Supporting Information

Surface Modification of Anatase Nanoparticles with Fused Ring Catecholate Type Ligands: A Combined DFT and Experimental Study of Optical Properties

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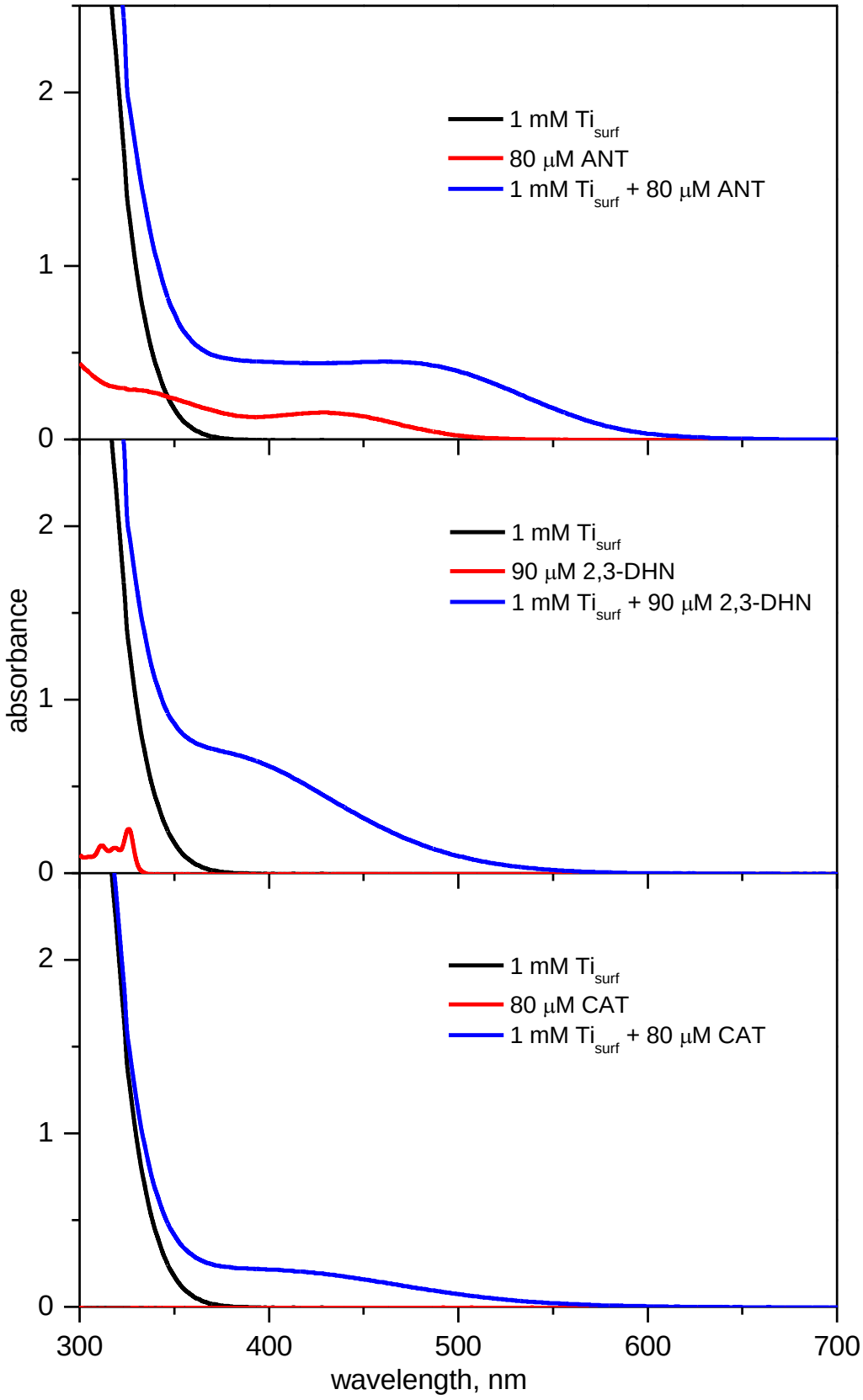

Fig. S1 Absorption spectra of TiO_2 nanoparticles (black), free ligands (red) and ligand-TiO_2 CT-complexes (blue) with 15% coverage in methanol/water=90/10, pH = 2.

