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GRK 2516 Soft Matter Seminar

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Research seminar of the DFG Research Training Group GRK 2516 (https://grk2516.uni-mainz.de).

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Molecular dynamics simulations of water and acetonitrile mixtures in external electric field

Electrochemistry is a discipline promising to advance material science towards more environmentally friendly and sustainable technologies for energy solutions. Electrochemical systems are usually composed of interacting complex molecules, making understanding collective effects limited for macroscopic experiments. Computer simulations offer a way to obtain insights in silico. In particular, molecular dynamics simulations, with detailed interatomic potentials, allow us to rationalize experimental results by exploring the dynamics of physical systems through virtual experiments. In the first part of this thesis, I systematically review molecular dynamics simulation methods providing the foundation for preparing our physical system in silico. I introduce the basic principles of an all-atom molecular simulation within the framework of statistical physics and discuss in detail the treatment of electrostatic interactions and the importance of dielectric boundary conditions. In the second part of this thesis, I present our molecular dynamics study of a liquid system composed of water and acetonitrile molecules and their response to an external electric field. This mixture exhibits unique properties, including a distinctive electrical conductivity detection in the absence of an electrolyte in novel electrolysis flow cells. However, the underlying physical mechanism behind this phenomenon remains unknown. As a first step to understanding this mechanism, this work focuses on the bulk system structure and how a macroscopic external electric field influences its properties.

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