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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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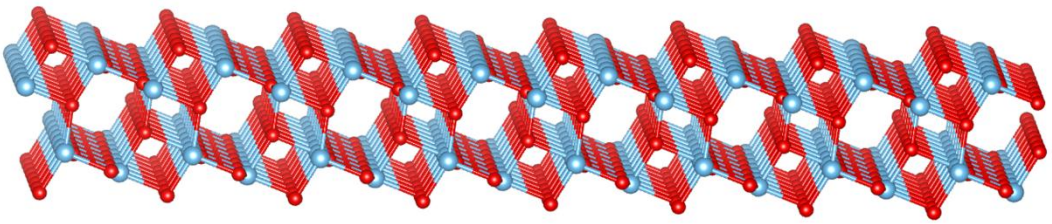

Fig. S1. Configuration of the periodical $(TiO_2)_{256}$ system.

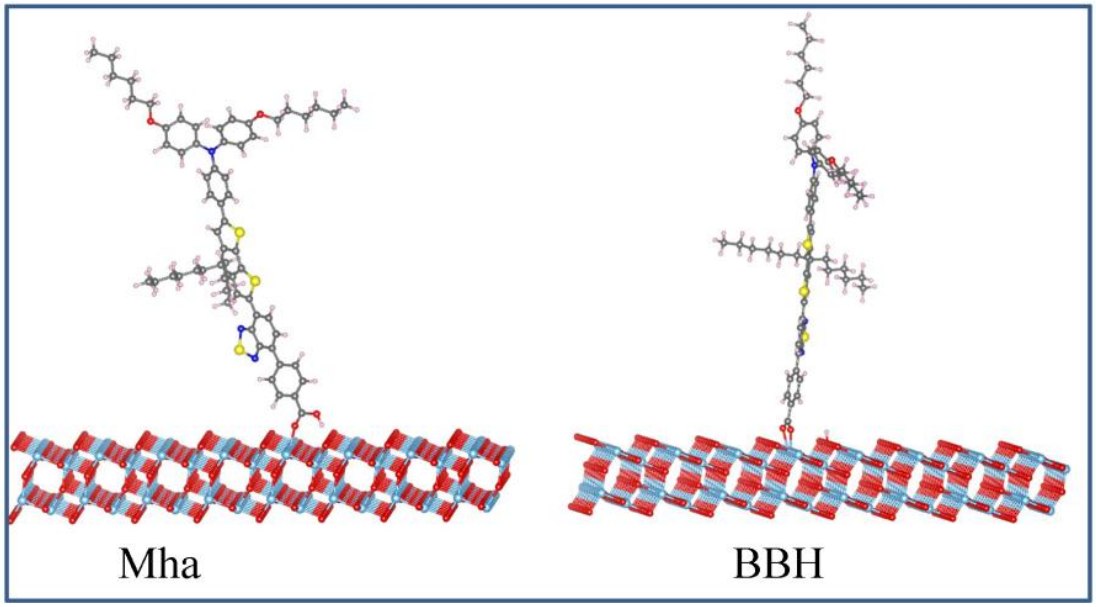

Fig. S2. Different adsorption modes on the surface of anatase (101) for C 258.

