PhD position

Institut Jean Lamour
Campus Artem Nancy

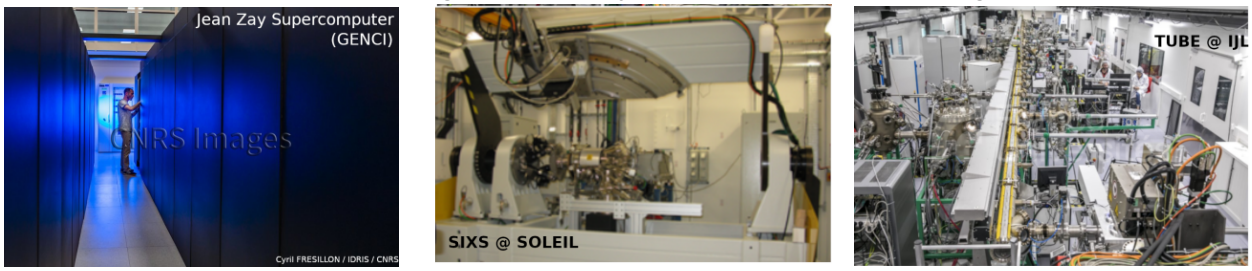
SIXS beamline
SOLEIL synchrotron, Saint Aubin

Surfaces of Intermetallic Catalysts: Surface Diffraction, Surface Science, and Density Functional Theory

Context : Greenhouse gas emissions drive climate change, leading to record-breaking temperatures, extreme weather events, and urgent calls for stronger climate action worldwide. Carbon dioxide is one of the most significant greenhouse gases. The primary objective of this project is to enhance the efficiency, sustainability, and environmental compatibility of CO_2 reduction to methanol through the development of advanced catalytic materials chosen among intermetallic compounds.

Intermetallic catalysts stand out for their exceptional stability and diverse atomic and electronic structures [1,2]. This versatility allows them to perform efficiently under harsh conditions, offering unique catalytic behaviors. Their structural diversity makes them ideal for tailoring high-performance catalysts for a wide range of chemical reactions, with strong potential in both industrial and environmental applications.

Objectives : This PhD thesis seeks to reveal fundamental surface structure–property relationships by bridging state-of-the-art experiments with predictive computational methods. The project will start with the investigation of (Ga,Sn)Pd_2 surfaces, using density functional theory (Fig. 1a), surface diffraction (experiments at SOLEIL, Fig 1b). The project will take place @ IJL (Fig. 1c).



(a) (b) (c)

Fig. 1 : Experimental and computational set-up available for the project : (a) EXPLOR High Performance Computing Center, (b) SIXS @ SOLEIL, TUBE @ IJL Nancy

Techniques/methods in use: Density Functional Theory, Surface X-ray Diffraction, Surface Science

Applicant skills: Strong background in chemistry, physical chemistry, materials science, or condensed matter physics. Experience in surface science, crystallography, Python programming, and/or quantum chemistry will be considered an asset. Excellent communication skills are essential, with the ability to work and exchange ideas effectively both orally and in writing. English speaking is required. The application should include a statement of research interest, a CV and Master's degree transcript

Supervisor(s) Emilie Gaudry (IJL), Alessandro Coati (SIXS SOLEIL). Interactions with Corentin Chatelier (CEA Grenoble) are also expected during the project.

[1] M Armbrüster, *et al.*, *Catalysis Reviews* (2013) 55 289
[2] F Brix *et al.*, *The Journal of Physical Chemistry Letters* (2020) 11 7672
[3] E. Gaudry *et al.*, *J. Mater. Chem. A* (2020) 8, 7422