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Electronic Supplementary Information

Charge Displacement Curves

**Fig. S1:** Left: CD curve of the L0-TiO$_2$ system anchored in BB geometry as a function of different solvents. Right: comparison between the CD curves calculated by SVP and 6-31G* basis sets for the same system.
**Fig. S2:** CD curve of the rh-L0-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.

**Fig. S3:** CD curve of the NKX-2587-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.
Fig. S4: CD curve of the NKX-2697-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.

Fig. S5: CD curve of the L1-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.
**Fig. S6**: CD curve of the D5-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.

**Fig. S7**: CD curve of the BA-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.
**Fig. S8**: CD curve of the NH$_2$-BA-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.

**Fig. S9**: CD curve of the NO$_2$-BA-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.
**Fig. S10:** CD curve of the AA-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.

**Fig S11:** CD curve of the AAF$_3$-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in BB geometry.
**Fig. S12**: CD curve of the L0-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in M geometry.

**Fig. S13**: CD curve of the NKX-2587-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in M geometry.
Fig. S14: CD curve of the NKX-2697-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in M geometry.

Fig. S15: CD curve of the BA-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in M geometry.
**Fig. S16**: CD curve of the NH₂-BA-TiO₂ system. The sensitizer is anchored on TiO₂ in M geometry.

**Fig. S17**: CD curve of the NO₂-BA-TiO₂ system. The sensitizer is anchored on TiO₂ in M geometry.
**Fig. S18:** CD curve of the AA-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in M geometry.

**Fig. S19:** CD curve of the AAF$_3$-TiO$_2$ system. The sensitizer is anchored on TiO$_2$ in M geometry.
**Fig. S20:** CD curve of the FA-TiO\(_2\) system. The sensitizer is anchored on TiO\(_2\) in M geometry.

**Fig. S21:** Comparison between CD curves of the NKX-2587 dye anchored on a (TiO\(_2\))\(_{38}\) and (TiO\(_2\))\(_{82}\) clusters. The sensitizer is anchored on TiO\(_2\) in BB geometry.
Partial Density of States (PDOS)

**Fig. S22**: Plots of Density Of States (DOS) for the complex containing the L0 dye in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

**Fig. S23**: Plots of Density Of States (DOS) for the complex containing the rh-L0 dye in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
**Fig. S24**: Plots of Density Of States (DOS) for the complex containing the NKX-2587 dye in the BB anchoring geometry: (red) \((\text{TiO}_2)_{38}\) cluster DOS, (green) DOS of the \((\text{TiO}_2)_{38}\) cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) \((\text{TiO}_2)_{38}\) cluster contribution to the total DOS.

**Fig. S25**: Plots of Density Of States (DOS) for the complex containing the NKX-2697 dye in the BB anchoring geometry: (red) \((\text{TiO}_2)_{38}\) cluster DOS, (green) DOS of the \((\text{TiO}_2)_{38}\) cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) \((\text{TiO}_2)_{38}\) cluster contribution to the total DOS.
Fig. S26: Plots of Density Of States (DOS) for the complex containing the L1 dye in the BB anchoring geometry: (red) (TiO₂)₃₈ cluster DOS, (green) DOS of the (TiO₂)₃₈ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO₂)₃₈ cluster contribution to the total DOS.

Fig. S27: Plots of Density Of States (DOS) for the complex containing the D5 dye in the BB anchoring geometry: (red) (TiO₂)₃₈ cluster DOS, (green) DOS of the (TiO₂)₃₈ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO₂)₃₈ cluster contribution to the total DOS.
**Fig. S28** : Plots of Density Of States (DOS) for the complex containing BA in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

**Fig. S29** : Plots of Density Of States (DOS) for the complex containing NH$_2$-BA in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
**Fig. S30**: Plots of Density Of States (DOS) for the complex containing NO$_2$-BA in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

**Fig. S31**: Plots of Density Of States (DOS) for the complex containing AA in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
**Fig. S32**: Plots of Density Of States (DOS) for the complex containing AAF$_3$ in the BB anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

**Fig. S33**: Plots of Density Of States (DOS) for the complex containing the L0 dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
Fig. S34: Plots of Density Of States (DOS) for the complex containing the NKX-2587 dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

Fig. S35: Plots of Density Of States (DOS) for the complex containing the NKX-2697 dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
**Fig. S36:** Plots of Density Of States (DOS) for the complex containing the BA dye in the M anchoring geometry: (red) (TiO₂)₃₈ cluster DOS, (green) DOS of the (TiO₂)₃₈ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO₂)₃₈ cluster contribution to the total DOS.

**Fig. S37:** Plots of Density Of States (DOS) for the complex containing the NH₂-BA dye in the M anchoring geometry: (red) (TiO₂)₃₈ cluster DOS, (green) DOS of the (TiO₂)₃₈ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO₂)₃₈ cluster contribution to the total DOS.
**Fig. S38:** Plots of Density Of States (DOS) for the complex containing the NO$_2$-BA dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

**Fig. S39:** Plots of Density Of States (DOS) for the complex containing the AA dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
Fig. S40: Plots of Density Of States (DOS) for the complex containing the AAF$_3$ dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.

Fig. S41: Plots of Density Of States (DOS) for the complex containing the FA dye in the M anchoring geometry: (red) (TiO$_2$)$_{38}$ cluster DOS, (green) DOS of the (TiO$_2$)$_{38}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) (TiO$_2$)$_{38}$ cluster contribution to the total DOS.
**Fig. S42**: Plots of Density Of States (DOS) for the complex containing the NKX-2587 dye in the BB anchoring geometry: (red) $(\text{TiO}_2)_{82}$ cluster DOS, (green) DOS of the $(\text{TiO}_2)_{82}$ cluster in the presence of the point charges reproducing the dye electrostatic potential, (blue) $(\text{TiO}_2)_{82}$ cluster contribution to the total DOS.

**Table S1.** Comparison between the amount of CT calculated from the CD curves and from the partial dye charges for the interacting dye/semiconductor assemblies.

<table>
<thead>
<tr>
<th>System</th>
<th>Charges CT</th>
<th>CD CT</th>
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<tr>
<td>L0-BB</td>
<td>0.43</td>
<td>0.36</td>
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<tr>
<td>NKX-2587-BB</td>
<td>0.39</td>
<td>0.40</td>
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<tr>
<td>NKX-2697-BB</td>
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<td>0.36</td>
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<tr>
<td>L1-BB</td>
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<tr>
<td>AA-BB</td>
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</table>
Additional fit

Fig. S43: Effect of charge donation/withdrawal on the energy position of the conduction band edge. When two electrons are added to TiO$_2$ we calculated the shifts relative to both singlet and triplet electronic states, finding almost coincident values.