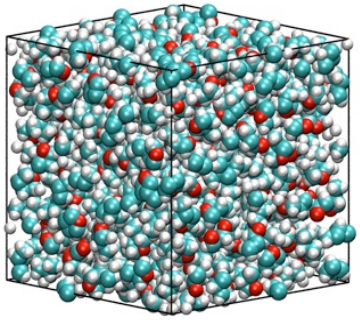
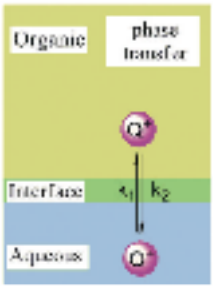
DIPLOMARBEIT/MASTERARBEIT PROJECT AVAILABLE

Multiphase Catalysis for the transformation of bio-renewables: Investigation on Transition-Metal Catalysts in Ionic Liquid-Organic Solvent Interface

Next-generation chemical processes will require a sustainable separation of reaction products from the reaction medium. In this respect, the application of multiphase systems represents an innovative approach, especially when ionic liquids for the transformation of highly polar bio-renewables are incorporated. Selective modifications of the ligand structure incorporated in the organometallic catalyst, enable us to control the diffusivity of the catalyst within the organic and ionic liquid phases, and additionally allow control of the catalyst location in the interphase.



This project will use molecular simulation methods to study a prototypical example of an organic-ionic liquid solvent system (e.g., hexane-[BMIM]Cl):



- What is the structure of the interface between these two liquids?
- What is the diffusivity of a catalyst molecule in the organic and ionic liquid phases?
- When placed at the interface between the two liquids, where does the catalyst particle go?
- How do changes in the structure of the catalyst molecule, or the ionic liquid, affect the behavior and positioning of the catalyst?

Students interested in this project should have:

- Basic familiarity with physics, thermodynamics, and physical and organic chemistry
- Experience with the Linux operating system
- Familiarity with programming in Fortran, C/C++, or another high-level language (knowledge of scripting languages such as Perl or Python is especially recommended)
- Prior experience with numerical modeling and simulation is desirable

For more information on this project, please contact:

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