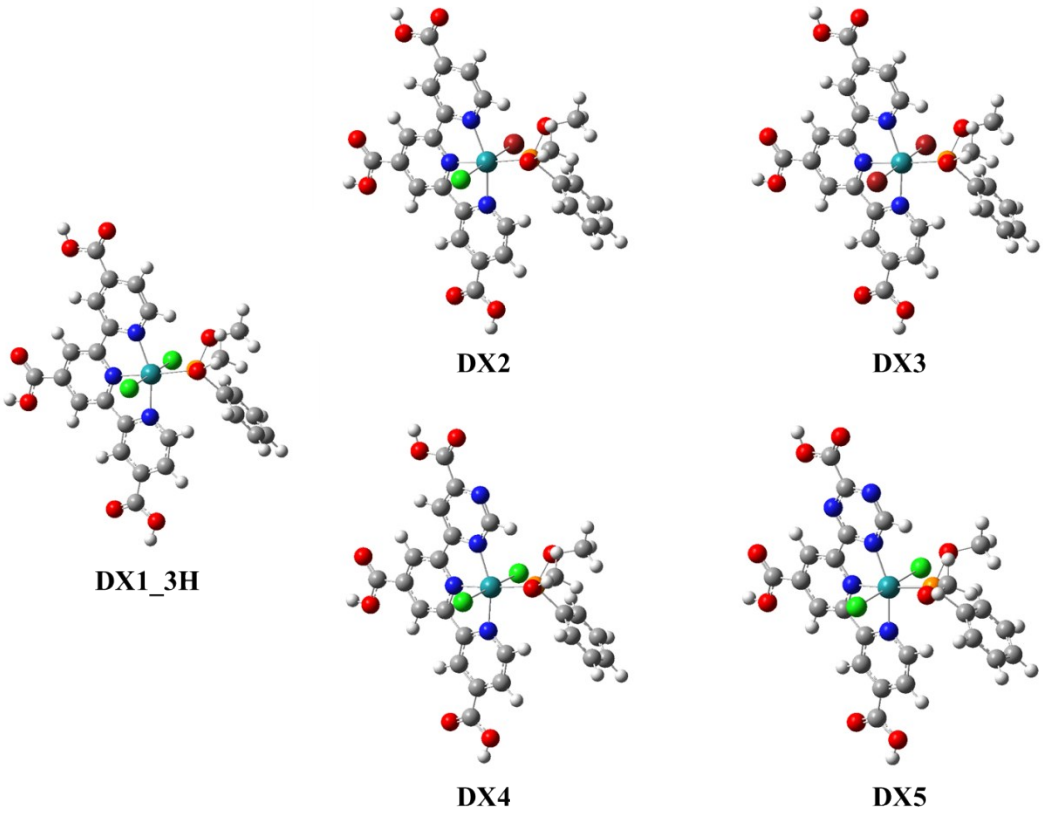

Fig.S1 The fully optimized structures of **DX1-5** in gas phase by PBE0. (The basis set for Ru is SDD and for non-metal atoms is 6-31G*)