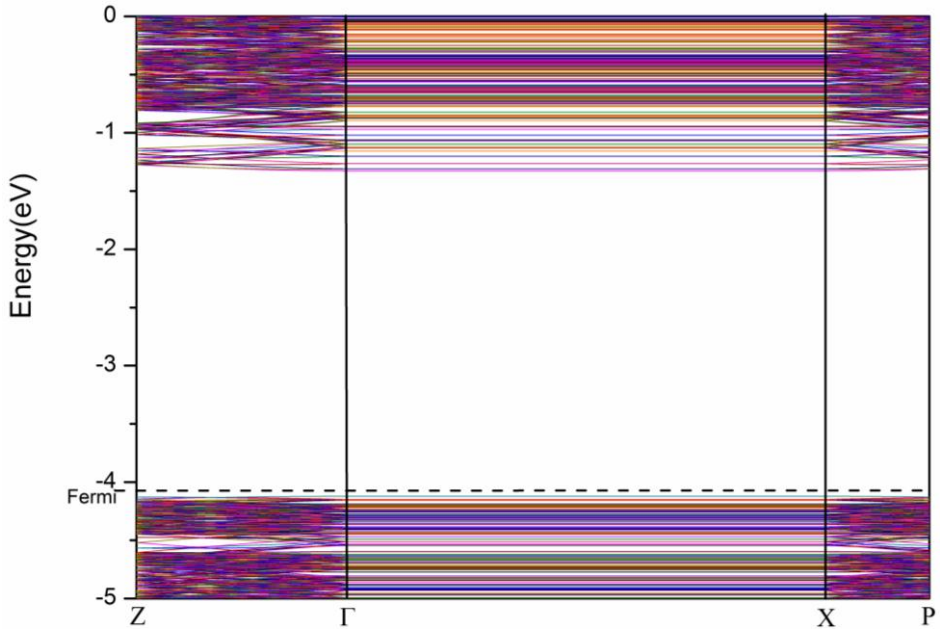

Fig. S3. The band structure of $(TiO_2)_{256}$ calculated by DFTB with Fermi level marked in dashed line.

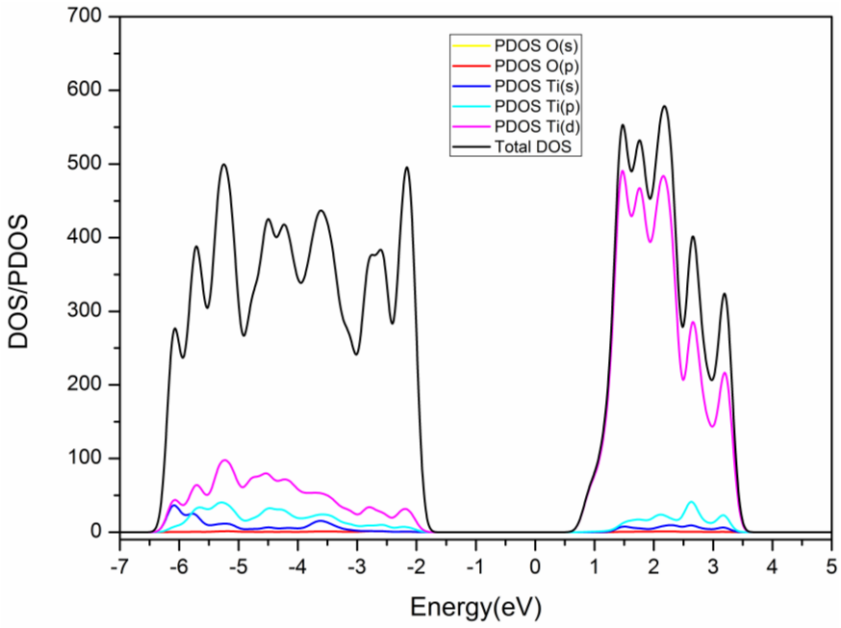

Fig. S4. Density of states (DOS) of $(TiO_2)_{256}$ system.

