

## Charge carrier dynamics in rutile $\text{TiO}_2(110)$ : role of oxygen vacancies probed by femtosecond transient absorption spectroscopy and x-ray photoelectron spectroscopy

**Keywords:** rutile  $\text{TiO}_2$  (110), oxygen vacancies, defect states, band bending, transient absorption spectroscopy (TAS), x-ray photoelectron spectroscopy (XPS)

### Scientific description:

Rutile  $\text{TiO}_2(110)$  single crystals are a model system for fundamental studies of defect-driven charge carrier dynamics in transition metal oxides. Oxygen vacancies ( $V_O$ ) and associated  $\text{Ti}^{3+}$  states strongly influence electron trapping, band bending, and surface reactivity [1]. While x-ray photoelectron spectroscopy (XPS) provides quantitative information on the density and nature of these defects at the surface [2], femtosecond transient absorption spectroscopy (TAS) allows direct monitoring of charge carrier lifetimes in the near-infrared.

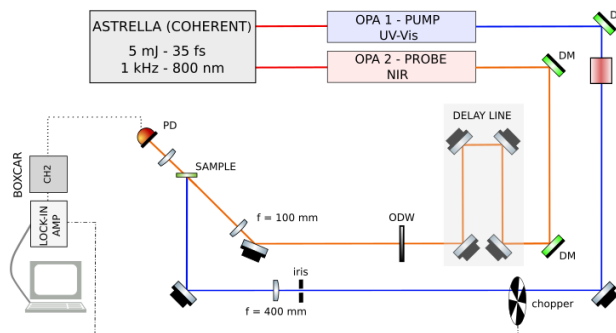


Figure 1. Experimental setup of transient absorption spectroscopy (TAS) on the femtosecond laser platform SUMO @INSP.

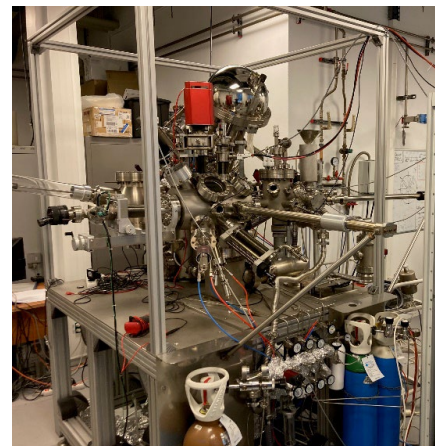


Figure 2. Experimental setup of the OXYDES team for XPS measurements.

The goal of this internship is to establish correlations between the density of oxygen vacancies and the ultrafast dynamics of photoexcited carriers in rutile  $\text{TiO}_2$ . Single crystals will be annealed under UHV to produce different reduction states, then exposed to air to stabilize the surfaces before optical measurements. XPS will quantify surface defect densities and chemical states, while UV-Vis spectroscopy will probe the gap and sub-gap absorption tails [3]. Femtosecond TAS (pump 340 nm, probe 1.3  $\mu\text{m}$ ) will be performed to measure electron relaxation dynamics as a function of vacancy concentration. HAXPES measurements may complement the study by accessing band bending and near-surface potential gradients.

This project will provide insight into the interplay between defect density, band structure, and charge carrier lifetimes in a model oxide system, with relevance for photocatalysis and oxide electronics.

[1] P. Maity *et al.*, J. Phys. Chem. C 122, 8925 (2018).

[2] Y. Gao *et al.*, JACS Au 5, 1822 (2025).

[3] P. R. Jubu *et al.*, Results in Optics 9, 100273 (2022).

**Techniques/methods in use:**

UHV annealing of rutile TiO<sub>2</sub>(110) single crystals. X-ray photoelectron spectroscopy (XPS). UV–Vis–NIR absorption spectroscopy. Femtosecond transient absorption spectroscopy (pump–probe). Hard X-ray photoelectron spectroscopy (HAXPES).

**Applicant skills:**

Good background in solid-state physics and optics. Strong motivation for experimental work, including ultrafast spectroscopy and surface science. Knowledge of photoelectron spectroscopy, laser–matter interaction, or semiconductor physics will be appreciated.

**Industrial partnership:** N

**Internship supervisor(s):** Anna Levy ([levy@insp.jussieu.fr](mailto:levy@insp.jussieu.fr)) – Gregory Cabailh ([cabailh@insp.jussieu.fr](mailto:cabailh@insp.jussieu.fr)) – Rémi Lazarri ([remi.lazzari@insp.jussieu.fr](mailto:remi.lazzari@insp.jussieu.fr))

**Internship location:** Institut des Nanosciences de Paris, 4 Place Jussieu, 75005 Paris.

**Possibility for a Doctoral thesis:** Y