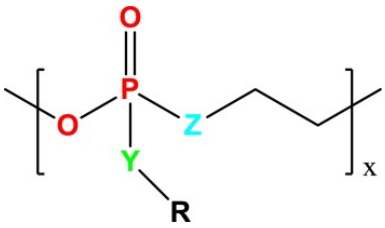
MSc Project

Molecular Modelling of Ion Permeability and Transport in Polyphosphoester Membranes

Introduction. Large-scale energy storage is needed in stable power-grid management and the integration of renewable sources. The redox *flow battery* (FB) provides a unique combination of high efficiency and long cycle life. The key FB components are redox pairs (usually vanadium ions), electrodes and a separating polymer membrane to prevent the electrolytes to cross mix and to transfer ions. High-quality, low-cost materials are vital to achieve large-scale acceptable FBs; ion chemistry and transport are the key factors in determining the final FB performance. In this project we use molecular-dynamics simulations to provide fundamental physical insights into the ion transport in *novel, polyphosphoester membrane for FB*.



(Y=O, CH2, NHR, NR2; Z=O, NH, CH2)

Polyphosphoesters (PPEs) are a class of (bio)degradable polymers with high chemical versatility and functionality. The linkage patterns and functionalization possibilities that further broadens the possible applications of PPEs ranging from biomedical to flame retardant materials. In the present project we think about the functionalization which will promote the cation (Li- or hydronium ions) transport and conductivity in final material. The applications are for the novel perspective membrane for new battery (Li-ion or flow).

Goal. In this Master project the student will carry out atomistic large-scale molecular-dynamics. The MSc. project should help to unravel the connection between the microscopic structure and structural changes in PPE membrane that explain their cation conductivity characteristics.

Task. In the groups of prof. dr. Lyulin and prof. dr. Wurm, the synthesis of the PPE membranes and molecular-dynamics (MD) simulations will be performed. The main task will be to carry out molecular simulations, and to perform the analysis of their results. The Gromacs/LAMMPS MD software package will be used for these purposes. We will use our own compute clusters with in total ~1000 CPU cores and Infiniband QDR interconnect and will apply for access to national supercomputer facilities of SurfSARA.

Requirements. Expertise in programming and knowledge of programming language(s) (as, for example, Python, Fortran,C,C++, Matlab, Mathematica, etc) and interest in performing numerical simulations.

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