

Ecole Doctorale - 104

Sciences de la Matière, du Rayonnement et de l'Environnement

### **UNIVERSITY:** Lille University

Scientific field: Heterogeneous catalysis, time resolved, Near Ambient Pressure X-ray Photoelectron Spectroscopy

Title of the thesis: Witness a catalyst in action using Time resolved NAP-XPS

Supervisor: Prof. Jean-François Paul, Dr. Pardis Simon, Dr. Héloise Tissot

Laboratory: Unité de Catalyse et Chimie du Solide (UCCS, UMR-CNRS 8181), https://uccs.univ-lille.fr/axes-de-recherche/catalyse-heterogene/modspec

Related research project (international/national/regional): ANR NAPTIME

## **PhD Project :**

This PhD project, based at the University of Lille within the UCCS laboratory, focuses on the dynamic behavior of photocatalysts under reaction conditions. It addresses a key challenge in heterogeneous photocatalysis: the limited fundamental understanding of how photocatalysts undergo structural and electronic changes during operation. While traditional mechanistic models often consider the catalyst as a static material, photocatalysts are inherently dynamic systems. They respond rapidly to variations in temperature, pressure, gas composition, and illumination, factors that critically influence their catalytic activity and selectivity. Capturing these transient processes requires time-resolved studies under realistic working conditions.

The objective of the PhD is to develop a time-resolved experimental methodology using Near Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS), leveraging the capabilities of a newly installed laboratory-based NAP-XPS instrument at the Institut Chevreul (Lille University). This state-of-the-art setup, the second of its kind in France after the TEMPO beamline at Synchrotron SOLEIL, enables operando surface chemistry investigations.

As a model system, the research will focus on a photocatalyst composed of three components: zinc (as the active metal site), tungstophosphoric acid (a polyoxometalate mediating electron transfer), and titanium oxide (a light-harvesting semiconductor). This hybrid catalyst has shown excellent performance in two benchmark reactions: the selective photocatalytic reduction of  $CO_2$  into CO in the presence of water, and the oxidation of CH<sub>4</sub> into CO.

Time-resolved NAP-XPS measurements will be used to identify the structure and nature of active sites, monitor the formation of intermediate species, and follow the catalyst's evolution and potential deactivation during operation. Beyond chemical identification, the methodology will allow the characterization of reaction kinetics and the timescales associated with competing processes on the same surface, offering insight into how selectivity arises under dynamic conditions. The outcomes of this







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work will contribute to advancing operando spectroscopy techniques and support the rational design of more efficient photocatalysts for sustainable chemical transformations.

## **Candidate Profile**

We are looking for a highly motivated candidate with:

- A Master's degree (or equivalent) in chemistry, materials science, spectroscopy or a related field.
- Background in catalysis, surface science, or spectroscopy techniques.
- Strong analytical skills and ability to work in an interdisciplinary environment.

**Application Process:** Interested candidates should submit their CV, cover letter, and academic transcripts to Dr. H. Tissot (University of Lille) heloise.tissot@univ-lille.fr. Applications will be reviewed on a rolling basis until the position is filled.

Planned recruitment date: October 2025-january 2026

**Profile:** Master in Material Science, Physical Chemistry or Inorganic Chemistry with knowledge in Spectroscopy and/or material synthesis.

#### Additional remarks/comments :

The position for which you are applying is likely to be located in a "restricted area" within the meaning of article R. 413-5-1 of the penal code. If this is the case, your appointment and/or assignment can only take place after access authorization has been issued by the head of the institution, in accordance with the provisions of article 20-4 of decree n°84-431 of June 6, 1984.



