

Support Information

Dependence of the Irradiation Conditions and Crystalline Phase of TiO₂ Nanoparticles on their Toxicity to *Daphnia magna*

Huiting Lu,^a Wenhong Fan,^{*a} Haifeng Dong^b and Lingling Liu^a

^a School of Space and Environment, Beihang University, Beijing 100191, P. R. China

^b Research Center for Bioengineering and Sensing Technology, University of Science and Technology Beijing, Beijing 100083, P. R. China

Correspondence: Wenhong Fan, Department of Environmental Science and Engineering, School of Chemistry and Environment, Beihang University, Beijing 100191, P. R. China. Tel.: +86 1082338630. Fax: +86 1082338630. E-mail: fanwh@buaa.edu.cn

Calculation about the Valence Band Edge (E_v) and the Conduction Band Edge (E_c) of Each TiO_2 NPs Sample

The energy band gap (E_g) is the energy interval between the valence band edge (E_v) and the conduction band edge (E_c). Hence, the relationship of E_g , E_v and E_c is as follows:

$$E_g = E_v + E_c \quad (S1)$$

Meanwhile, the relationship between the band edge energies (E_v , E_c) and the absolute electronegativity (χ) can be calculated according to the following equation¹:

$$E_c = -\chi + 0.5 E_g \quad (S2)$$

$$E_v = -\chi + 0.5 E_g \quad (S3)$$

The absolute electronegativity of TiO_2 is 5.81 eV. Then according to the value of E_g , the value of E_v and E_c can be calculated by equation S2 and S3.

Table S1. Zeta potential of TiO₂ nanoparticles.

Sample	Zeta potential (mV)
A-S	-1.5400
M1	-6.7000
M2	-6.1400
M3	-10.5000
R-S	-6.2900

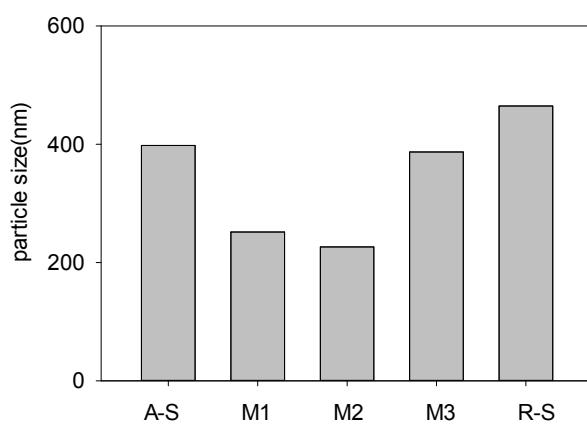


Figure S1. Average diameters of TiO_2 nanoparticles on the basis of the DLS data.

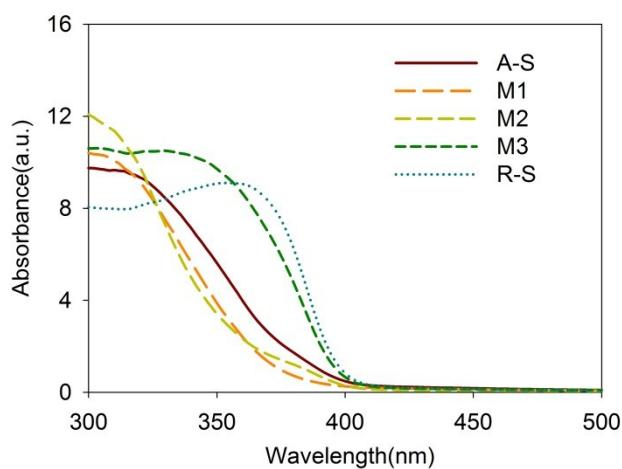


Figure S2. UV-visible spectra of the five TiO_2 nanoparticles.

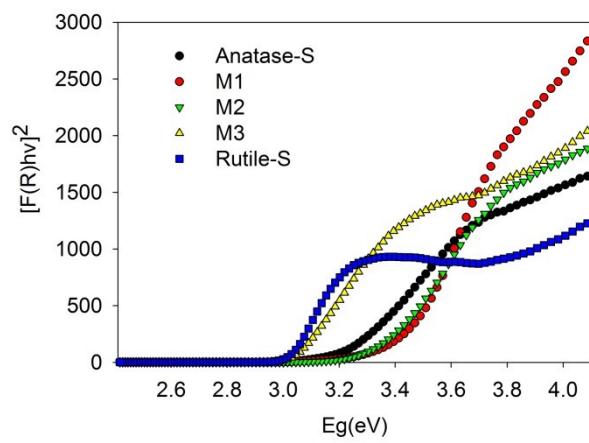


Figure S3: Band gap determination using Kubelka–Munk function of the five TiO_2 nanoparticles.

