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Supporting Information for: Ru(II)-phthalocyanine sensitized solar cells: the influence of co-adsorbents upon interfacial electron transfer kinetics

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1. Dye characterization: Absorption, Emission and CV Data

Table S1

Sample	Absorption maximum Q band (nm)	Emission maximum (nm)[a]	$E_{1/2}^{ox}$ vs SCE (V)[b]
RuPcA1	635	680-830	0.67
RuPcA2	630	680-825	0.55
RuPcA3	625	710-830	0.53
RuPcA4	640	700-820	0.61
RuPcA5	625	700-830	0.54
RuPcA6	630	710-830	0.55

[a]: the first maximum is attributed to fluorescence and the second to phosphorescence. λexc corresponds to the maximum of the Q band measured in the absorption spectra.
[b]: Measurements done in 1mM CH_2Cl_2 (except RuPcA1 in DMSO) solutions using $TBAPF_6$ as electrolyte.

2. Comparison of the absorption spectra of RuPc in solution and adsorbed onto TiO_2

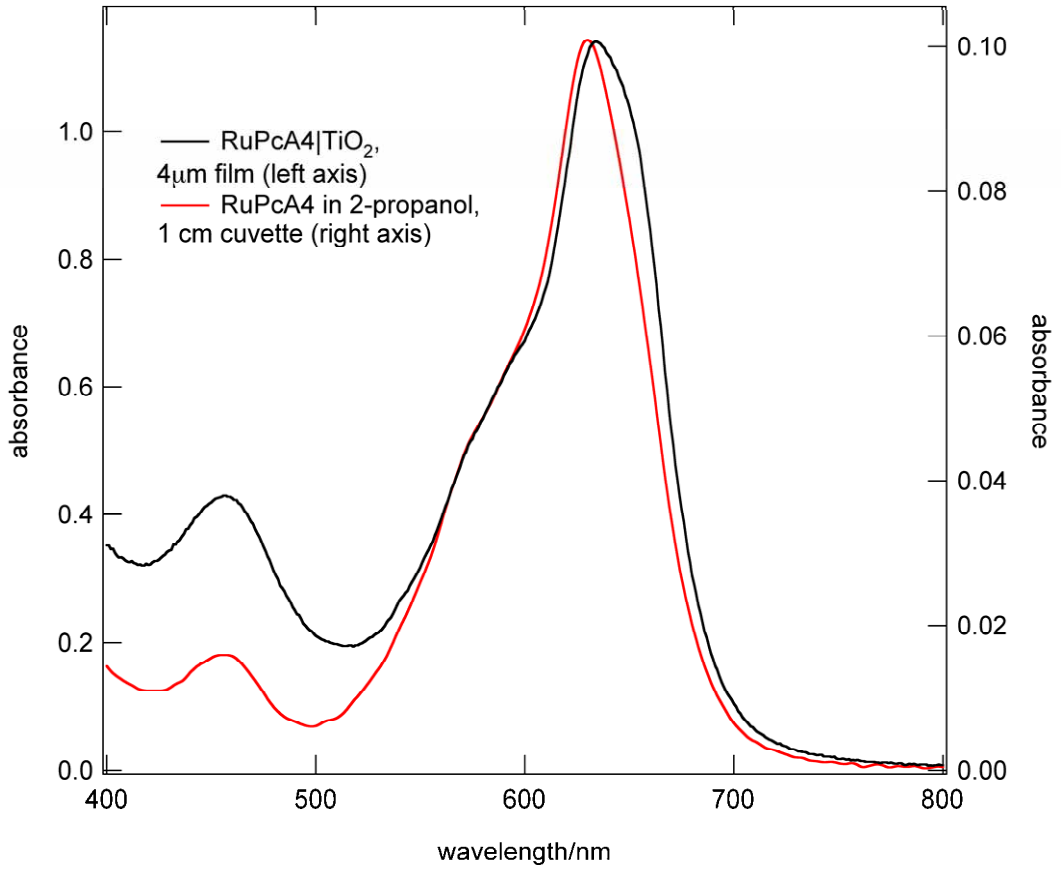

Fig. S1 Comparison of the absorption spectra of RuPcA4 in isopropanol and adsorbed onto TiO_2 (no coadsorber added). There are no significant changes on the absorption spectra of the dye in spite of the large difference on dye concentration. This suggests that even at high dye concentrations and in the absence of CHENO, no significant amount of dye aggregates are formed. The other RuPc dyes show a similar behaviour.