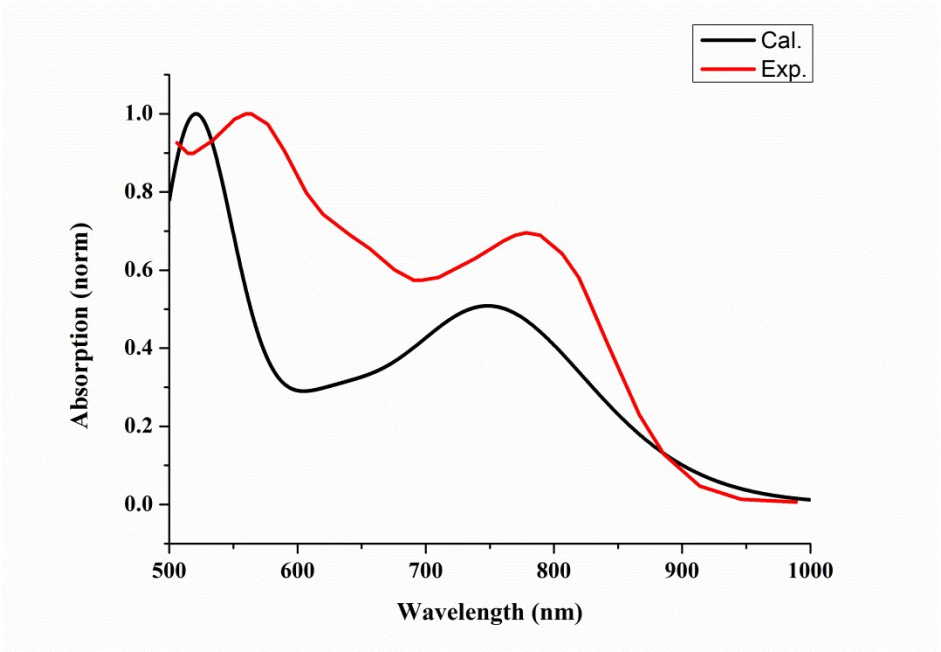

Fig.S2 The calculated absorption spectrum (the black line) and experimental one (the red line) of **DX1**.

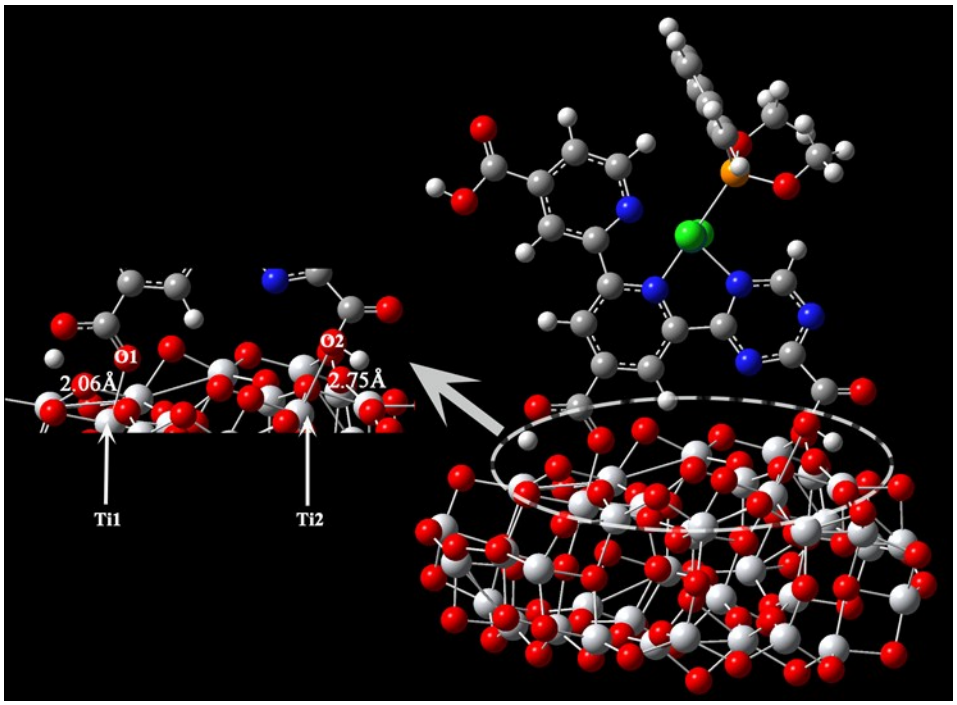

Fig. S3 Optimized configuration of **DX5/TiO_2** complex (binding patterns with respect to the triazine ring). The left structure represents a magnified image of the selected part of **DX5/TiO_2** (dashed circle). The distances between O atoms of **DX5** and Ti atoms of the **TiO_2** are also shown.

Table S1 The O1-Ti1 and O2-Ti2 distances of the **DX4/TiO_2** and **DX5/TiO_2** complexes **(**binding patterns with respect to the pyrimidine and triazine ring, respectively**)** (the unit is Å).

