

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%)

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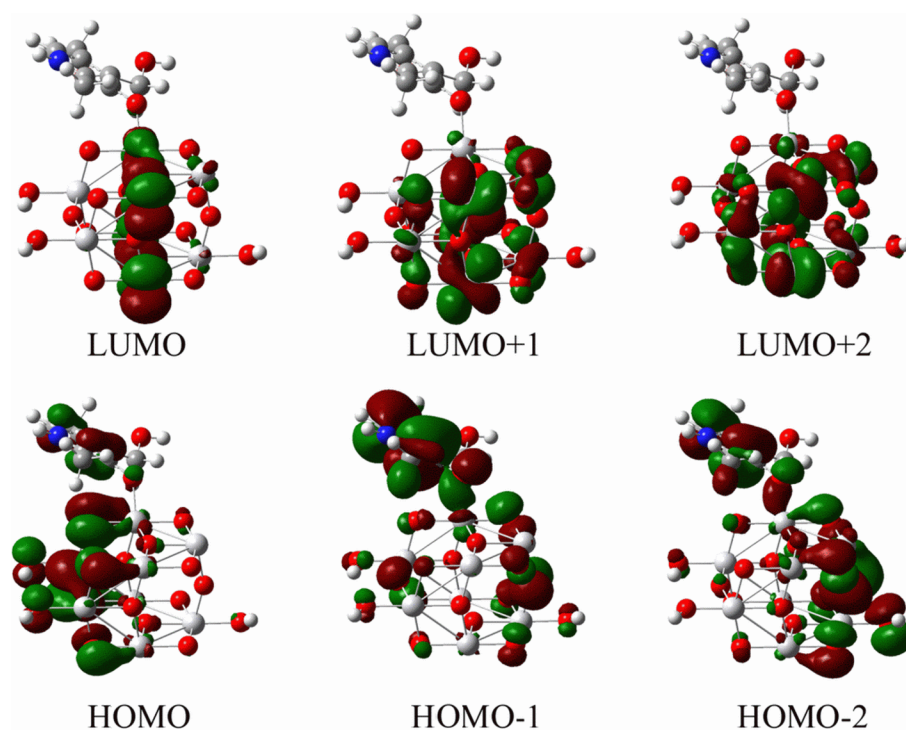


Fig. S-1. Spatial distributions of highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) for $B_6/[Ti_8O_{14}(OH)_3]$ clusters.