Post-doctoral position at IC2MP, Poitiers (France)

Reactivity of water and radicals at crystalline cellulose surfaces

A 1 year postdoc position in the field of QM/MM simulations of water-cellulose interfaces is available at the Theoretical Chemistry group of Dr. Gilles Frapper at IC2MP (U. Poitiers - CNRS, France). The position is funded by the ANR CelloPlasm. The net salary will be around 2.3 k€ per month (depending on experiences). Partly health insurance (70% in charge of French Social Security), and a social housing support are a plus.

Project: the postdoc work will consist of applying DFT and/or QM/MM molecular dynamics simulations to the chemical reactivity at water liquid/crystalline cellulose interfaces. Modelling of the solvation effects will be considered as the water-cellulose interactions play a crucial role in the depolymerization process of cellulose. Activation of C-O bonds by water molecules and radicals (ex. OH excited state in plasma) will be studied. Periodic systems are envisaged, *ie* use of DFT codes as CP2K, VASP, …

Desired qualifications: solid background in physics and chemistry and understanding of quantum mechanics with experience in computational material modeling at the atomic scale and interfaces; requirements: expertise in the modelling of reaction pathways at surfaces through AIMD simulations, experience in computational tools (elaboration of scripts in bash, python,...). Knowledges in QM/MM approaches to model liquid or gas/solid interfaces will be appreciated (CP2K experiences, …); possess a solid track record of research accomplishments. Excellent communication skills in English, both verbal and written, are required.

How to apply: Applications should be sent to gilles.frapper@univ-poitiers.fr as early as possible with the mail subject " **Post-doc position**". The application should include:

- a detailed Curriculum Vitae, including a transcript of PhD diploma,
- a cover letter describing why you should be considered for this position, answering the following questions: What QM/MM modeling technique(s) do you have expertise in? What liquid or gas/solid interfaces did you look at? What is your experience with molecular dynamics, transition state characterization (if any)? When might you start?
- a list of three professors who have supervised you in M.Sc. and PhD research projects or current employers and who are willing to provide a letter of recommendation.

All documents should be in PDF format and written in English. A short-list of candidates will be made, who will be contacted for an interview over Skype (In CV, Skype address must be included).

The selected candidate is expected to start ***asap*** and before 31 december 2018.