Aggregation of organic dyes on extended TiO_2 models: a DFT/TDDFT investigation

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Supporting Information

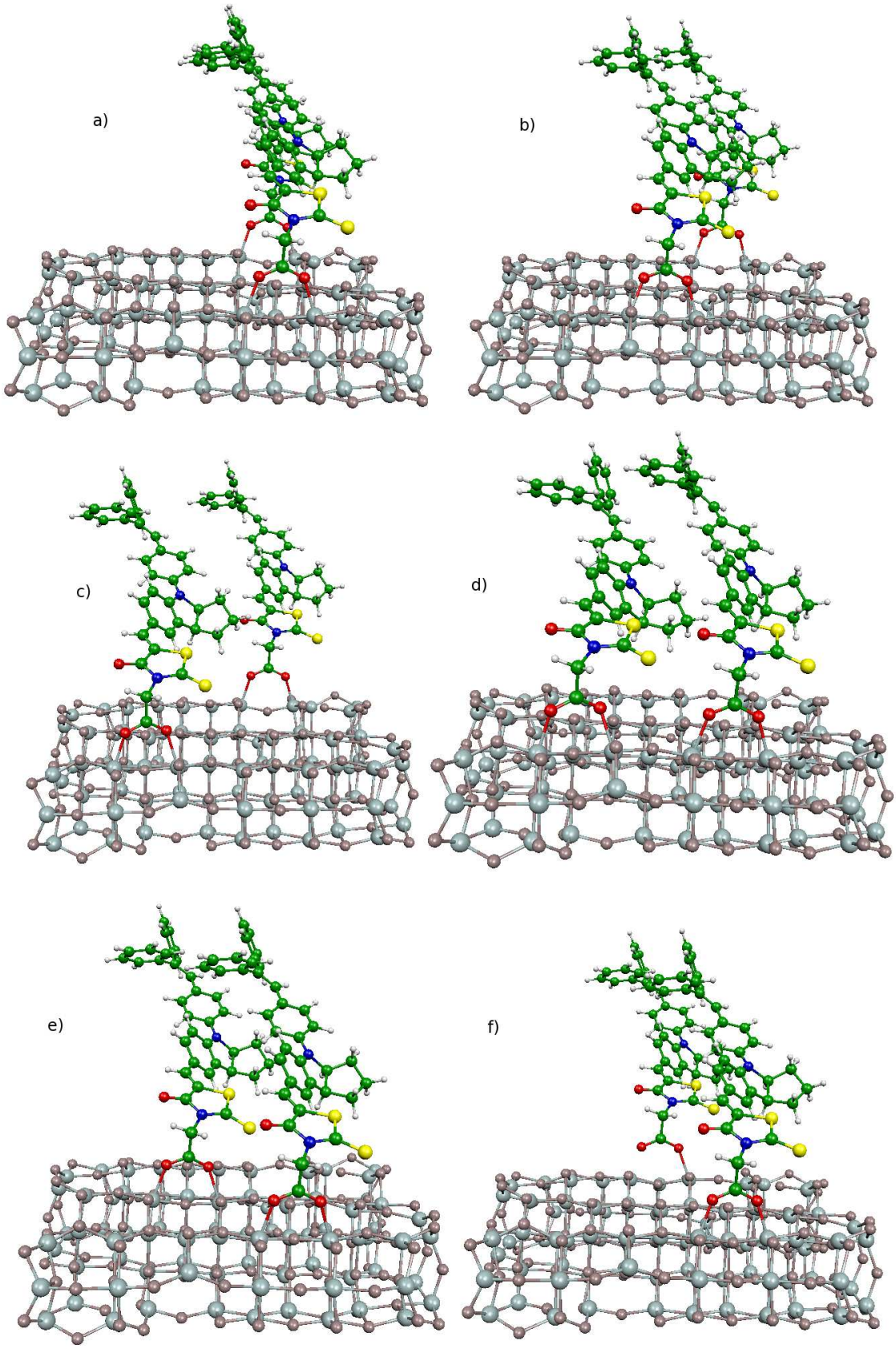

Figure S1: Optimized structure of (a) (2,0)-D102, (b) (2,2)-D102, (c) (2,4)-D102, (d) (4,0)-D102, (e) (-1,1)-D102 and (f) (-2,2)-D102 on the $(TiO_2)_{82}$ cluster.

