

Plasticization mechanism of bio based materials: a molecular modeling approach.

Postdoc, molecular simulation, Rhodia, Lyon, FR

Description of the context of the post-doctoral offer:

The post-doctoral position presented here is part of collaboration between Rhodia Technology Center in Lyon (CTRL) and the CNRS laboratory CERMAV in Grenoble.

Description of the project:

Cellulose based polymers, like cellulose acetate, cannot be easily processed (through classical processing tools like extrusion and injection molding) without the help of plasticizing additives. Depending on the amount added and the quality of the interactions involved, the global effect of these additives can be very different and can even sometimes prevent the polymer from being processed. Consequently it is of prior necessity to identify and classify these systems in terms of the interactions they can develop with the polymer matrix.

Description of the work proposed within the post-doctoral position:

In order to get a better understanding of these interactions, we propose a twofold project based on atomistic simulations.

- Calculation of the enthalpy of mixing between model compounds of cellulose acetate and different candidates for plasticizing additives. Even though the enthalpy of mixing of synthetic polymer models can be experimentally accessible (mainly with micro-calorimetry), the experimental approach would have to be developed in the case of sugars which justifies the simulation strategy employed here. In order to investigate the structural diversity of cellulose acetate (acetylation degree, position of the acetylated group on the glucopyranosic cycle ...) different molecular models will be used (mono or disaccharides with various substitutions).
- Molecular dynamics of cellulose acetate models (with and without plasticizers) at different temperature in order to calculate thermo-mechanical transitions and their evolution with the amount and nature of additives. The identification of the amount of excess free volume induced by the plasticizer will be a key parameter in these simulations. For these additives, we will define the role of both sterical and energetic interaction on this phenomenon.

Practical details of the post-doctoral position:

- The candidate will perform the calculation through the use of commercial simulation codes, essentially Materials Studio from Accelrys. He will be based on the Research Centre of Rhodia in Saint-Fons, in the neighborhood of Lyon, France and will have a close contact with the CERMAV in Grenoble (possible travel there).
- The candidate must have a PhD either in computational physics/chemistry or in polymer physics/chemistry with an emphasis on numerical simulation methods.
- Net salary / month: 2200€/month.
- To apply to the present offer, please send your resume and have recommendation letters sent to the following persons :
Jean-Yves DELANNOY (RHODIA, +33(0)472896383, jean-yves.delannoy@eu.rhodia.com), Caroll VERGELATI (RHODIA, +33(0)472896925 caroll.vergelati@eu.rhodia.com), Karim MAZEAU (CERMAV-CNRS, +33(0)47603763933, karim.mazeau@cermav.cnrs.fr),
- Do not hesitate to send any questions concerning this post-doctoral offer.