

**PostDoc position in Computational Chemistry
at ENS Lyon in collaboration with Total, France**

Starting Date: as soon as possible.

Title: Understand action mechanism of detergent additives by molecular simulation

Advisors: Dr. C. Michel, Dr. S. Steinmann, Dr. S. Loehlé

Description: One postdoc position of 18 month is available to work with Dr. Carine Michel & Dr. Stephan Steinmann in the laboratory of computational chemistry of ENS Lyon (France). It is financed by Total.

The development of high performance fuel is an important challenge in the optimization of engine work, energetic consumption decrease, etc. The knowledge of how fuel additives are working is becoming crucial. Among additives that are used in the formulation, detergents are very important in the 'clean up' process of the engine. Relying on molecular simulations (DFT and DFT-B), the objective here is to obtain a better understanding at the nanoscale of the action of detergents toward soot and metallic surface in order to identify key parameters and to screen molecules for highest efficiency. This will enable to design optimal detergents. Frequent exchange with Total will be needed and parallel experimental studies at Total will be performed in order to validate the theoretical results

We invite candidates with a completed PhD degree (or equivalent) in computational 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 and would be creative, curious, initiative taker and open-minded person. Strong knowledge of DFT or semi-empirical methods are required, with preferentially both and some knowledge of classical simulations and physical-chemistry of interfaces is a plus. Interest and ability for scripting with Python will be appreciated. We further expect good written and oral communication skills in English, the ability to work independently, and cooperate with partners.

ENS Lyon has a strong track record in the modeling of heterogeneous catalysts using periodic DFT and is currently developing novel strategies to describe solid/liquid interfaces. This top-ranked French university is located in the beautiful city of Lyon in the south of France (UNESCO Heritage Site). The work-contract of 18 month includes French Social Welfare (basic health insurance, unemployment 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) or Dr. Sophie Loehlé (sophie.loehle@total.com).

Selected References :

Steinmann*, S. N.; Sautet, P. & Michel, C. "Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models" PCCP, 2016, 18, 31850-31861

Steinmann*, S. N.; Ferreira de Morais, R.; Götz*, A. W.; Fleurat-Lessard, P.; Iannuzzi, M.; Sautet, P. & Michel, C. "A Force Field for Water over Pt (111): Development, Assessment and Comparison" JCTC, 2018, 14, 3238-3251