

## MD Simulations of Diffusion coefficients in electrochemical cell for Electrofuel synthesis

### Description:

The project “Fundamentals of ElectroFuel Synthesis for Aviation” is combining experimental and molecular dynamics studies for the systematic and tailored generation of liquid aviation fuels. Therein, MD simulations are performed to study various properties of the reaction system of an electrochemical cell which is used for hydrogenation of furfural and 5-HMF. This electrochemical cell contains two metal electrodes and specific electrolyte composition in between, as shown in the figure below.

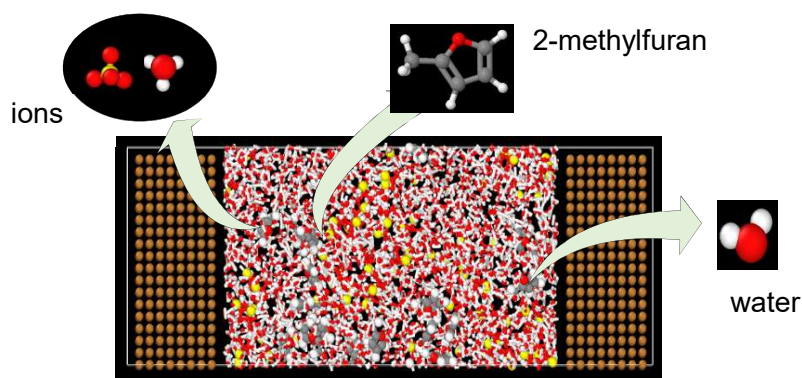


Fig. 1. The configuration of an electrochemical cell containing water, ions and 2-methylfuran with the copper electrodes

A systematic study on the diffusivity of different molecules in the electrochemical cell is essential to understand the behavior and impact of the electrolyte.

Therefore, in this work, the LAMMPS software shall be used to calculate the diffusion coefficients of different moieties in the electrochemical system in the bulk phase and near the electrodes. The diffusivities will be computed for various working conditions of the electrochemical cell, e.g., various voltages, different electrolyte compositions, different electrodes.

### Requirements

- knowledge in molecular dynamics simulations
- experience in using the MD simulator LAMMPS

### Contact information

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