Electronic Supplementary Information

Theoretical design and characterization of high-efficiency organic dyes with different electron-withdrawing groups based on C275 toward dye-sensitized solar cells

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Table S1 The maximum absorption wavelength E_λ of **C275** calculated by different functionals with the 6-311G** basis set compared with experimental value.

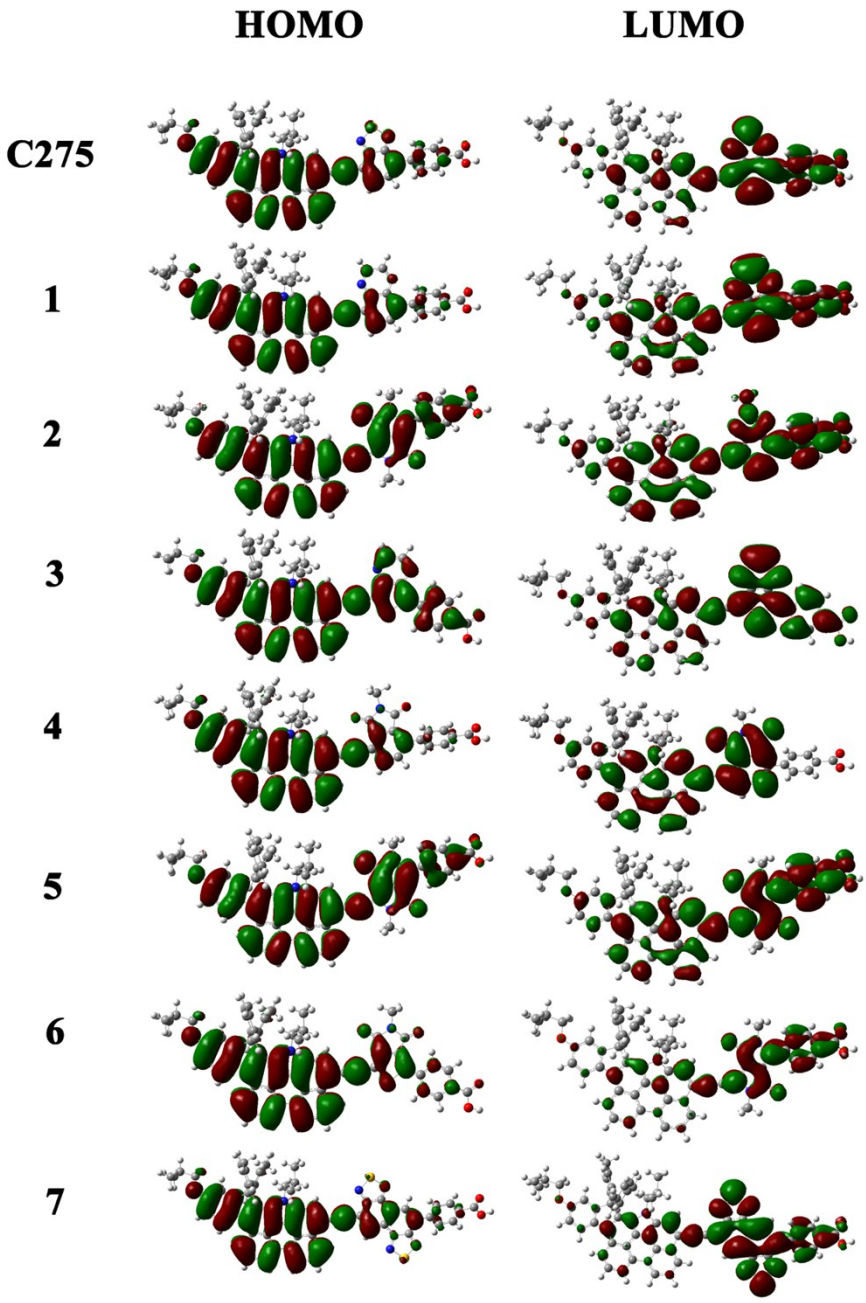
Fig. S1. Illustration of the frontier molecular orbitals of organic dye **C275** and dyes **1-7** obtained at B3LYP/6-311G** level in gas phase with the isodensity surface of 0.01 au.

