# PhD position at IFP Energies nouvelles (IFPEN)

Chemical sciences

# Theoretical Studies on the Adsorption of Phosphoric Acid on γ-$Al_2O_3$ at the Solid Liquid Interface

The ever growing increase in both, the demand of transportation fuels and the necessity to overcome environmental issues related to their combustion, has made catalysis a research topic of paramount importance in our society. Molybdenum sulfide based hydrotreating catalysts are one of the most efficient systems in the removal of unwanted nitrogen and sulfur in combustion fuels.

$MoS_2$ active phases are mostly supported by γ-$Al_2O_3$ and contains other promoters such as phosphorous. However, although this element is known to enhance the catalyst properties, it also renders the catalyst preparation difficult, since there is an interplay between many complicated chemical reactions at the Solid-Liquid Interphase (SLI), not fully controlled by experimentalists..

In this PhD project we aim at the characterization and simulation of the γ-$Al_2O_3$ impregnation by P by means of state of the art Ab initio Molecular Dynamics simulations (AIMD). These simulations will allow a comprehensive analysis of the acid-base properties of the modified support at the SLI, hence giving us insights on the preparation of $MoS_2$-P catalysts and on innovative ways to improve this process.

During her/his research, the applicant will use advanced AIMD techniques for the computation of thermodynamic properties at the SLI, use this thermodynamic data to compute the adsorption phenomena and speciation of the impregnation solutions, simulate the vibrational spectra of adsorbed species and the zeta-potential of relevant systems. Therefore, at the end of the PhD, the applicant will master some of the most advanced simulation techniques in this domain and will have a strong expertise that will allow the candidate to share results with peer experimental and theoretical researchers in the growing community of scientists working on SLI phenomena.

**Keywords**: Theoretical Chemistry, Molecular Dynamics, Heterogeneous Catalysis, Surface Chemistry, Solution Chemistry, Speciation.

| | |
|---|---|
| **Academic supervisor** | Dr. MICHEL, Carine, Laboratoire de Chimie, ENS-Lyon |
| **Doctoral School** | ED206 Chimie, Procédés, Environnement / www.edchimie-lyon.fr |
| **IFPEN supervisor** | Dr. CORRAL VALERO, Manuel, Dép. Génie des Matériaux Divisés manuel.corral-valero@ifpen.fr |
| **PhD location** | IFPEN and ENS Lyon, France |
| **Duration and start date** | 3 years, starting preferably on October 1, 2018 |
| **Academic requirements** | Master degree in Theoretical Chemistry, Physical Chemistry or Materials Sci. |
| **Language requirements** | Fluency in French or English, willing to learn French |
| **Other requirements** | Knowledge of computer and scripting languages are an important asset |

For more information or to submit an application, see theses.ifpen.fr or contact the IFPEN supervisor.

## 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 www.ifpen.fr.