

# Supporting Information of

## Water-Driven Micromotors for Rapid Photocatalytic Degradation of Biological and Chemical Warfare Agents

*Jinxing Li, Virendra V. Singh, Sirilak Sattayasamitsathit, Jahir Orozco, Kevin Kaufmann,  
Renfeng Dong, Wei Gao, Beatriz Jurado-Sanchez, Yuri Fedorak, Joseph Wang\**

Department of Nanoengineering, University of California San Diego, La Jolla, CA 92093 (USA)

\*Correspondence to: [josephwang@ucsd.edu](mailto:josephwang@ucsd.edu)

### **1. Photocatalytic degradation mechanism**

Figure S1 displays the mechanism for the photocatalytic degradation involved in the operation of the TiO<sub>2</sub>/Au/Mg-micromotor. The new micromotors consist of a photoactive TiO<sub>2</sub> surface layer embedded with Au nanoparticles for photodecomposition. Under UV irradiation, the photogenerated positive holes react with adsorbed water and produce strong oxidizing hydroxyl radicals. In addition, the photogenerated free electrons react with adsorbed molecular O<sub>2</sub> to produce superoxide anions that could also contribute to the production of peroxide radicals, hydroxyl radicals, and hydroxyl anions. The complete mineralization of CWAs has been achieved due to coupled oxidation-reduction carried out by the highly active radicals and anions. The presence of the Au nanoparticles can effectively shift the Fermi level of TiO<sub>2</sub> and enhance the charge carrier separation to extend the lifetime of the generated radicals and anions, which results in an enhanced photocatalytic efficiency.

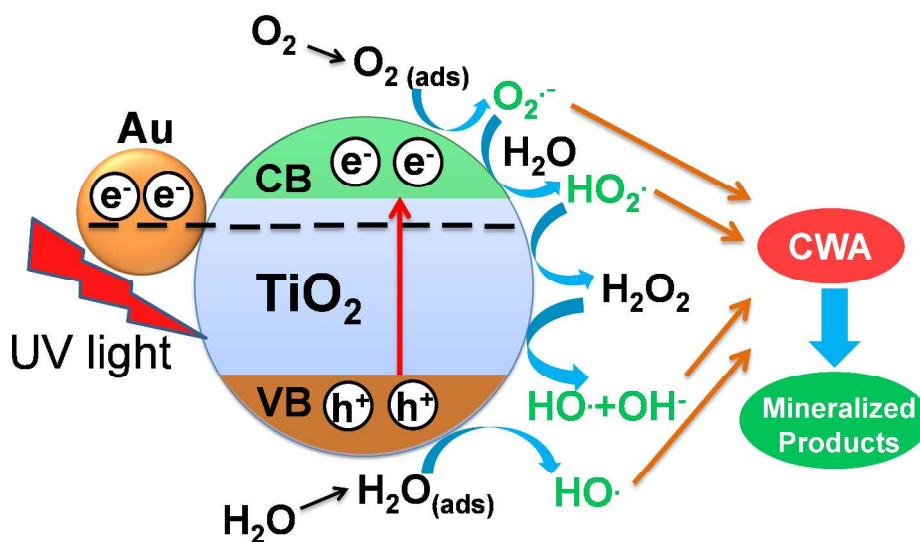
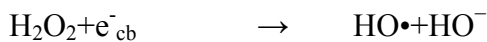
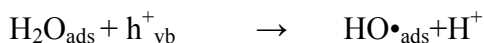


Figure S1. Proposed mechanism for the photocatalytic CWA degradation involved in the operation of the  $\text{TiO}_2/\text{Au}/\text{Mg}$ -micromotor.

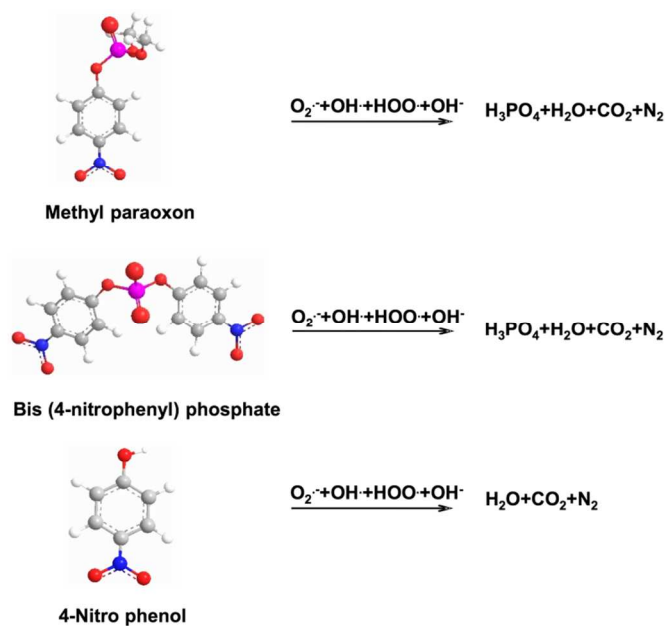
The reaction process was proposed as follows:



According to the above reactions, the generated active species  $\text{HO}\cdot$ ,  $\text{HO}^-$ ,  $\text{HO}_2\cdot$  and  $\text{O}_2\cdot^-$  are responsible for the mineralization of b-NPP, MP and 4-NP.