Fig. S2. The distance between dye cation hole and TiO_2 surface of dye **1**, **2**, **4** and **6**.

Fig. S3. Total and Partial Density of State (DOS) for dyes **1-7** and **C275** adsorbed on $(TiO_2)_{38}$ cluster. The dash line intercepts with the energy axis correspond to calculated E_{CB} edges.

Table S1 The maximum absorption wavelength λ_{max}(nm) of **C275** calculated by different functionals with the 6-311G** basis set compared with experimental value.

Functional	B3LYP	MPW1PW91	PBE0	MPW1K	BHandHLYP	M062X	CAM-B3LYP	LC-ωPBE	LC-BLYP	ωB97X	ωB97XD	Exp.
λ_{max}(nm)	693	644	642	543	522	505	505	440	437	455	483	536



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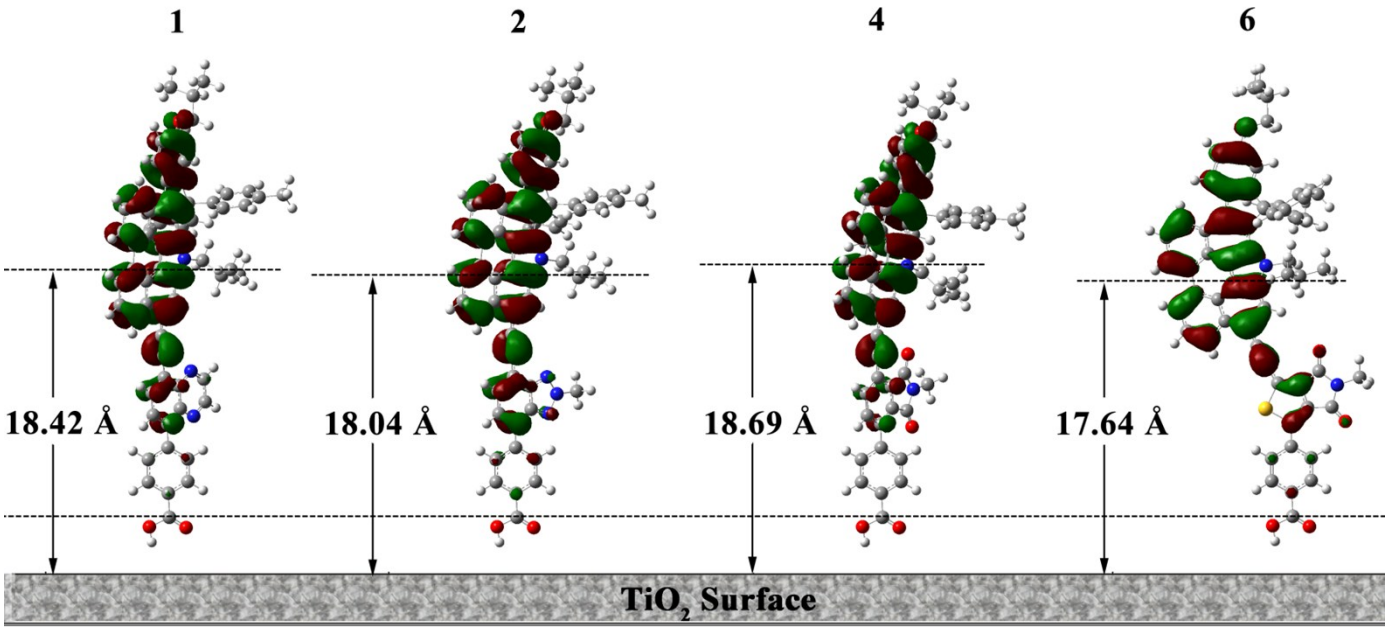

Fig. S2. The distance between dye cation hole and TiO_2 surface of dyes **1**, **2**, **4** and **6**.

