Institut de Chimie des Milieux et Matériaux de Poitiers

Post-doctoral position available

DFT prediction of the reactivity and selectivity of the catalytic alkylation of furfural with alkyl alcohols

Starting: Autumn 2022
Duration: 12 months
Location: Applied Quantum Chemistry group - Catalysis and unconventional media (Mediacat) Team, IC2MP, Poitiers - https://ic2mp.labo.univ-poitiers.fr/la-recherche/mediacat/
Contact: Dr. Frédéric Guégan, frederic.guegan@univ-poitiers.fr

Project:

Furfural is a molecule of particular interest, as it is one of the rare potential platform chemical to be produced in large scale from biomass waste. It is currently used in several end-use industries (paints and coatings, agriculture…), although only a limited chemical diversity is now at hand. Expanding the latter in an eco-efficient manner is thus of interest.

Within the CATALFUR ANR project, we propose to combine experimental and theoretical studies to evaluate the potential of the catalytic alkylation of furfural derivatives with various alkyl alcohols.

The objective of this post-doctoral project is thus to evaluate the reactivity and selectivity of the target reaction, for a series of furfural derivatives and under acidic conditions. The recruited fellow will thus compute reaction profiles for the various possible reactions (screening reactive position on the furfural derivative), at the DFT level, first on simple models (*e.g.* methylfuran and methanol), and then on more realistic ones. The detailed list of reagents will be discussed with the experimental team within IC2MP (F. Jérôme, DR CNRS). Rationalisation of the observed selectivities/reactivities will be sought on the basis of electron-density and MO-based descriptors (conceptual DFT, NBO, ELF, QTAIM), and the obtained results will be confronted to experiments.

Candidates:

Candidates should have a PhD in Chemistry, with experience in computational chemistry and molecular modelling. Knowledge in electronic structure analyses (ELF, NBO, CDFT, QTAIM…) will be an advantage, as well as previous experience in interacting with experimentalists.

Candidates are invited to send a CV and two recommendation letters to F. Guégan (frederic.guegan@univ-poitiers.fr).

Position details

The CNRS post-doctoral position is available for 12 months, starting from autumn 2022. Net salary (per month) ranging from 2141€ to 3050€ depending on experience (health insurance fully covered). The project is funded by the ANR (ANR-21-CE43-0005, https://anr.fr/Project-ANR-21-CE43-0005). The recruited fellow will be granted access to local computational facilities (IC2MP cluster, regional mesocenter), as well as national ones (applications to GENCI). Opportunities to diversify their computational/theoretical chemistry skills will also be proposed (yearly training actions within the frame of the Western Section of the research federation Themosia).

Last but not least, Poitiers is a nice small city, with an easy access to Paris (~1h10 by TGV), the Atlantic Ocean and the Southwest of France.