

Copper Single Atom-diimine Catalytic centers immobilized on TiO₂ for water purification under-visible-light irradiation.

Georgia Pantela¹, Panagiotis Tzevelekidis¹, Christiana A. Mitsopoulou¹

¹Laboratory of Inorganic Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimioupolis, Zografou 15771, Greece

[*cmitsop@chem.uoa.gr](mailto:cmitsop@chem.uoa.gr)

Titanium dioxide (TiO₂) is the most investigated nanomaterial due to its excellent photocatalytic properties, non-toxicity, chemical stability and low cost. It exhibits a large band gap of ~3.2eV, which limits its absorption capacity in the UV light spectrum. To enhance the catalytic efficiency of TiO₂ for water purification, it is crucial to reduce its bandgap. This modification enables the material to effectively harness sunlight, including the visible light spectrum, thereby improving its photocatalytic performance.

[1]

Single-atom catalysts (SACs) exhibit remarkable catalytic efficiency due to their unique electronic structure and maximum utilization of individual atoms, which improves selectivity and activity in various chemical processes. Cu-based SACs (Cu-SACs) can expose more accessible active sites which are utilized more efficiently. When combined with TiO₂ the photocatalytic performance is improved due to the transfer of electrons on the Cu SACs and the suppression of exciton recombination. [2,3].

In this study, we employed an innovative approach for the modification of the Cu SACs centers on TiO₂ by bonding them with various diamine ligands. A variety of analytical techniques were used for characterizing the generated TiO₂ oxide nanoparticles, including X-ray diffraction (XRD) and thermogravimetric analysis (TGA) to determine the crystal structure and composition. Optical properties were assessed using UV-DRS, while spectroscopic characterization were performed using IR-ATR and Raman techniques. The resulting Cu SAC:[diimines]/TiO₂ nanoparticles demonstrated high degradation efficiency under LED visible light for the removal of toxic dyes from water, such as Methylene Blue (MB) and Rhodamine B (RhB).

References:

- [1] M. Nolan, A. Iwaszuk, A. Lucid, J. Carey, M. Fronzi, *Advanced Materials* 28 (2016) 5425-5446
- [2] Y. Zhao, L. Tao, *Chinese Chemical Letters* 35 (2024) 108571
- [3] P. Zhang, H. Zeng, D. Wen, X. Sui, Z. Wang, Y. Wang, H. Chen, Y. Weng, J. Long, *ChemSusChem* 17 (2023) e202301041