International PhD offer in Chemistry

Green chemistry and biomass valorization

Contact information

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Keywords

- Green Chemistry
- Biomass and CO_2 valorization
- Heterogeneous catalysis
- Surface chemistry
- Computational chemistry
- Machine learning

Supervisors and advisors

Supervisor 1	Jeremie Zaffran	E_2P_2L	https://www.e2p2l.com
Supervisor 2	Benjamin Katryniok	UCCS	https://uccs.univ-lille.fr
Advisor	Philippe Sautet	UCLA	https://www.chemistry.ucla.edu/directory/sautet-philippe

Contract details

- *Duration*: 3 years
- *Salary*: ~1800-2300 €/month
- *Location*: Lille (France), potential research stay at UCLA (USA)
- *Starting date*: October 2024 (flexible)

Requirements

- Wet-lab experience (catalysis): *intermediate*
- Density functional theory calculation: *basics*
- Solid state and surface chemistry: *intermediate*
- Machine learning and scripting abilities: *basics*

Topic of the thesis

A PhD thesis, funded by the CNRS (The French National Center of the Scientific Research), under the joint supervision of UCCS (Unit of Catalysis and Chemistry of Solids, in Lille—France) and E_2P_2L (Eco-Efficient Products and Processes Lab, in Shanghai—China) labs, with the participation of UCLA (University of California, Los Angeles, in the USA), is currently available. The student will be based at Lille in France, with the possibility for a short-term research stay at UCLA to be organized (upon funding availability). While UCCS is a leading lab in the field of catalysis and an academic unit mainly involving the CNRS and University of Lille, E_2P_2L is a joint unit between academy and industry developing green chemistry processes and including many partners, especially the CNRS and Solvay (recently renamed "Syensqo") company. This thesis is based on an international collaboration and interdisciplinary research, bringing together experimental and computational chemistry with machine learning.

In the current environmental context and the shortness of fossil resources, biomass valorization and CO_2 disposal are a promising alternative. Glycerol is an abundant compound stemming from plants and green waste, and can be upgraded into high value-added products. In this project, we aim at finding an original process to achieve the direct carboxylation of glycerol through CO_2, to obtain glycerol carbonate, a green solvent of interest for industrials. While different processes have already been proposed to achieve this molecule, most of them involve toxic halide precursors and proceed through indirect routes. Here, in the framework of heterogeneous catalysis, we plan to develop computational tools, joining density functional theory (DFT) calculations and machine learning algorithms, to predict the reactivity of surfaces according to their chemical compositions,[1] in order to design efficient solid catalysts for the direct carboxylation of glycerol.

Our work will be based on recent publications demonstrating the promising activity of CeO_2, doped with some specific metals.[2] At the first stage of the project, the precise reaction mechanism will be elucidated, under a synergic investigation between experimentalists and theoreticians, with a special care on the effect of CO_2 coverage at the surface. Then a database correlating the nature and the ratio of several dopants with the surface activity will be elaborated, in order to fit an efficient machine learning predictive model. Finally, this numerical model will be used to screen the catalytic properties of a wide number of surface compositions, the most promising ones being ultimately validated by experiment.

[1] Zaffran, J.; Jiao, M.; Wischert, R.; Streiff, S.; Paul, S., *The Journal of Physical Chemistry C* **2024**, *128*, 5084-5092.
[2] Kulal, N.; Vetrivel, R.; Ganesh Krishna, N. S.; Shanbhag, G. V., *ACS Applied Nano Materials* **2021**, *4*, 4388-4397.