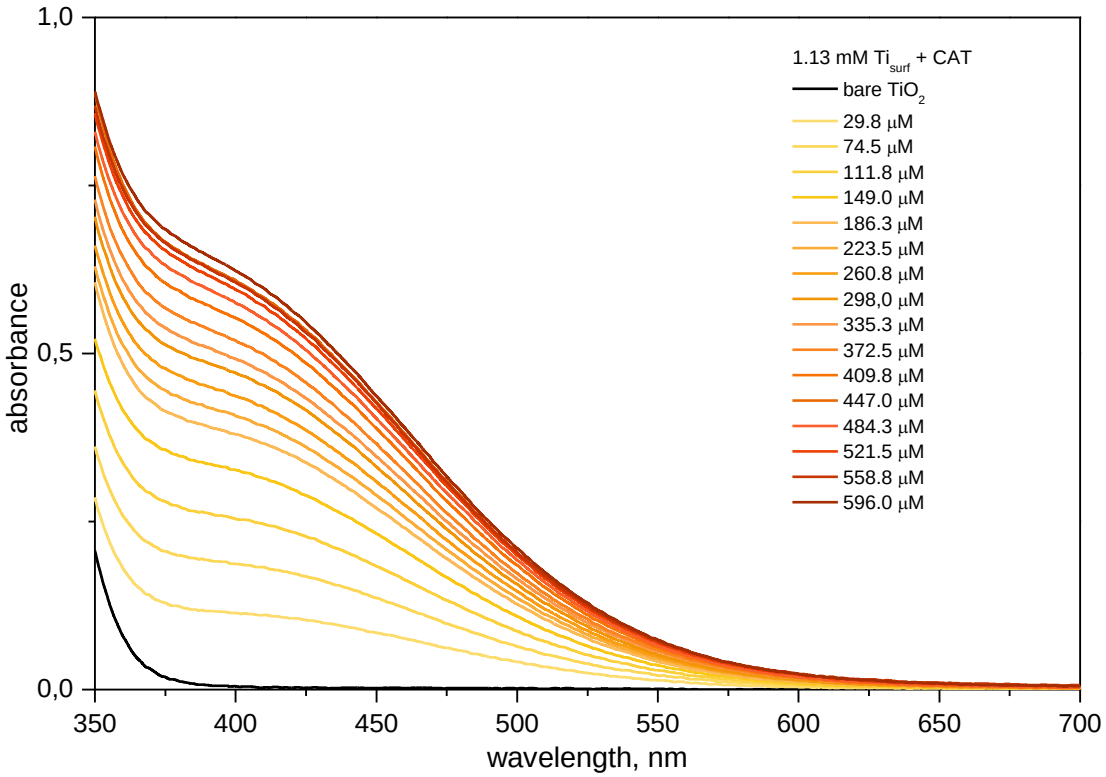

Fig. S2 Absorption spectra of 4 mM TiO_2 nanoparticles before and after surface modification with catechol (0 – 0.6 mM in 0.04 mM steps) in methanol/water=90/10, pH = 2 (data recorded 20 h after surface modification).

