

**PhD position in heterogeneous catalysis (70% experiments + 30% computation)**

**at École Centrale Lille, France, in strong collaboration with E2P2, Solvay, Shanghai**

*Starting date:*

As soon as possible

*Title:*

Machine Learning-Aided Experimental/Computational Design of Solid Catalysts for Hydrogen Peroxide Production

*PhD Advisors:*

Pr. Sébastien Paul (Ecole Centrale Lille), Dr. Jérémie Zaffran (CNRS)

*Description:*

A joint experimental–theoretical PhD position is available in the Unité de Chimie et de Catalyse du Solide (UCCS) lab, located at École Centrale Lille (France), within the framework of an industrial collaboration with E2P2 laboratory in Shanghai (China), a collaborative unit between Solvay industry and the CNRS (the National Scientific Research Center of France). The objective of the project is to provide in-depth understanding of the catalytic two-step autoxidation in hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) production, through anthraquinone hydrogenation. The experimental side of the program will be supervised by Pr. Sébastien Paul, while the computational aspect of the research will be handled by Dr. Jérémie Zaffran. High throughput (synthesis conditions such as temperature, reagent concentrations, reaction time, etc.) experiments combined with *ab initio* calculations (density functional theory, DFT) will be led together to get a deep understanding of usual noble metal-based catalysts used for anthraquinone hydrogenation, and to develop efficient earth abundant-based multi-metallic catalysts for that purpose. This work will be assisted by machine learning (ML) algorithms to speed-up the design of solid catalysts, predicting their activity and selectivity from a set of various computed and measured descriptors. Ultimately, such a research is expected to produce relevant tools to academics and industrials to address the reactivity issue in H<sub>2</sub>O<sub>2</sub> production and in several other areas.

**Profile and skills required:** We invite candidates with a completed Master of Science degree (or equivalent) in chemistry, physics or materials science. The successful candidate is expected to bring strong interest in the study of catalytic mechanisms and applying experimental and simulation methods (especially DFT) to solve problems of industrial and scientific interest. We further expect good written and oral communication skills in English, the ability to work independently, and cooperate with partners. French language skills will be an advantage. The main thesis supervisor will be Pr. Sébastien Paul. He is a Full Professor at Centrale Lille, a generalist engineer school, where he was the head of the Sciences of the Matter department between 2009 and 2016. After his PhD in Chemical Engineering at the University of Technology of Compiègne, France (1996), he was hired by Centrale Lille as Assistant Professor (1998). From 2004 to 2009 he was at the head of the “Chemical Engineering” Department, which then became the “Sciences of the Matter” Department. In 2009 he was nominated Associate Professor and in 2011 Full Professor. His research work is carried out at UCCS. More particularly he is the head of the VAALBIO group (standing for VALorization of ALkanes and BIOmass). Sébastien Paul is also the coordinator of the REALCAT project (‘Advanced High-Throughput

Technologies Platform for Biorefineries Catalysts Design'; 9.4 M€). He is involved in the development of a large variety of catalytic processes starting from compounds issued from the biomass or hydrocarbons in the frame of academic and industrial collaborations. Finally, he has supervised or co-supervised 16 PhD, 16 post-docs, is co-author of more than 60 scientific articles ( $h_{index}=20$  – more than 1500 citations), 17 patents, and more than 80 oral communications. He is also the co-founder of the start-up TEAMCAT SOLUTIONS.

The thesis co-supervisor will be Dr. Jérémie Zaffran. He is a full researcher at the CNRS since 2020. The CNRS is the main scientific center of research in France, including various different labs from mathematics to physics or chemistry. J. Zaffran obtained his PhD in 2014 at Ecole Normale Supérieure de Lyon, in France. Then, he stayed at the Technion—Israel Institute of Technology (IIT), a famous research institute in Israel for a three year postdoc position, followed by a first academic position at ShanghaiTech University in China. His area of expertise is related to computational catalysis, and more specifically to the elaboration of joint ML-DFT models to study catalytic properties of surfaces for various applications. All along his career, he has collaborated with many experimental and industrial groups from several countries in the world. He is the author and co-author of more than 25 peer-reviewed publications with a *h-index* of 16 and close to 1000 citations

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In France, a PhD is completed in three years and does not include teaching duties. The work-contract of three years includes French Social Welfare (basic health insurance, un-employment insurance, etc).

*Contact information:*

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*Application materials:*

- CV
- 1 page research statement
- 1-2 contact references

Please entitle you application mail "peroxide\_phd\_application"

*A few relevant links:*

**E2P2 Lab:** <https://www.e2p2l.com/en/who-we-are/contacts>

**UCCS Lab:** <https://uccs.univ-lille.fr/index.php/fr/annuaire/111-paul-sebastien>