LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisor(s)**
Fernando Lugo	Maarten Sabbe Paul Van Steenberge

Understanding aqueous phase radical polymerization processes through computational chemistry

Aim

Studying polymerization reactions in aqueous phase in order to deepen the knowledge of the process in environmental friendly media, focusing on rare events polymerization, to provide accurate data for further development of kinetic models through the use of first principle models and DFT.

Justification

Polymer materials are indispensable in modern society and contribute to many high-end applications such as 3D printing for tailored medical applications as implants or external protheses. These materials have to be carefully synthesized to provide the necessary structural properties, while at the same time be biologically compatible with the patient's tissue. To achieve these special properties detailed control of the polymer structure is necessary; predicting this structure requires accurate modelling of the polymerization reactions. This process starts with obtaining rate coefficients of the main and secondary reactions to be able to construct a highly detailed model. For this matter, the first principle methods provide a computational procedure with rather small effort, and they allow to determine rate coefficients that are experimentally very difficult to access, such as those of some side reactions with a large effect on the resulting polymer structure.

In principle, the tailored polymers with detailed structures can be synthesized by radical polymerizations, and normally, these reactions are carried out in solvents. Due to environmental regulations, new feasible procedures have to be developed to fulfil the demand of industrial size production of these materials. This is the reason behind the proposal of using aqueous media for the reactions, hence the importance of acquiring accurate data to be able to construct better models.

Program

1) Understand reactivity of the propagation and rare events of different chemistries in aqueous phase
2) Obtaining rate coefficients of propagation and rare events for the polymerization of different chemistries through DFT methods and modelling the condensed phased interactions through the COSMO-RS model.
3) Evaluation of the obtained kinetic data in existing kinetic models and comparison with the available experimental data