Supplementary Material (ESI) for Journal of Materials Chemistry


**Supplementary material**

# Visible-light C –heteroatom bond cleavage and detoxification of chemical warfare agents using titania-supported gold nanoparticles as photocatalyst

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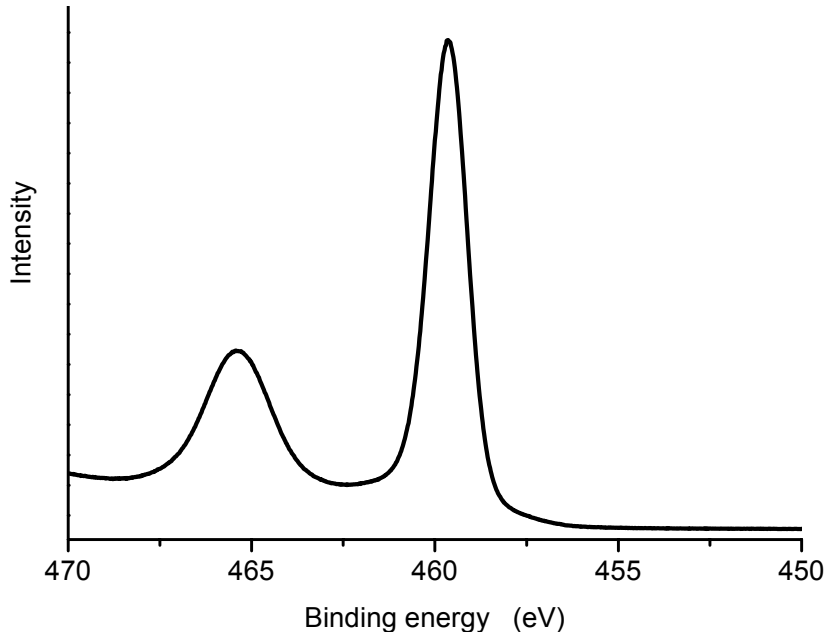



**Fig. S1.** XPS spectrum of the 0.7 wt % $Au/TiO_2$ sample in the Ti(2p) region.

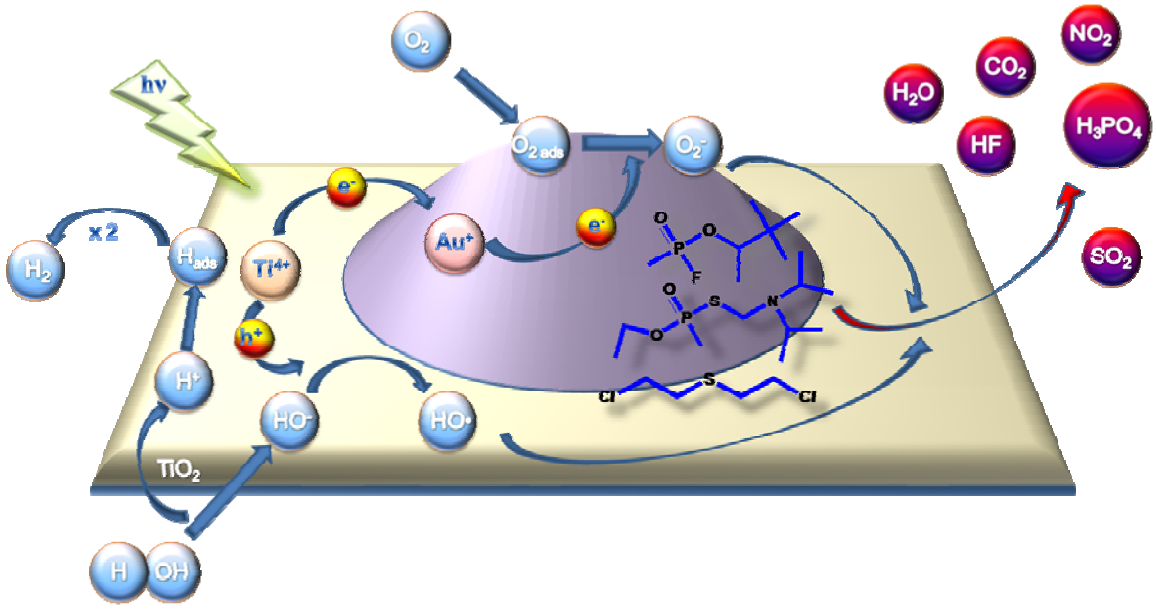



**Fig. S2.** The possible mechanism of photodegradation of the neurotoxic compounds over $Au/TiO_2$ photocatalysts under UV irradiation.

