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Understanding aqueous phase radical polymerization processes through first principle methods

Aim

Obtaining rate coefficients of propagation reactions in aqueous phase in order to better understand reactions in environmental friendly media, mainly focusing on acrylamide and acrylonitrile polymerization reactions.

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 reactions of each chemistry intended to study. 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) Obtaining rate coefficients of propagation reactions of the polymerization of acrylamide and acrylonitrile through first principle methods in aqueous phase.
2) Assessment of the calculated rate coefficients in comparison with the available experimental data.
3) Accurately modelling the kinetics of these reactions using available micro-kinetic models to simulate microstructural characteristics.