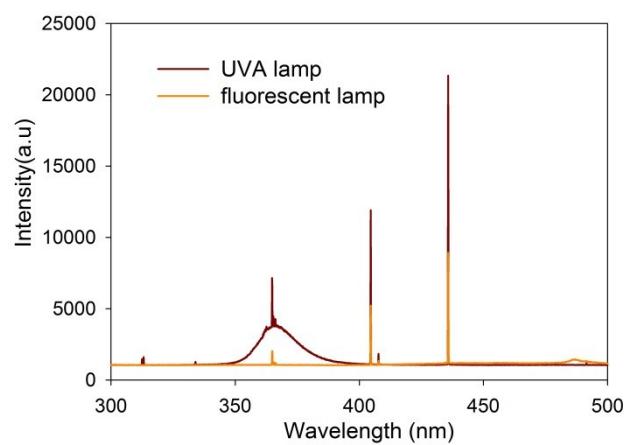


Figure S4. Emission spectra of the UVA lamp and fluorescent lamp.

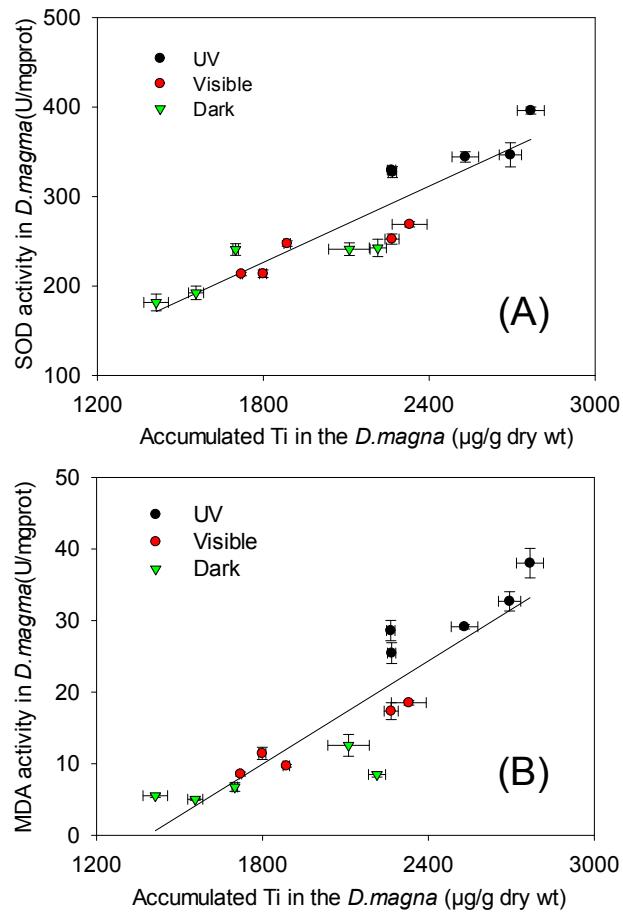


Figure S5. Relationship among SOD (A), MDA (B) and accumulated Ti in *D. magna* after 48 h of exposure to the five TiO_2 nanoparticles. Mean \pm standard deviation ($n = 3$).

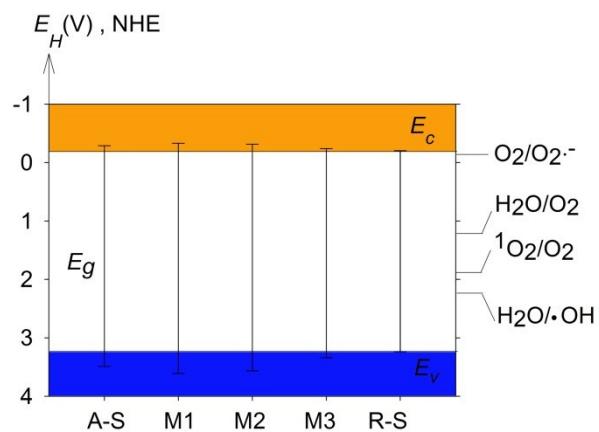


Figure S6. Band edge positions of the five TiO_2 nanoparticles in contact with an aqueous solution.

REFERENCES

- S1. Y. Xu and M. A. A. Schoonen, *American Mineralogist*, 2000, **85**, 543-556.