

**Post-doctoral position at LASIR with IFP Energies nouvelles
(IFPEN)
Chemical science**

**Applications of EPR techniques in studying the
active sites in Photocatalysis**

Photocatalysis is a sustainable approach to wastewater and air decontamination, to contribute to solve the energy issue by means of water splitting, photoreforming and photoelectrochemical processes or by reducing the atmosphere CO₂ concentration by photoconverting this greenhouse gas into valuable products. These photocatalytic reactions are initiated through band-gap photo excitations of semiconducting materials (such as TiO₂), generating excitons which are trapped in surface states during a sufficiently long time to allow electron transfer to adsorbed reactants, initiating reaction. All of these events involve single electron which, can be characterized by Electron Paramagnetic Resonance (EPR) spectroscopy.

EPR technique is highly sensitive and can be easily applied (in the conventional continuous wave, CW, mode) *in situ* or *operando* to characterize and identify directly the species during illumination and make the link between the nature of the active site and the photocatalytic activity (in the case of *operando* EPR). Besides, EPR can also be used in pulsed mode to get access to the chemical environment of the electron in order to better describe the structure of the active site. The other asset of pulsed EPR is that measurements are performed at low temperature which allow to study processes which are slowed down at 4K and cannot be studied at room temperature. Finally, EPR can also be used in imaging mode (such as MRI for nuclear spin) in order to better identify the localization of trapped holes and electrons. The objective of this post-doctoral internship is first to apply EPR spectroscopy in CW and pulsed mode on several semi-conductors designed by IFPEN in order to perform a detailed characterization of the active site. Complementary analyses such as XRD, UV-visible, infrared spectroscopies will be also done to determine the relevant parameters of the material that affect the photoreactivity. The second objective will be to develop a device which allows to perform *operando* EPR to better understand the working semiconductor and make directly the link with the activity. The last objective of this internship will be to apply EPR imaging in order to better understand the influence of the illumination on the number of trapped electron in the depth of the shaped material.

This internship in partnership with LASIR (Hervé Vezin's group) will be localized in Lille except a few stays in Lyon.

Keywords: EPR, Photocatalysis, *operando*, imaging

Academic supervisor	Dr, BEN TAYEB, Karima Laboratoire de Spectrochimie Infrarouge et Raman (LASIR) Lille
IFPEN supervisors	Dr BONDUELLE, Audrey, Chef de projet, Département Catalyse par les sulfures, audrey.bonduelle@ifpen.fr Dr DELPOUX, Olivier, Responsable du Pôle Structure Surface Réactivité, Département Caractérisation des matériaux, olivier.delpoux@ifpen.fr
PhD location	Laboratoire de Spectrochimie Infrarouge et Raman, Université des Sciences et technologie de Lille
Duration and start date	12 months from 1 st of may
Employer	CNRS
Academic requirements	Ph-D in EPR or in catalysis in relevant disciplines
Language requirements	Fluency in French or English, willingness to learn French