

PhD position at IFP Energies nouvelles (IFPEN) Chemical sciences

Molecular simulations of mechanisms involved in the recycling of heterogeneous catalysts

Catalysts are very often made of active phases containing metallic elements (such as platinoids, cobalt, nickel...) considered as strategic or even critical because of the economic strain induced by a growing usage in multiple sectors (industrial chemistry, energy storage, electrolyzers, ...) Hence, the quest for a circular economy approach brings new scientific challenges, like the molecular scale understanding of the chemical phenomena involved in the key stages of catalytic metal recycling processes. In particular, within the context of heterogeneous supported catalysts, complex chemical mechanisms of metal leaching are used to recover the metal atoms from the surface of an oxide support, which knowledge remains rather empirical.

By focusing on the strategic case study of cobalt supported on alumina, the PhD project aims at rationalizing this knowledge by using quantum molecular modelling-based methods to address two major scientific challenges. Firstly, the chemical nature of refractory cobalt oxide species, formed in interaction with alumina sites during the thermal pretreatment step that precedes the leaching step, will be identified. Secondly, the chemical bonds (Al-O-Co) breaking mechanisms, involved during the leaching of the as formed oxide cobalt species, will be investigated. Various levels of molecular modelling will be employed: state-of-the-art Density Functional Theory, for the determination of the surface phase diagrams of supported cobalt oxides, molecular dynamics (biased or unbiased) either ab initio or using Machine Learning interatomic potentials for the identification of reaction mechanisms. The results will provide new insights into catalyst eco-design by an optimal choice of the alumina support's nanostructure.

This thesis will be integrated within the scientific program of the Common Research Laboratory ERACLECE between IFPEN and ENS de Lyon. The PhD student will benefit from the complementary expertise of the two laboratories on these systems and methodologies. Three previous relevant publications:

A. Hühn et al. Catal. Sci. Technol. 15 (2025) 878 <https://doi.org/10.1039/D4CY01152J>

R. Réocreux et al. Nature Communications 10 (2019) 3139. <https://doi.org/10.1038/s41467-019-10981-9>

K. Larmier et al. Angew. Chem. Int. Ed. 54 (2015) 6824. <https://doi.org/10.1002/anie.201502069>

Keywords: active sites, cobalt, alumina, quantum simulation, computational catalysis, molecular dynamics

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Doctoral School	Ecole Doctorale de chimie de Lyon (ED 206), ENS Lyon
PhD location	IFP Energies nouvelles (Solaize) and ENS de Lyon, France
Duration and start date	3 years, starting in autumn 2026
Employer	IFP Energies nouvelles
Academic requirements	Master degree in Catalysis, Theoretical Chemistry, Physical Chemistry, or Materials Science.
Language requirements	English level B2 (CEFR), willingness to learn French
Other requirements	Knowledge of computer and scripting languages are an important asset

To apply, please send your cover letter and CV to the Pascal RAYBAUD, pascal.raybaud@ifpen.fr

About IFP Energies nouvelles

IFP Energies nouvelles is a French public-sector research, innovation and training center. Its mission is to develop efficient, economical, clean and sustainable technologies in the fields of energy, transport and the environment. For more information, see [our WEB site](#).

IFPEN offers a stimulating research environment, with access to first in class laboratory infrastructures and computing facilities. IFPEN offers competitive salary and benefits packages. All PhD students have access to dedicated seminars and training sessions.