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SUPPLEMENTARY MATERIAL TO

# Visible light absorption of $TiO_2$ nanoparticles surface-modified with vitamin $B_6$: A comparative experimental and DFT study

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TABLE S-I. Wavelengths, oscillator strengths, and wave functions of electronic excitations calculated for the $[Ti_8O_{14}(OH)_3(B_6)]^+$ clusters

| Excited state | Wavelength, nm | Oscillator strength | Wave function (\|coefficient\|$^2$ ≥ 10 %) |
|---|---|---|---|
| 1 | 388 | 0.0002 | HOMO → LUMO (70 %) |
| 2 | 378 | 0.0003 | HOMO-2 → LUMO (26 %) |
| | | | HOMO-1 → LUMO (10 %) |
| 3 | 369 | 0.0007 | HOMO-6 → LUMO (20 %) |
| | | | HOMO-5 → LUMO (18 %) |

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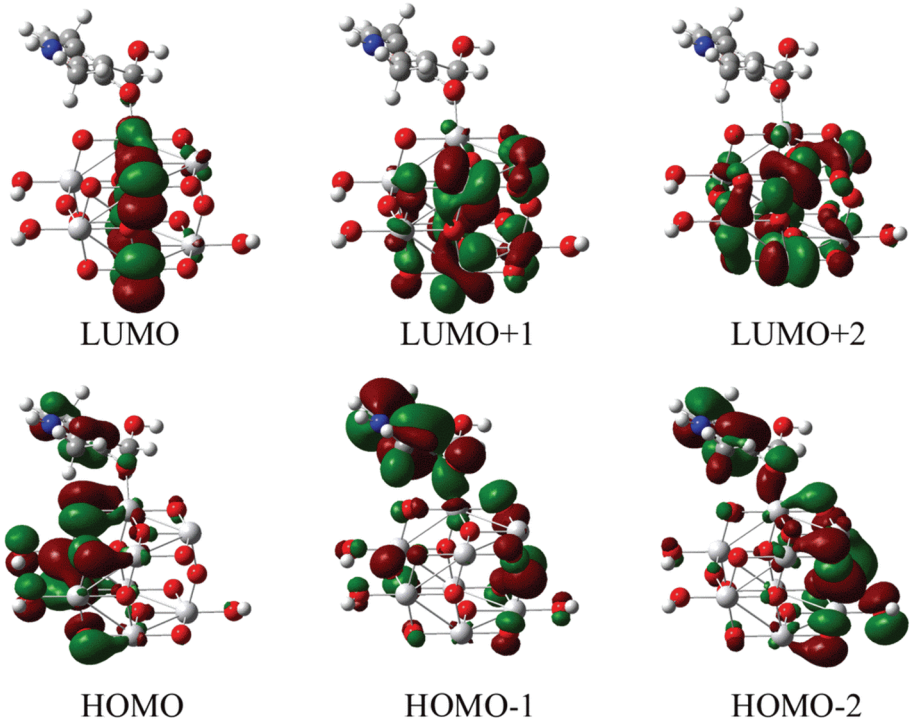


Fig. S-1. Spatial distributions of highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) for $[Ti_8O_{14}(OH)_3(B_6)]^+$ clusters.