Nerve agent simulants such as b-NPP and MP have strong P=O and P-O-C bonds. The photocatalytic degradation of these molecules on  $\text{TiO}_2/\text{Au}/\text{Mg}$  micromotors begins with cleavage of the P-O-C bond and makes secondary products. Subsequently, P-O bond, C-C bond, P and C atoms were oxidized gradually in the presence of active oxidative species, which finally lead to

the formation of mineralized products such as carbon dioxide, water and phosphoric acid. The pH value decreased from 6.0 at the beginning of the reaction to 4.0 at the end of the reaction, indicating the formation of acidic products. Based on the above results, the reaction mechanism of photocatalytic degradation of b-NPP, MP and 4-NP, is presented in Scheme S1.



**Scheme S1.** Chemical reactions involved in the photocatalytic destruction of the different pollutants.

## 2. Photocatalytic degradation of 4-NP

In order to expand the versatility and practical utility of the  $TiO_2/Au/Mg$  micromotors towards diverse environmental applications and confirm their complete mineralization capacity, we also examined their ability to fully remediate the persistent phenolic pollutant 4-NP, which is also a hydrolysis product of MP and b-NPP. Remarkably, as displayed in Fig. S2A, we found that 0.13 mM 4-NP can be completely decomposed within 10 minutes by the moving photocatalytic micromotors, while negligible elimination is observed in control experiments without the active surface or the motion of the motors. Furthermore, the complete color removal of the 4-NP solution after treatment by photocatalytic micromotors (Fig. S2B) also confirms that the decomposition process is mainly through redox reactions that promote complete mineralization rather than hydrolysis. Overall, this data clearly suggests that such enhanced photocatalytic

degradation by micromotors is a complete mineralization process which is highly efficient for persistent phenolic compound remediation.

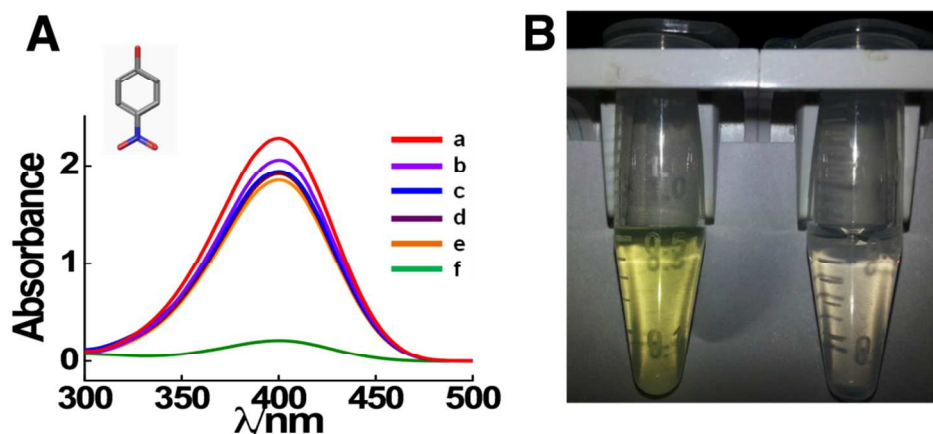


Figure S2. (A) Absorbance spectra of 4-NP ( $C_0=0.13$  mM) after a 10 min treatment with the  $\text{TiO}_2/\text{Au}/\text{Mg}$  motors in UV (green, f), as compared with different control experiments, including operation (a) without any treatment in dark, (b) moving  $\text{TiO}_2/\text{Au}/\text{Mg}$  motors in dark, (c) moving  $\text{Al}_2\text{O}_3/\text{Au}/\text{Mg}$  micromotors (with passive surface) in UV light, (d) UV light only, and (e) static  $\text{TiO}_2/\text{Au}/\text{Mg}$  micromotor in UV light. Conditions for each test: total volume of the contaminated solution is 600  $\mu\text{L}$ ; micromotor amount, 2.25 mg; 0.08 M NaCl and 0.075% Triton X-100 is added for propulsion. All experiments were performed at room temperature. (B) Image of a solution polluted with 0.13mM 4-NP (left), and a solution with 0.13 mM of 4-NP after 10min treatment with moving  $\text{TiO}_2/\text{Au}/\text{Mg}$  motors in UV irradiation (right). Conditions, as in A.

### 3. Supporting Videos

3.1 Supporting Video S1: Propulsion of  $\text{TiO}_2/\text{Au}/\text{Mg}$  micromotor in water containing a 0.08 NaCl.

3.2 Supporting Video S2: Propulsion of  $\text{TiO}_2/\text{Au}/\text{Mg}$  micromotor in seawater.

3.3 Supporting Video S3: Long-time propulsion of  $\text{TiO}_2/\text{Au}/\text{Mg}$  micromotor in seawater.