Multiscale modelling of heterogeneous chemical reactions

Summary

Chemical reactions in heterogeneous solid-liquid systems will be modelled using a combination of quantum chemistry, molecular mechanics and fluid dynamics approaches. Systems relevant for carbon dioxide capture and storage will be the primary subject of research.

Research field:	Chemistry and biotechnology
Supervisor:	Toomas Tamm
Availability:	This position is available.
Offered by:	School of Science Department of Chemistry and Biotechnology
Application deadline:	Applications are accepted between May 03, 2021 00:00 and May 31, 2021 23:59 (Europe/Zurich)

Description

Many chemical reactions occur in heterogeneous environments, in particular on the solid/liquid boundary. Heterogeneous catalysis, absorption and desorption are common examples. The solid phase is not necessarily an ideal surface, but may be a nanoparticle or a larger grain, possibly immobilized on an inert carrier. Porous materials reacting with liquids or dissolved molecules are also included here. Such reactions are frequently diffusion limited, with the flow of liquid phase restricted by size of pores and inter-grain channels. Capillary effects also play an important role.

As the reaction proceeds, the solid grain may undergo physical changes, such as accumulation of primary or side products, clogging of pores, crack formation, etc. Models of such processes involve a combination of chemical and physical phenomena and combine approaches on molecular and microscopic scales. In certain situations, such as chemical reactor design, macroscopic level mixing may also be included.

In the proposed doctoral project, the student will develop methods of multiscale modelling of chemical reactions in heterogeneous environments, with feedback through change of properties of the solid phase due to physical and chemical changes therein. Potential applications include carbon dioxide capture and storage with use of silicate, carbonate and other sorbents, and CO_2-rich aqueous solutions as well as supercritical CO_2 as the liquid phase. The surface reactions will be modelled using traditional computational chemistry techniques, primarily density functional theory. Results from these calculations will be scaled up via use of molecular mechanics.

Computational fluid dynamics will be used to model liquid flows. Due to limited availability of software specifically tailored for this kind of modelling, it is expected that the work will involve significant amount of programming in order to implement the combined methods, interface diverse software packages and process and visualize the results.

Applicants should fulfil the following requirements:

- Master's degree (or equivalent) in chemistry or related field, with experience in computational chemistry (quantum mechanics and/or molecular mechanics methods)
- Familiarity with computational chemistry software (eg Gaussian, Turbomole, Orca, Gromacs, Tinker)
- Strong programming skills (C, C++, Fortran and/or Python)
- Experience in using computational fluid dynamics methods is a plus

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