	DX4	DX5
O1-Ti1	1.90	2.06
O2-Ti2	3.58	2.75

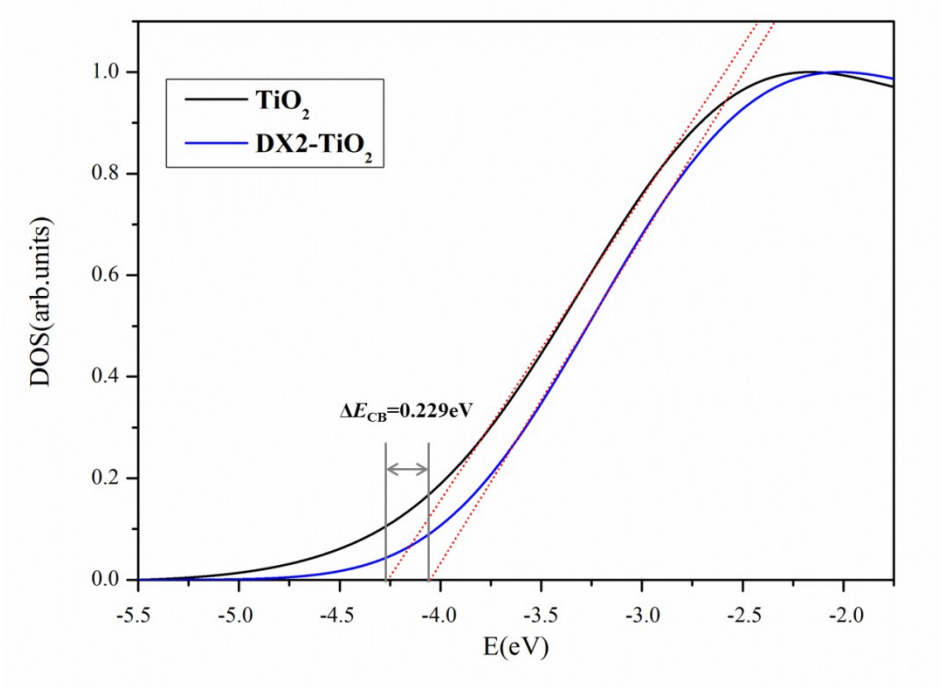

Fig.S3 Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for **DX2** in DMF. (The black line represents $(TiO_2)_{38}$ cluster DOS. The blue line represents $(TiO_2)_{38}$ cluster contribution to the total DOS.)

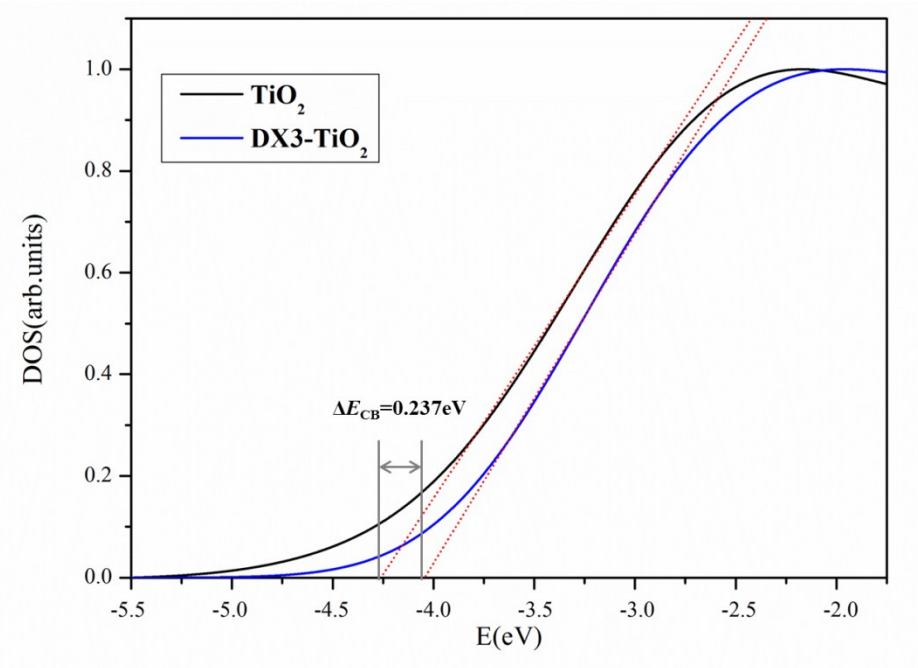

Fig.S4 Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for **DX3** in DMF. (The black line represents $(TiO_2)_{38}$ cluster DOS. The blue line represents $(TiO_2)_{38}$ cluster contribution to the total DOS.)

