

**Experiment title: UNRAVELING THE LOCAL STRUCTURE AND OXIDATION STATE OF VANADIUM (V) IN V-DOPED TiO<sub>2</sub> NANOSTRUCTURED THIN FILMS FOR PHOTOCATALYTIC APPLICATIONS**

**Experiment number:**  
HC-1860

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**Report:** Doping with transition metals is an effective method to enhance visible-light absorption in TiO<sub>2</sub> nanoparticles and to improve the efficiency of many photocatalytic processes under solar radiation. A determination of the incorporation site of the dopant and an understanding of the local bonding arrangement and electronic structure is a necessary step for knowledge-based materials design. In this paper [1], we report an in-depth X-ray absorption spectroscopy study of V dopants in TiO<sub>2</sub> nanoparticles deposited by gas-phase condensation with a local structure similar to anatase, rutile, or intermediate. The combination of K- and L-edge spectra in the pre-edge, edge, and extended energy regions with full potential ab initio spectral simulations shows that V ions occupy substitutional cationic sites in the TiO<sub>2</sub> structure, irrespective of whether it is similar to rutile, anatase, or mixed.

- [1] G. Rossi, M. Calizzi, V. Di Cintio, S. Magkos, L. Amidani, L. Pasquini, F. Boscherini, Local Structure of V Dopants in TiO<sub>2</sub> Nanoparticles: X-ray Absorption Spectroscopy, Including Ab-Initio and Full Potential Simulations, *J. Phys. Chem. C.* 120 (2016) 7457–7466. doi:10.1021/acs.jpcc.5b12045.

