# Modelling and Simulation for the Search for New Active Materials for Redox Flow Batteries - Results of the International Project SONAR

Jens Noack[1,2,*], Emmanuel Baudrin[3], Rocco Fornari[4], Alejandro Franco[3], Daniel Gerlach[1], Xinjie Guan[2], Jan Hamaekers[5], Astrid Maaß[5], Chris Menictas[2], Gael Mourouga[6], Hermann Nirschl, Nataliya Roznyatovskaya[1], Roman Schaerer[6], Juergen Schumacher[6], Piotr de Silva[4], Maria Skyllas-Kazacos[2], Jakub Wlodarczyk[6], Amadeus Wolf, Jia Yu[3]

[1]Fraunhofer-Institute for Chemical Technology, Joseph-von-Fraunhofer-Str. 7, 76327 Pfinztal, Germany; [2]University of New South Wales (UNSW), UNSW Sydney NSW 2052 Australia; [3]Denmark Technical University, Anker Engelunds Vej 1, 2800 Kgs. Lyngby, Denmark; [4]Université de Picardie Jules Verne, Chemin du Thil, 80000 Amiens, France; [5]Fraunhofer-Institute for Algorithms and Scientific Computing, Schloss Birlinghoven, 53757 Sankt Augustin, Germany; [6]Zurich University of Applied Sciences, Wildnachstrasse 21, Postfach 805, CH-8401 Winterthur, Switzerland; [7]Karlsruhe-Institute of Technology, Chemieingenieurwesen und Verfahrenstechnik, Kaiserstr. 12, 76131 Karlsruhe, Germany

*Corresponding author: jens.noack@ict.fraunhofer.de

Due to the characteristics of flow batteries, this technology is ideally suited for low-cost storage in the range of a few hours and thus for load balancing as stationary storage in grids with high amounts of renewable energy [1]. Today, a large number of different active materials for flow batteries are known, although only a few have been commercialised [2]. Basically, the energy supply and thus also the required storage should be sustainable, i.e. not cause resource problems and not be harmful to humans and the environment. A potential for a huge range of possibilities is offered by organic active materials, which should be used especially in aqueous solutions. Due to the immense possibilities, classical synthesis and testing is extremely lengthy and costly. An alternative can be model-based high-throughput screening, where by simulating the properties of active materials in the electrolyte and the battery itself, computer-based simulations can be used to conduct the search.

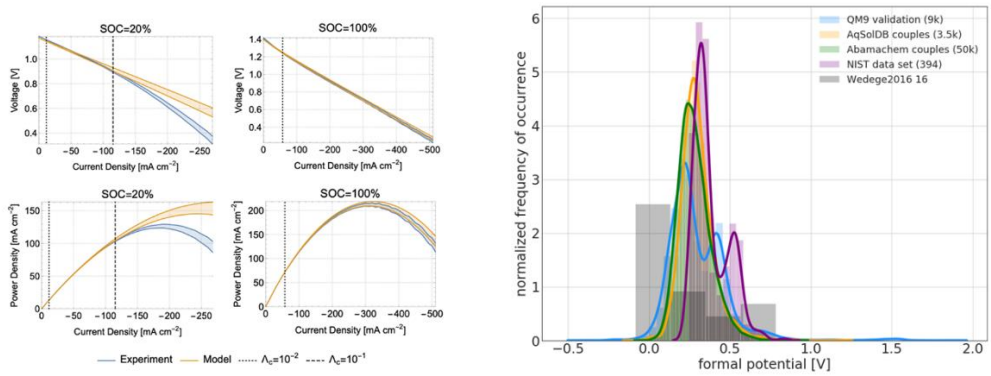


*Figure 1: left) Simulated vs. experimental polarisation curves based on a 0D cell modell for MV/TMA-TEMPO, right) ML-based calculated formal potentials vs. database-based potentials of a dataset with 9000 quinone based redox couples*

The SONAR project is an EU-funded project in which 7 different institutions from the EU, Switzerland and Australia are developing a high-throughput screening method capable of finding new active materials for redox flow batteries. The principle is a serial coupling of different size scales, combined with molecule generation and machine learning. The chemical structure of a candidate is generated by a molecule generator and then its atomistic properties, kinetics, side reactions and cell properties are iteratively calculated with exclusion criteria.

In this talk we will give an overview of 2 years of research in this project in the areas of machine learning for high throughput screening, DFT based quantum mechanics modelling, kinetics Monte Carlo methods for meso-scale, 0D cell modelling, 3D cell modelling, stack modelling and techno-economics.

[1] B. Dunn, H. Kamath, J.-M. Tarascon, Science 2011, 334, 928–935.
[2] J. Noack, N. Roznyatovskaya, T. Herr, P. Fischer, Angew. Chem. Int. Ed. 2015, 54, 9776–9809.