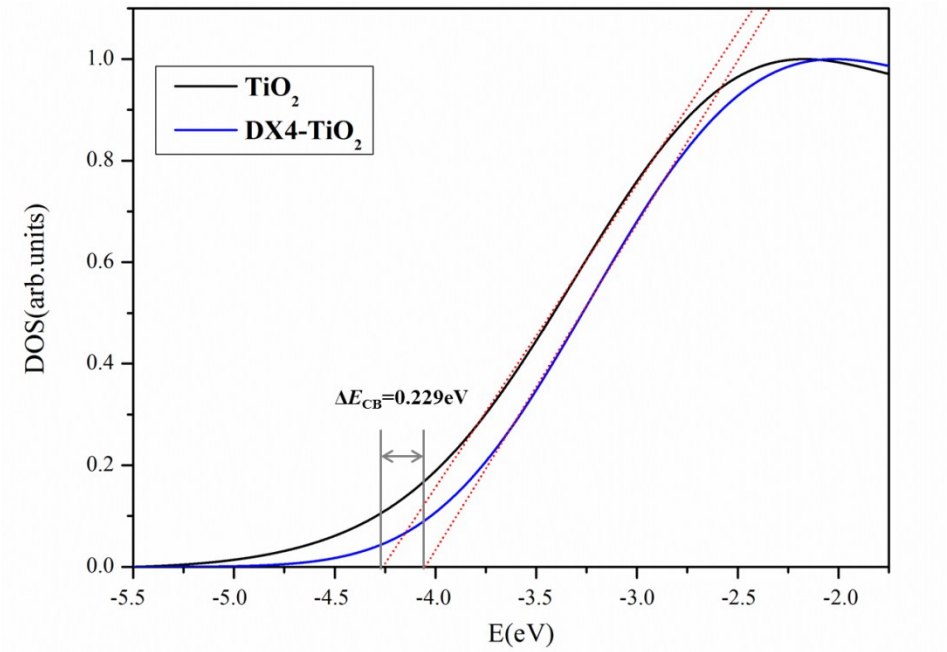

Fig.S5 Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for **DX4** in DMF. (The black line represents $(TiO_2)_{38}$ cluster DOS. The blue line represents $(TiO_2)_{38}$ cluster contribution to the total DOS.)

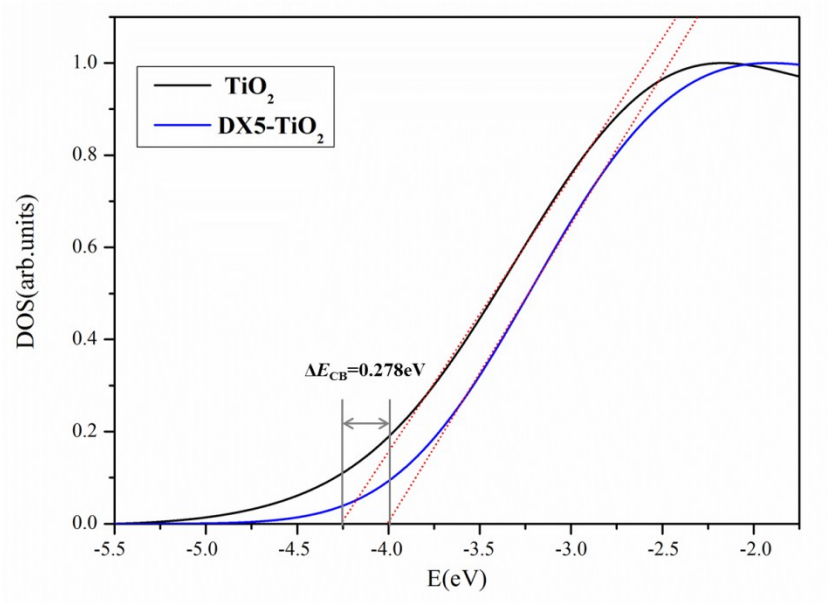

Fig.S6 Schematic representation of the model used to evaluate the CB shift caused by the sensitizer adsorption for **DX5** in DMF. (The black line represents $(TiO_2)_{38}$ cluster DOS. The blue line represents $(TiO_2)_{38}$ cluster contribution to the total DOS.)