**Table S1.** Products characterized in the photocatalytic Soman detoxification over $Au/TiO_2$ catalysts.

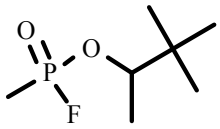
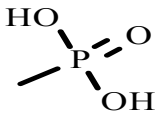
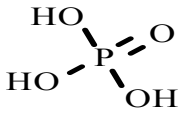
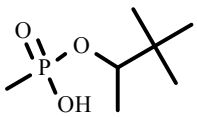
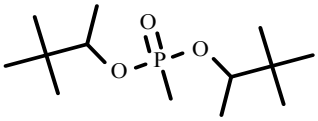
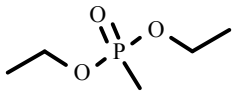
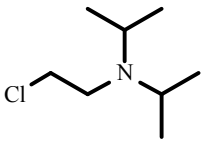
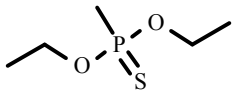
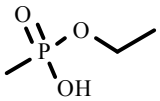
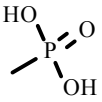
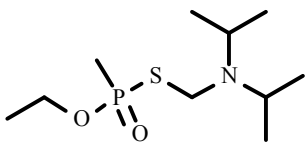
| Nr. Crt. | Product | Retention time (min.) | Chemical structure |
|---|---|---|---|
| **1** | O-Pinacolyl methylphosphonofluoridate | 8.84/8.90 |  |
| **2** | Methylphosphonic acid | 10.23 |  |
| **3** | Phosphoric acid | 12.17 |  |
| **4** | Pinacolyl methylphosphonate | 12.78 |  |
| **5** | O-Pinacolyl O- Pinacolyl methylphosphonate | 15.38 |  |

**Table S2.** Products characterized in the photocatalytic VX detoxification over $Au/TiO_2$ catalysts. catalysts.

| Nr. Crt. | Products | Retention time (min.) | Chemical structure |
|---|---|---|---|
| **1** | Diethylmethane phosphonate | 8.42 |  |
| **2** | Diisopropylaminoethyl chloride | 9.05 |  |
| **3** | Diethyl methylphosphonothioate | 9.23 |  |
| **4** | O- Ethylmethyl phosphonate | 9,40 |  |
| **5** | Methylphosphonic acid | 10.23 |  |
| **6** | O-Ethyl-S2-diisopropylamino ethyl methyl phosphonothionate | 17.98 |  |

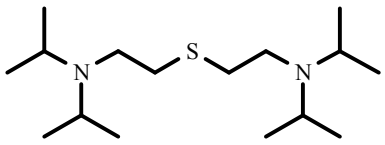
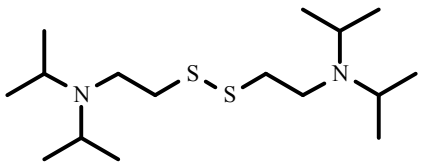
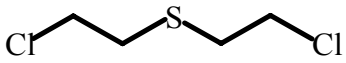
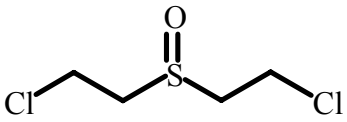
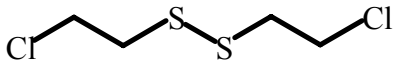
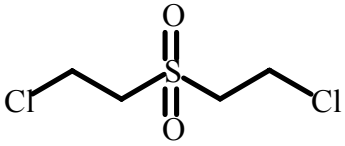
| | | | |
|---|---|---|---|
| **7** | Bis(diisopropylaminoethyl)sulfide | 19.66 |  |
| **8** | Bis(diisopropylaminoethyl)disulfide | 21.79 |  |

**Table S3.** Photodegradation products characterized in the sulfur mustard detoxification over $Au/TiO_2$ catalysts.

| Nr. Crt. | Product | Retention time (min.) | Chemical structure |
|---|---|---|---|
| **1** | Bis(2-chloroethyl)sulfide | 7.63 |  |
| **2** | Bis(2-chloroethyl)sulfoxide | 9.35 |  |
| **3** | Bis(2-chloroethyl)disulfide | 13.05 |  |
| **4** | Bis(2-chloroethyl)sulfone | 16.88 |  |