SUPPLEMENTARY MATERIAL TO

**Visible light absorption of surface-modified TiO2 nanoparticles with vitamin B6: a comparative experimental and DFT study**

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Table S-I. Wavelengths, oscillator strengths, and wave-functions of electronic excitations calculated for B6/[Ti8O14(OH)3]clusters.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Wavelength (nm) | Oscillator strength | Wavefunction  (|coefficient|2 ≧ 10%) |
| Excited State 1 | 388 | 0.0002 | HOMO → LUMO (70%) |
| Excited State 2 | 378 | 0.0003 | HOMO-2 → LUMO (26%)  HOMO-1 → LUMO (10%) |
| Excited State 3 | 369 | 0.0007 | HOMO-6 → LUMO (20%)  HOMO-5 → LUMO (18%) |



Fig. S-1.Spatial distributions of highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) for B6/[Ti8O14(OH)3]clusters.

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