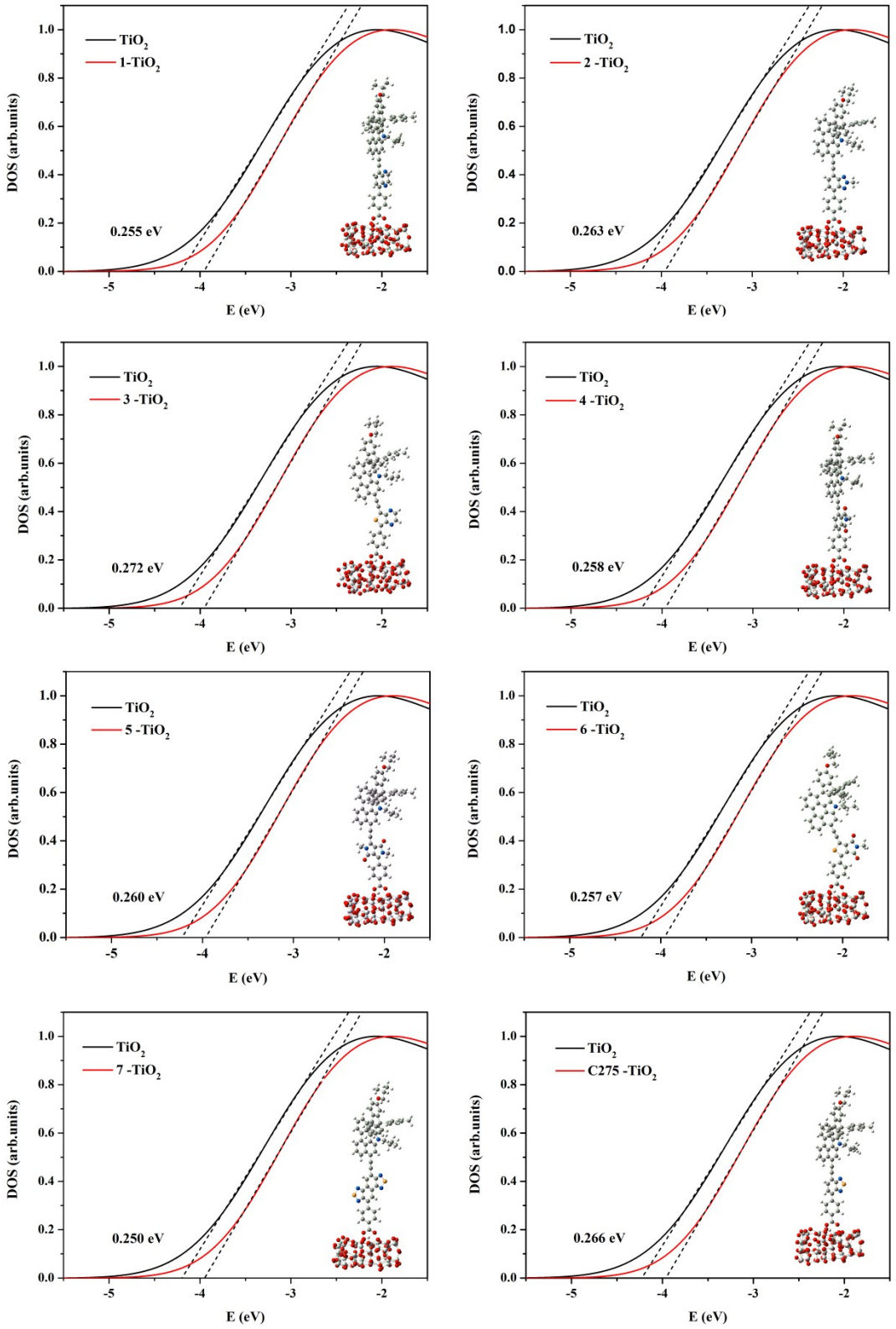

Fig. S3. Total and Partial Density of State (DOS) profiles for dyes **1-7** and **C275** adsorbed on $(TiO_2)_{38}$ cluster. The dash line intercepts with the energy axis correspond to calculated E_{CB} edges.