PhD Offer

Joint computational-experimental design of solid photo(electro)catalysts for waste CO_2 mediated aromatic molecule carboxylation

Expected starting date

September 2023 (Flexible)

Place

UCCS (Lille in France) in strong collaboration with E2P2L (Shanghai in China)

Supervisors

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Keywords

Photo(electro)catalysis, CO_2 valorization, Density Functional theory, Machine Learning

Abstract

A PhD position is available at UCCS (Unité de Catalyse et de Chimie du Solide) lab in France, in strong collaboration with E2P2 Lab in China. E2P2L is a joint unit between various academic partners, especially the CNRS and Solvay Company. This structure is specialized in the development of eco-efficient processes for the production of many kinds of chemicals. **CO_2 is an important industrial waste** responsible of major environmental issues. Various strategies have been investigated to **valorize it into valuables**. Here, we propose to use it to functionalize aromatic molecules, upgrading them into high value-added compounds. Indeed, aromatic derivatives are present in many fields of the chemical industry, from pharmaceutical products to polymers and plastics materials, also including aromas and fragrances. However, due to the aromatic ring high stability, the synthesis of such chemicals is not easy, usually involving high temperature processes and polluting precursors. In this project, focusing on a few aromatic molecules of interest for Solvay industries, we intend to develop an eco-friendly method of preparation, based on CO_2 **photo(electro)reduction** and bio-based aromatics. This technique is known to give access to a wide variety of product species, operating at room temperature and in soft chemistry conditions. Considering their high photo(electro)activity, hydrotalcite materials are catalysts of choice for such an application. They present a layered structure, with partially hydrogenated metal oxide layers stacked on each other. Since they can be easily exfoliated, their reactivity is strongly dependent on their chemical composition and on the support. In this work, we aim at combining computation and experiment to design efficient photo(electro)catalysts for aromatics carboxylation. **Density functional theory (DFT) calculations**, aided by **machine learning** algorithms will be first used to perform a fast and systematic screening of various hydrotalcite and support compositions. Then, the most promising formulations will be tested and validated by experiment. Above the development of ecological processes of interest for the industry, this work is also expected to have significant implications in the academic area. Indeed, our strategy combining machine learning and DFT can be decisive in the future to speed up quantum calculations, hence rendering easier the systematic study of surface reactivity.

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