Using Density Functional Theory to Model Realistic TiO_2 Nanoparticles, Their Photoactivation and Interaction with Water.

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SUPPLEMENTARY MATERIAL

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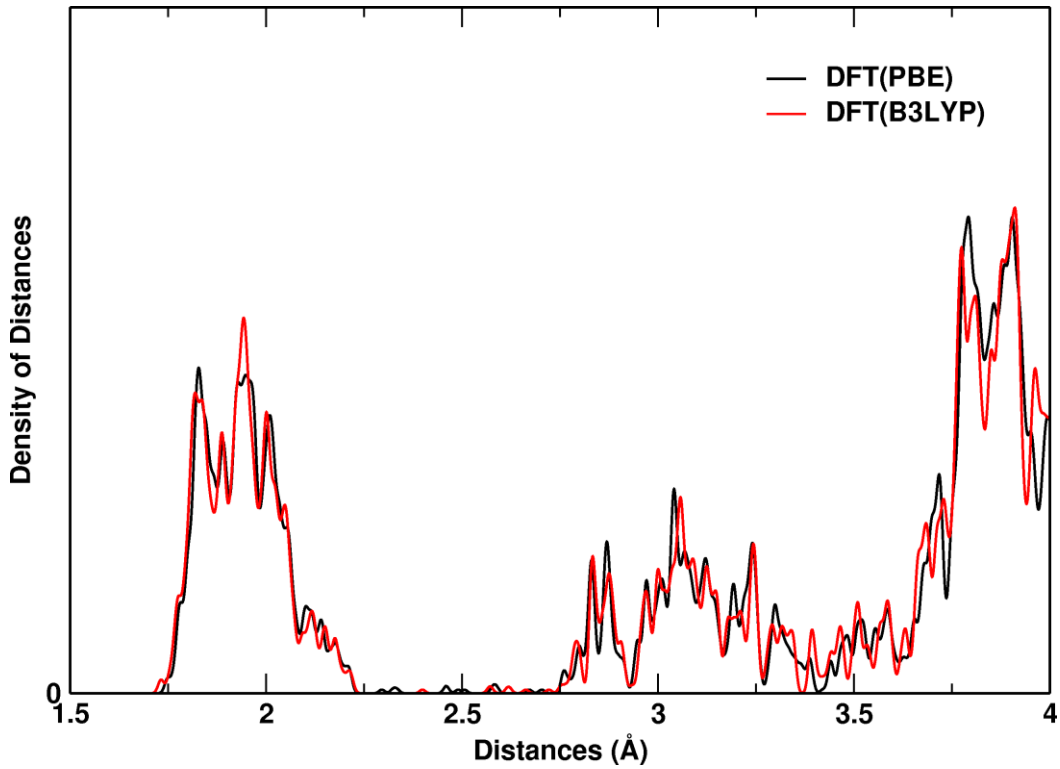

Figure S1. Comparison of the distances distribution (simulated EXAFS) computed with DFT(PBE), in black and DFT(B3LYP) in red, for the 2.2 nm NS produced at 300 K.

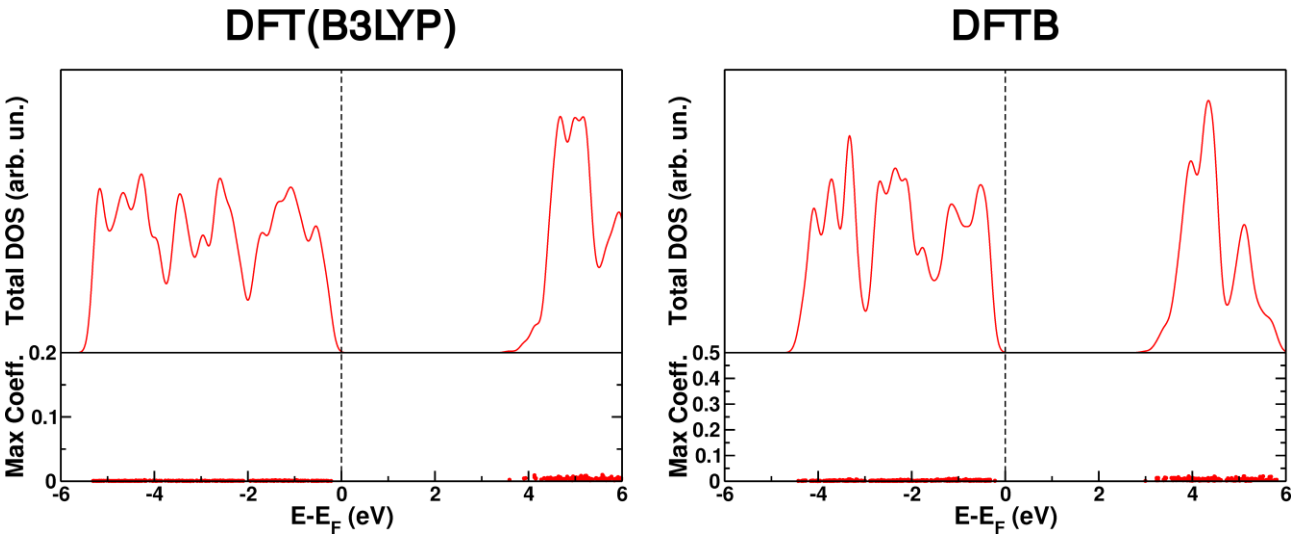

Figure S2. DFT(B3LYP) and DFTB total (DOS) density of states for anatase bulk TiO_2. The maximum atomic orbital coefficient (max_c) of each eigenstate is also reported.