Electronic Supplementary Information

Theoretical investigation on structural and electronic properties of organic dye C258 on TiO$_2$ (101) surface in dye sensitized solar cells

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**Fig. S1.** Configuration of the periodical (TiO$_2$)$_{256}$ system.
**Fig. S2.** Different adsorption modes on the surface of anatase (101) for C 258.

**Fig. S3.** The band structure of $(\text{TiO}_2)_{256}$ calculated by DFTB with Fermi level marked in dashed line.
Fig. S4. Density of states (DOS) of (TiO$_2$)$_{256}$ system.

Fig. S5. DOS and PDOS for Mha configuration system.
Fig. S6. DOS and PDOS for BBH configuration system.

Fig. S7. Selected frontier molecular orbitals of C258.