3. Molecular orbital (MO) plots obtained from the DFT calculations

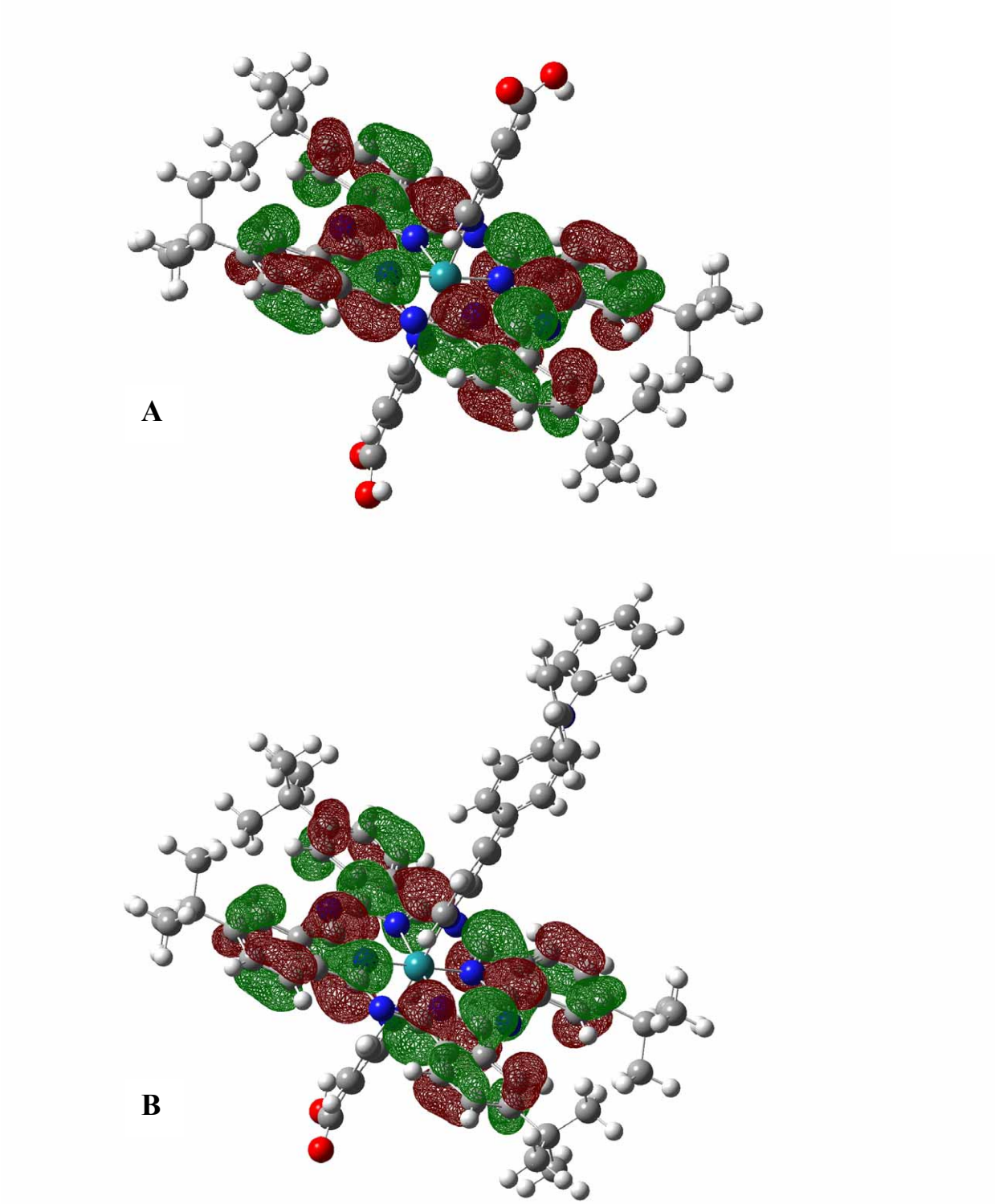

Fig. S2 Graphical representation of the HOMOs of RuPcA1 (**A**) and RuPcA2 (**B**) as determined from DFT calculations. Independently of the nature of the axial ligand, either electron acceptor (RuPcA1) or electron donor (RuPcA2), the HOMO seems to be exclusively located on the Pc ring. This is an indication that upon oxidation of the dye, the resulting hole will be located in the Pc ring. Since dye cation-TiO_2 (e-) recombination is strongly dependent on the hole-semiconductor surface distance and

this distance can be inferred to be the same for all the studied dyes, similar dye cation-TiO_2 (e-) recombination dynamics are expected for all the dyes. For the calculations we used the B3LYP functional as implemented in Gaussian 03, a general basis set with 6-31G(d) for nitrogen, oxygen, and carbon atoms, 6-31G for hydrogen atoms, and an effective core potential basis set LANL2DZ for the ruthenium atoms.