ÉCOLE NORMALE SUPÉRIEURE DE LYON

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Laboratoire de Chimie – UMR CNRS 5182

PostDoc Position (1 year)

MUSIC - Multiscale Simulations of bi-functional catalysts

Context

The project MUSIC is conducted in collaboration with two American partners (D . Vlachos and A. Goetz) 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 (1 year)

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 PostDoc fellow will be involved in the developement of force field and DFT-B parameters dedicated to the project (Pt/water and Pt/sugar interactions) in strong collaboration with A. Goetz (San Diego). A stay in San Diego is planned.

Applicant

The successful applicant is expected to have strong background in physical chemistry and strong interest in the developement of computational modeling techniques. A PhD in theoretical chemistry degree is required. The PostDoc will be supported for 1 year with a net salary of around 2000€/month, possibly higher depending on the working experience. Lyon's listing by UNESCO as a World Heritage Site gives recognition to the long history heritage of the city. It is also recognized for its gastronomy and last but not least, Lyon is a vivid city with thousands of students.

Contact/Application

To apply, please send a detailed CV and the names and addresses of at least

three references to :

Dr. Carine MICHEL & Dr. Philippe SAUTET

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www.ens-lyon.fr/CHIMIE