POSTDOC OFFER

Computational design of efficient metallic catalysts for plastic waste recycling:

A joint *ab initio* calculation and machine learning project

Plastic wastes are a major issue for our modern societies. Indeed, due to their outstanding life expectancy and their poor biodegradability, they are a significant source of environmental pollution and toxic emissions. A challenging alternative is to recycle plastic wastes in value-added products, relevant to chemical industries. In the context of a joint research program (ANR PLASTILOOP 2.0) between E2P2L lab and Solvay industries, a biochemical method is already investigated to decompose polymers in their elementary constitutive units. However, such monomers must be functionalized, *a posteriori* in order to be used by industry and transformed in various other organic materials.

Here, we are proposing a postdoctoral project to design efficient metal solid catalysts to address monomer functionalization. This work will be mainly computational, combining density functional theory (DFT) calculations and machine learning (ML) tools. The ultimate goal is to elaborate an ML tool enabling fast predicting of surface reactivity regarding several key reactions such as oxidation/hydroxylation and carbonylation/carboxylation. The method is based on the "descriptor approach" and consists in estimating the key reaction intermediate energies from a set of descriptors, without explicit DFT calculations. The descriptors can be of different natures, geometric, thermodynamic or electronic, and are in general easily reachable. Hence, providing an accurate predictive ML model is known, it is possible to plot energy diagrams of a specific reaction pathway at various surfaces, hence allowing a fast screening of a considerable number of catalytic surfaces in a very short time.

The first step of the project will aim at constituting a database of descriptors and DFT calculated energies for several reactions at some noble metals (Rh, Pd, Pt, Ru), known for they activity and selectivity. Then, at the second stage of this program, accurate predictive algorithms shall be established on the base of this data. And finally, at the last stage of this work, such models will be applied to perform a fast screening of multiple mono- and bi-metallic surfaces, hence providing guidelines to experimentalists in their catalyst synthesis.

All along this project, VASP software will be used for DFT calculations, and mainly Python and R will be necessary for ML. The expected candidate will have a good knowledge in DFT computation applied to surfaces, and a previous experience is required in machine learning. The project will take place at Centrale Lille, a prestigious Engineering School in France for a total duration of two years. E2P2L lab is a joint unit including various French and Chinees partners, especially CNRS, the French National Research Center and UCCS, an important lab specialized in catalysis and solid state study in Lille.

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