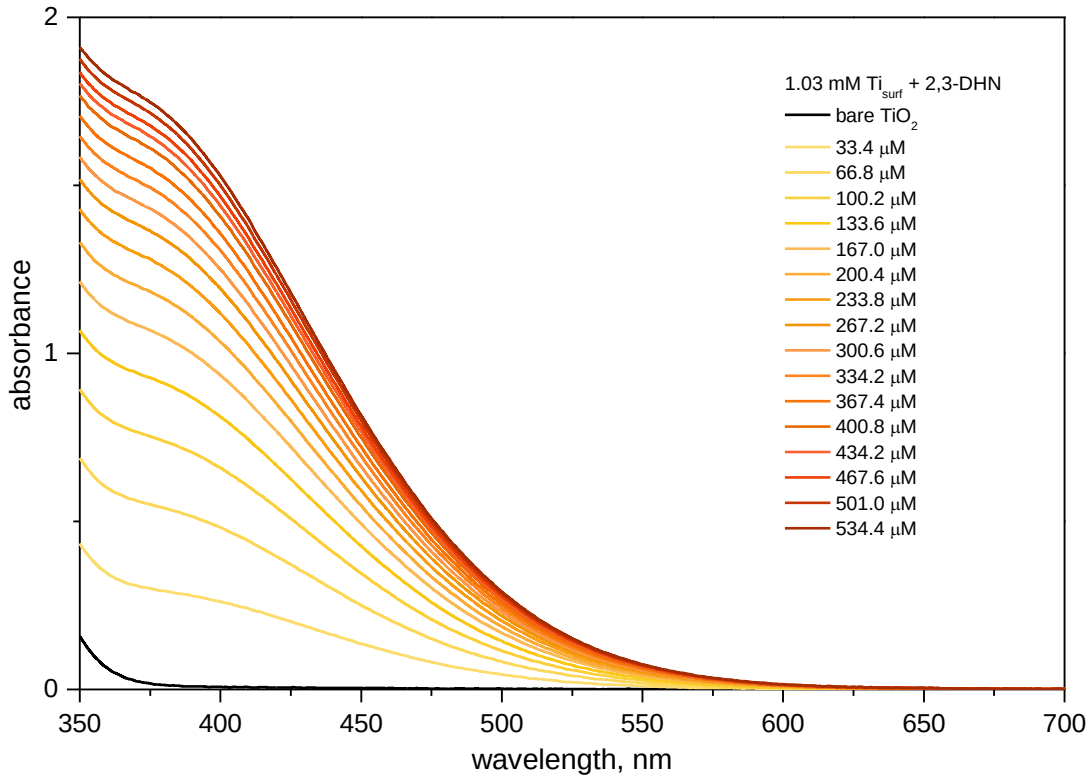

Fig. S3 Absorption spectra of 4 mM TiO_2 nanoparticles before and after surface modification with 2,3-dihydroxynaphthalene (0 – 0.55 mM in 0.035 mm steps) in methanol/water=90/10, pH = 2 (data recorded 20 h after surface modification).

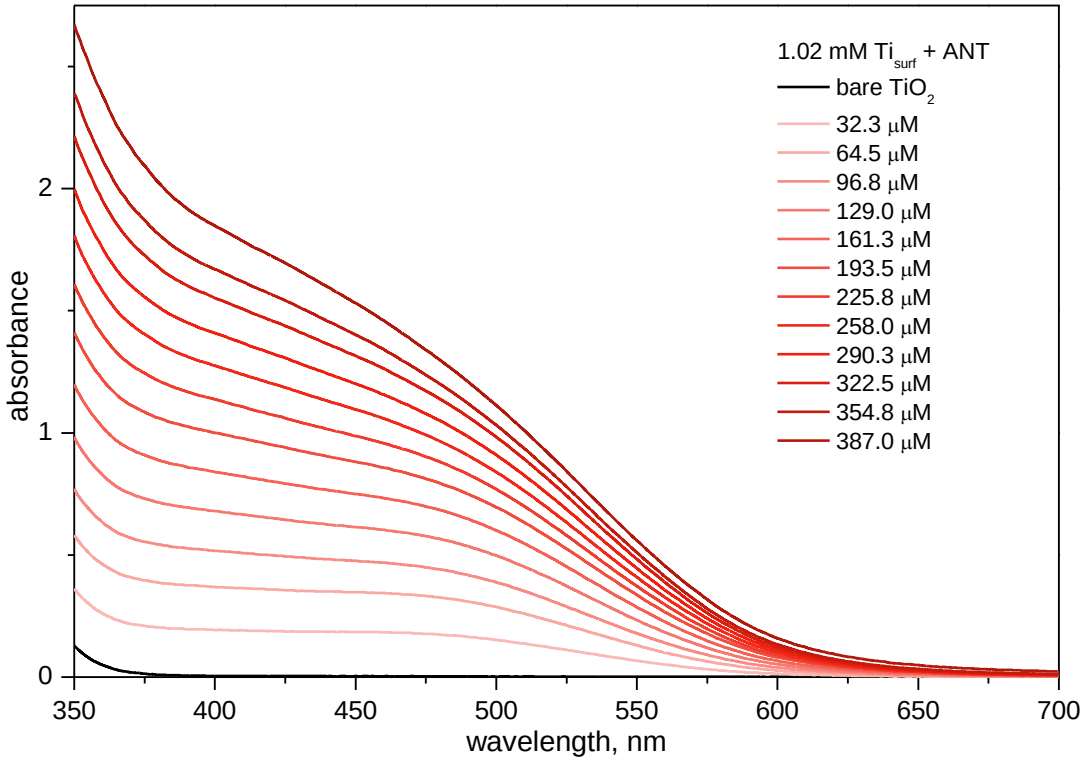

Fig. S4 Absorption spectra of 4 mM TiO_2 nanoparticles before and after surface modification with anthrarobin (0 – 0.4 mM in 0.035 mM steps) in methanol/water=90/10, pH = 2 (data recorded 20 h after surface modification).