Electrofuel Synthesis for Aviation

Fundamental Investigation of Electrofuel Synthesis by Molecular Dynamics Simulations

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In Short

- Studying the structure and dynamics of the reaction systems of the hydrogenation and hydrodeoxygenation of furfural and 5-hydroxymethylfuran (5-HMF) in a polarizable electrochemical cells by MD simulations;

- Investigating the effect of electrode material, electrolyte, and applied voltage;

- Combining the results from experimental studies and findings from molecular simulations to provide recommendations for optimal synthesis process based on the molecular structure.

The project C2.1, *Fundamentals of Electrofuel Synthesis for Aviation*, is part of the interdisciplinary SE^{2}A cluster of excellence at TU Braunschweig, in which technologies for sustainable and environmentally friendly aviation are studied. The objective of the project C2.1 is to lay the scientific foundation for producing aviation fuels via electrosynthesis.

Among all sources of greenhouse gases emission, aviation is one that has a great climate impact [1]. Therefore, it is a global objective to find methods and technologies for significantly reducing emissions of aviation. An important way to decrease the flight emission is to change the type of energy resources of the flight vehicles. In this regard, two alternatives to fossil fuels are 2-methylfuran and 2,5 dimethylfuran which have high efficiency and low hydrocarbon emissions [2].

The synthesis of these fuels, so-called electrofuels, from hydrogenation and hydrodeoxygenation of furfural and 5-hydroxymethylfuran (5-HMF) were widely investigated [3–5]. A reaction scheme for hydrogenation of furfural on a metallic electrode is shown in Figure 1. As shown in this figure, the 2-methylfuran (2-MF) can be achieved directly by hydrogenation of furfural or after an intermediate step by producing furfuryl alcohol (furol). However, during the hydrogenation process of furfural and 5-HMF, other species such as furan, tetrahydrofurfural or 2,5-Bis(hydroxymethyl)furan can be obtained, which are not desirable as an alternative fuel. Therefore, the production of these electrofuels with high yield

and efficiency needs a systematic and efficient procedure for achieving a sufficient amount of these fuels to be utilized in the aviation industry.
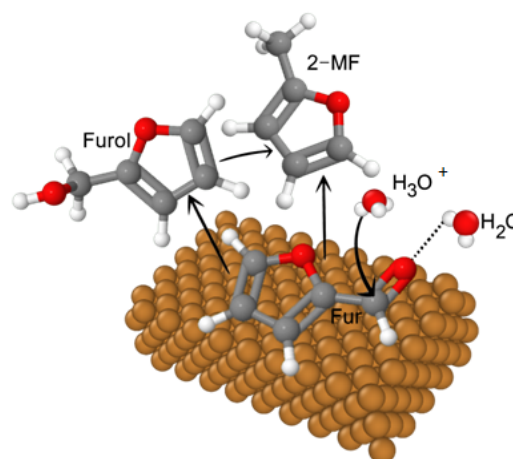

Figure 1: *Scheme of furfural (Fur) hydrogenation to 2-methylfuran (2-MF) or furfurylalcohol (Furol) on a metalic electrode.*

Within this context, in this study, the molecular dynamics simulation (MD) approach is utilized to complement the experimental electrochemical research of the project partners to gain insight into the behaviours of different moieties in an electrochemical cell. Accordingly, recommendations for optimal synthesis process will be deduced based on these investigations.

All MD simulations for this project are performed by LAMMPS [6] and GROMACS [7] to provide an atomic-level understanding on the behaviours of different molecules or ions in an electrochemical cell. In this project each simulated electrochemical cell consists of two electrodes and a liquid phase. The liquid phase contains water as solvent, electrolyte such as sulfuric acid or hydrochloric acid, and reactant molecules (i.e., furfural or 5-HMF as educt and/or 2-methylfuran or DMF as product). The scheme for an electrochemical cell configuration is presented in Figure 2. It consists of copper electrodes on the right and the left side of the simulation box, water solution with ionized sulfuric acid (i.e., hydronium and sulfate), and furfural molecules.

During this HLRN project, MD simulations are performed to provide an insight into behavior of systems with different electrode materials, electrolyte compositions, and applied potentials between two electrodes. These electrochemical systems are analyzed by determining the following characteristics of the systems.
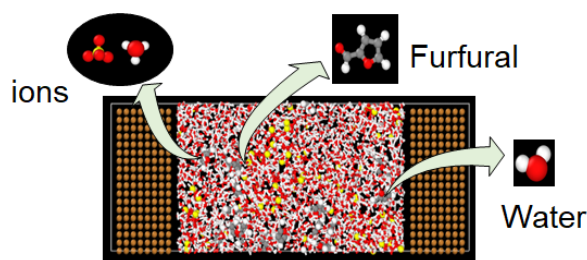
Figure 2: Setup configuration of an electrochemical cell containing furfural, water and ionized sulfuric acid with Cu electrodes.

1. Molecular arrangements of different molecules at the surface

2. Density profiles of different atoms in the absorbed layer

3. Radial distribution functions (RDF)

4. Transport properties, i.e., diffusivity

5. The potential of mean force (PMF) educts and products as a function of their distance from the electrode surface,

A depiction of a PMF curve for furfural and 2-methylfuran molecule in water solution near copper electrode is given in Figure 3.
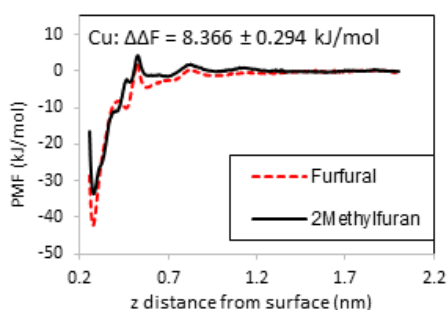
Figure 3: PMF curve furfural and 2-methylfural molecule at the copper electrode with water electrolyte

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https://www.tu-braunschweig.de/se2a

More Information

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Project Partners

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