# Multi-phase lattice Boltzmann simulations of transport processes in porous gas diffusion electrodes for lithium-air batteries

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## ABSTRACT

Lithium-air batteries have the potential to become the future energy source for electric vehicles. Typically, the battery consists of a lithium metal negative electrode, a porous separator soaked with liquid electrolyte, and a porous air electrode where oxygen from the surrounding atmosphere is reduced during battery discharge. This configuration yields the highest theoretical capacity of all Li batteries [1].

In our approach we focus on systems employing aqueous electrolytes [2]. $O_2$ is fed to the battery via so-called gas diffusion electrodes (GDEs) in which gas and liquid phase coexist. The use of hydrophobic binders ensures a fast transport of $O_2$ in the gas phase. The distribution of the liquid electrolyte in the porous structure has a strong influence on effective transport parameters and active surface areas which finally determine the performance of the battery.

In our contribution we present results of 2D and 3D lattice-Boltzmann simulations [3], [4] which are conducted on tomographic reconstructions of Ag-GDEs. In our simulations we explicitly take into account the heterogeneous wetting properties of hydrophilic Ag substrate and hydrophobic polymeric binder. The 3D simulations are used to extract effective transport parameters and specific surface areas at various saturations of the GDE with liquid electrolyte. The calculated $p_c$-$s_w$ curves of the 3D simulations are compared to a series of independent 2D simulations. We show that the computationally less demanding 2D simulations can be used as an effective tool for the screening of wetting properties of different new electrode geometries.

Finally, we present a short outlook on how the results of the LBM simulations can be used to predict the electrochemical performance of GDEs and full virtual battery cells, demonstrating the capabilities of our multi-scale approach for the development of novel battery materials.

## REFERENCES

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