

Internship/PhD topic: “Piezocatalysis for wastewater remediation and green fuels production”

Lab: Structures, Properties and Modelling of Solids (SPMS)

Keywords: piezo-photo-pyro-catalysis, water cleaning, CO₂ reduction, H₂ production

Topics: ferroelectrics and related materials, piezo-photo-pyro-catalysis

Supervision: B. Dkhil

Quick summary of the internship/thesis project:

Piezocatalysis, a cousin of photocatalysis that uses light stimulus to trigger oxydo-reduction, is an emerging and complementary technology that harnesses the mechanical energy generated by cavitation process, issued, e.g., from an ultrasonic bath, to catalyze chemical reactions. It offers promising solutions for environmental and energy challenges, in particular for applications in wastewater treatment and green fuels production, both of which are crucial for sustainable development. At SPMS, we have recently developed several materials design approaches, based on ferroelectrics and related materials (oxides, polymers, 2D systems), to significantly increase the piezo- and the piezo-photo-catalytic responses, enabling to break down harmful substances in water, such as organic contaminants (e.g., PFAS), dyes, and pharmaceuticals (e.g., endocrine disruptors), with some record efficiency values [1,2]. In parallel to our research strategy, our findings on water cleaning are also exploited in the development of a startup, we are closely working with. In the realm of green fuels production, piezocatalysis has also shown promise in facilitating key reactions such as water splitting for hydrogen generation or CO₂ reduction for CH₄ production, offering a clean and sustainable alternative to fossil fuels.

During this PhD, the candidate will:

- Join a dynamic and internationally recognized team
- Elaborate materials design strategies and synthesize the materials
- Fully characterize the as-design materials and study their piezo-photo-pyro-catalytic performances using a broad set of techniques available at SPMS and at many partners at Paris-Saclay University and also in the world (USA, Slovenia, Luxembourg, Romania, Turkey, Tunisia...), as well as at synchrotron facility sources. Some stays at partners will be planned.
- Use modelling tools and/or collaborate with theoretician partners in the framework of a joint laboratory between SPMS and Physics department of Arkansas, USA.
- Contribute and participate to the work dissemination by writing papers and participating to international conferences and workshops

Main experimental techniques/simulation tools/methods:

in situ XRD, Raman spectroscopy, SEM/TEM, STEM, EELS/EDX, XPS, EPR, ferroelectric, dielectric, piezoelectric, pyroelectric measurements, piezo-photo-pyro-catalytic measurements....and possibly computational tools ranging from first- and second-principles calculations (DFT, Monte Carlo, Molecular dynamics) to finite elements methods

Bibliography:

[1] W. Amdouni et al., Adv. Mater. **35**, 2301841 (2023)

[2] W. Amdouni et al., Small **20**, 2406425 (2024)