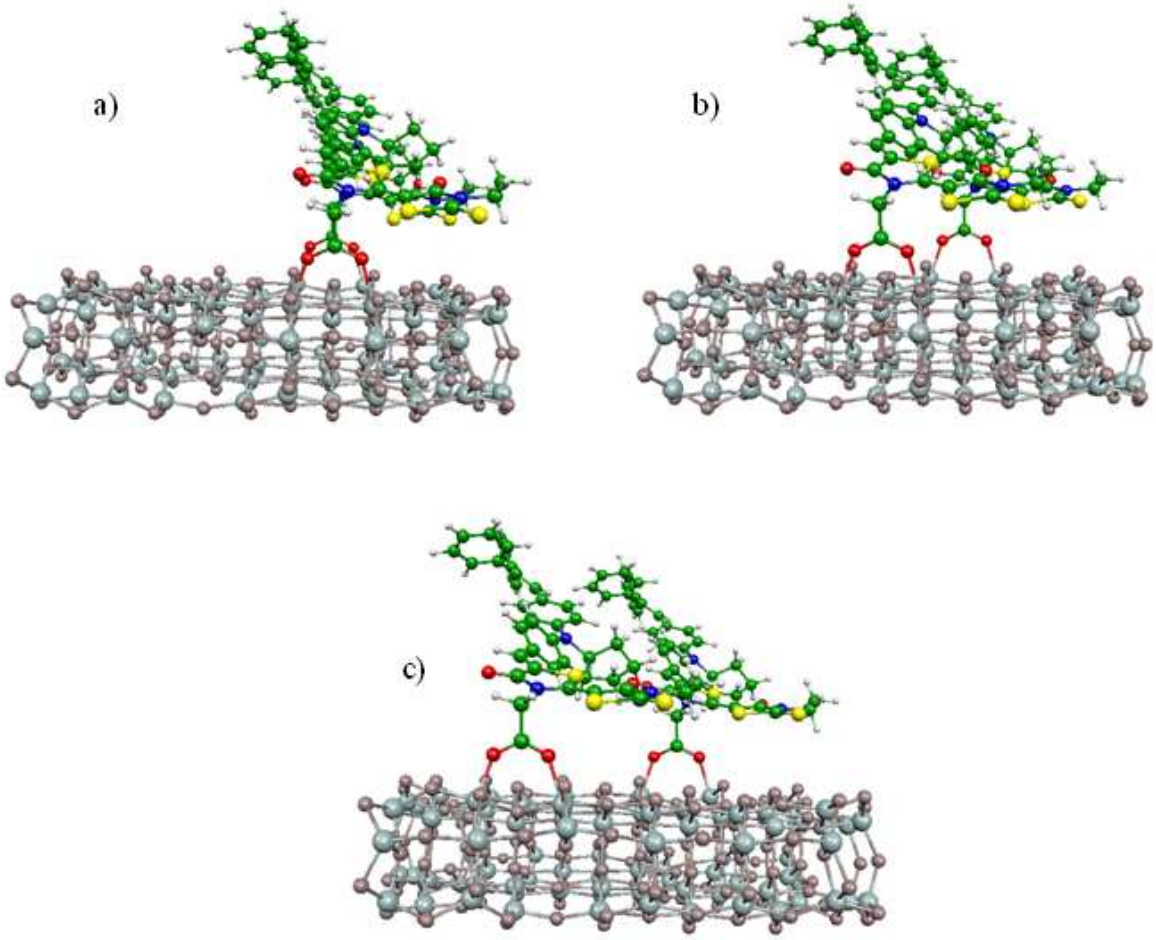

Figure S2: Optimized structure of (a) (0,2)-D149, (b) (2,2)-D149 and (c) (4,2)-D149 on the $(TiO_2)_{82}$ cluster.

Computational details:

Geometry optimizations have been performed by means of the Car-Parrinello method implementing Vanderbilt "ultrasoft" pseudopotentials. A cubic supercell of 60 a.u. side was employed. A plane wave kinetic energy cutoff of 25 (200) Rydberg was used to expand the Kohn-Sham orbitals (charge density). The size of the "little boxes" containing the ultrasoft cores was selected to ca. 4 a.u.