

PhD position in Computational Chemistry

at ENS Lyon in strong collaboration with E2P2, Solvay, Shanghai

Starting Date: September-October 2018

Title: Ab initio simulations of catalytic transformation of biomass-derived molecules to building blocks of industrial interest

PhD Advisor : Dr. C. Michel

Description: One PhD position is available in the group of Dr. Carine Michel in the laboratory of computational chemistry of ENS Lyon (France). The research will take place within the framework of an industrial collaboration with SOLVAY's E2P2 laboratory in Shanghai (China), and the University of Poitiers (France). The objective of the project is to provide in-depth understanding of the catalytic transformation of biomass-derived molecules to building blocks of industrial interest, using density functional theory (DFT) and other techniques (kinetic monte carlo, force-field based techniques to describe the catalyst-solvent interface), as appropriate. Both supported metal catalysts and homogeneous catalysts will be investigated and compared. The modeling study will be strongly aligned with experimental work carried out at partners, and it will involve frequent interaction with industrial stakeholders, including stays at SOLVAY's facilities in Shanghai.

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 applying simulation methods to solving problems of industrial and scientific interest. Previous experience in simulation or computer programming is not required, but is clearly a plus. 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.

ENS Lyon has a strong track record in the modeling of heterogeneous catalysts using periodic DFT and is currently developing novel strategies to describe the solvent/catalyst interface. This top-ranked French university is located in the beautiful city of Lyon in the south of France (UNESCO Heritage Site), an internationally recognized center for Catalysis.

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).

Please send your application (including a 1-page motivation letter illustrating your research interests, CV, and contact information of at least two references) to Dr. Carine Michel (carine.michel@ens-lyon.fr). Since the expected starting date is soon, priority will be given to candidates available as soon as possible.

Selected References :

R. Réocreux and C. Michel, "Rational Design of Heterogeneous Catalysts for Biomass Conversion—inputs from computational chemistry," *Curr. Opin. Green Sus. Chem.*, vol. 10, pp. 51–59, 2018.

S. N. Steinmann, P. Sautet, and C. Michel, "Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models," *Phys. Chem. Chem. Phys.*, vol. 18, no. 46, pp. 31850–31861, 2016.