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Laboratoire de Chimie – UMR CNRS 5182

PhD Position

Multiscale Simulations of bi-functional catalysts

Context

This project is in collaboration with two American partners and is sustained by the ANR and the NSF agencies as an international project. Two positions are opened at the Laboratoire de Chimie of ENS- Lyon, one PhD position and one post-doc position.

Project

In sustainable chemistry, the switch towards biomass-based resources requires to develop new catalysts for new reactions. Although simulation could be an excellent tool for the design of novel catalysts, the large size of the reaction network and the solvated conditions render brute force first principle calculations hopeless. In this project, we propose a novel multi-level and multi-scale approach to solve this issue and explore the complex pathways of the catalytic transformation of sugar molecules extracted from biomass using bifunctional catalysts. The complete reaction pathway, with hundreds of reactions, will first be mapped with a simple, approximate but very fast force-field approach. Kinetic simulations on that reaction array will reveal the few important elementary steps that need to be accurately calculated. The barriers for these steps will be estimated with state of the art hybrid multi-scale free energy simulations, including full treatment of the solvent.

The PhD student is expected to generate an extensive database of geometries and energies using Density Functional Theory in collaboration with a student working at the University of Delaware. This database will be used to fit a fast but approximate computational method (classical force field and semi-empirical approach). The database will also be used to parameterize fast screening methods based on scaling correlations and Bell-Evans-Polanyi (BEP)-type relationships. The PhD student will then be involved in the kinetic simulations and the multiscale free energy barriers simulations.

Applicant

The successful applicant is expected to have strong background in physical chemistry and strong interest in the application of computational modeling techniques to study chemical reactivity and spectroscopies. A Master degree is required. The student will be supported for 3 years to work towards a Ph.D. degree in Chemistry within the graduate program of the Universite de Lyon (www.edchimie-lyon.fr/). He/she will also benefit of the Ecole Normale Supérieure de Lyon environment (www.ens-lyon.eu).

Contact

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