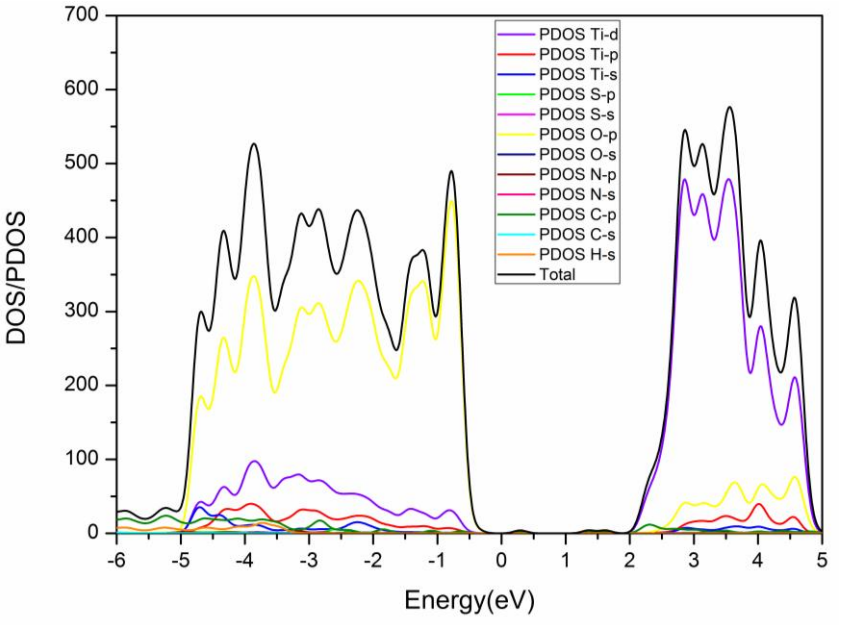

Fig. S5. DOS and PDOS for Mha configuration system.

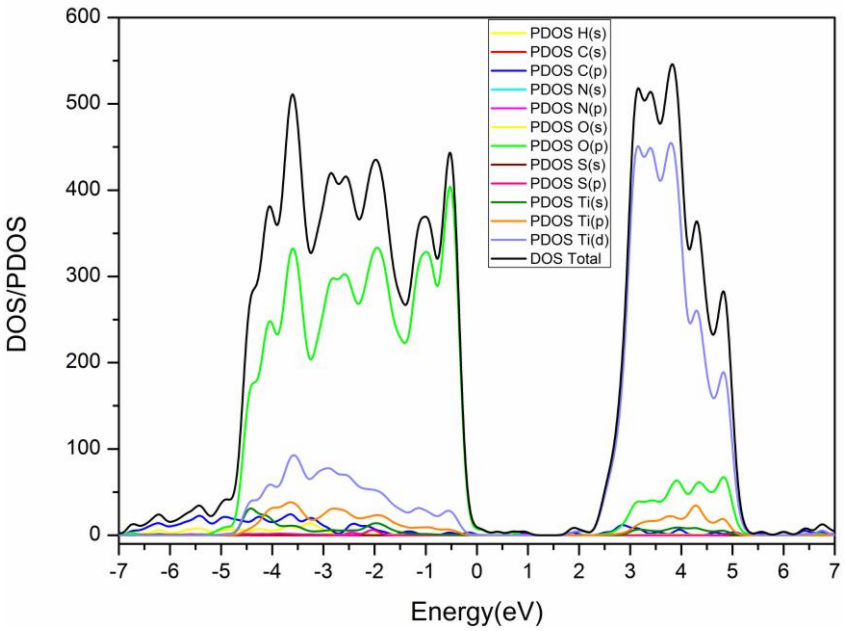

Fig. S6. DOS and PDOS for BBH configuration system.

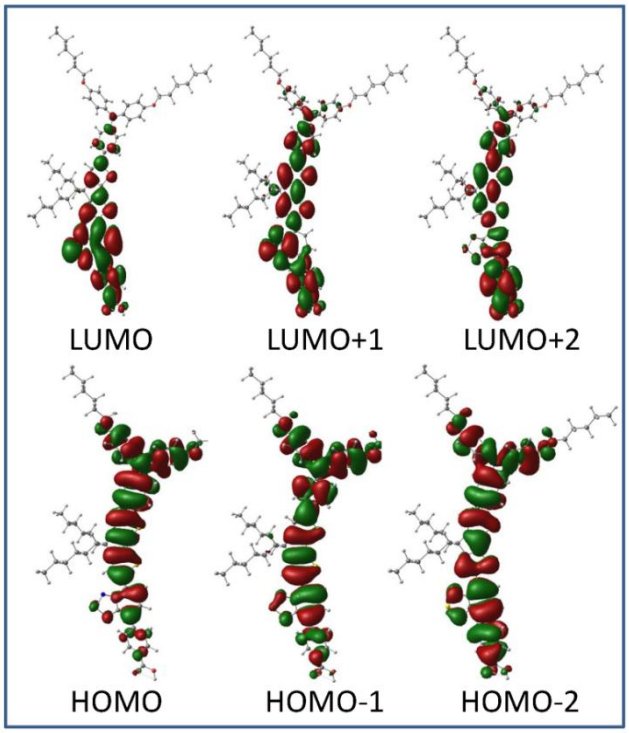

Fig. S7. Selected frontier molecular orbitals of C258.