

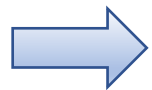


# **Modelling for the search for new active materials for redox flow batteries**

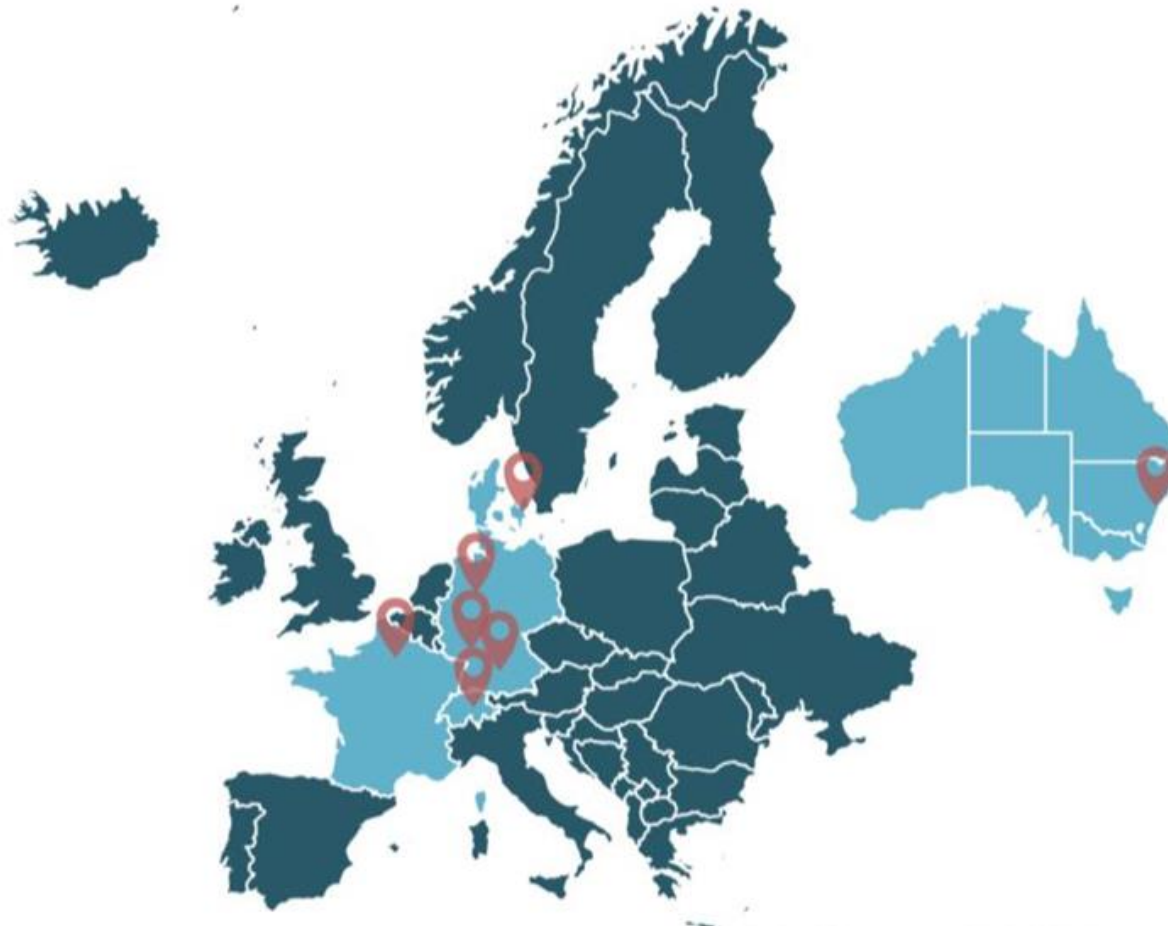
Jens Noack  
Fraunhofer ICT

**31st ISE Topical Meeting  
Aachen/Germany 2022  
May 18th 2022**

- **Huge number of possibilities of organic active materials for redox flow batteries**
- Laboratory testing is time consuming and costly
  - Chemical tests (e.g. solubility, stability)
  - Electrochemical half-cell tests (e.g. potentials, kinetics)
  - Cell & system tests (performance)
- Techno-economics ? -> CAPEX ?
- Behavior in the grid ? -> Levelised cost of storage?
- Only LCOS (levelised cost of storage (lifetime cost / lifetime energy throughput)) gives compareable values!



**Development of a model-based high-throughput screening method**



Fraunhofer-Institute for Chemical Technology (ICT)

GERMANY

Fraunhofer-Institute for Algorithms and Scientific Computing (SCAI)

GERMANY

Technical University of Denmark (DTU)

DENMARK

CNRS-Laboratoire de Réactivité et Chimie des Solides (LRCS)

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Zurich University of Applied Science (ZHAW)

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Karlsruhe-Institute for Technology (KIT)

GERMANY

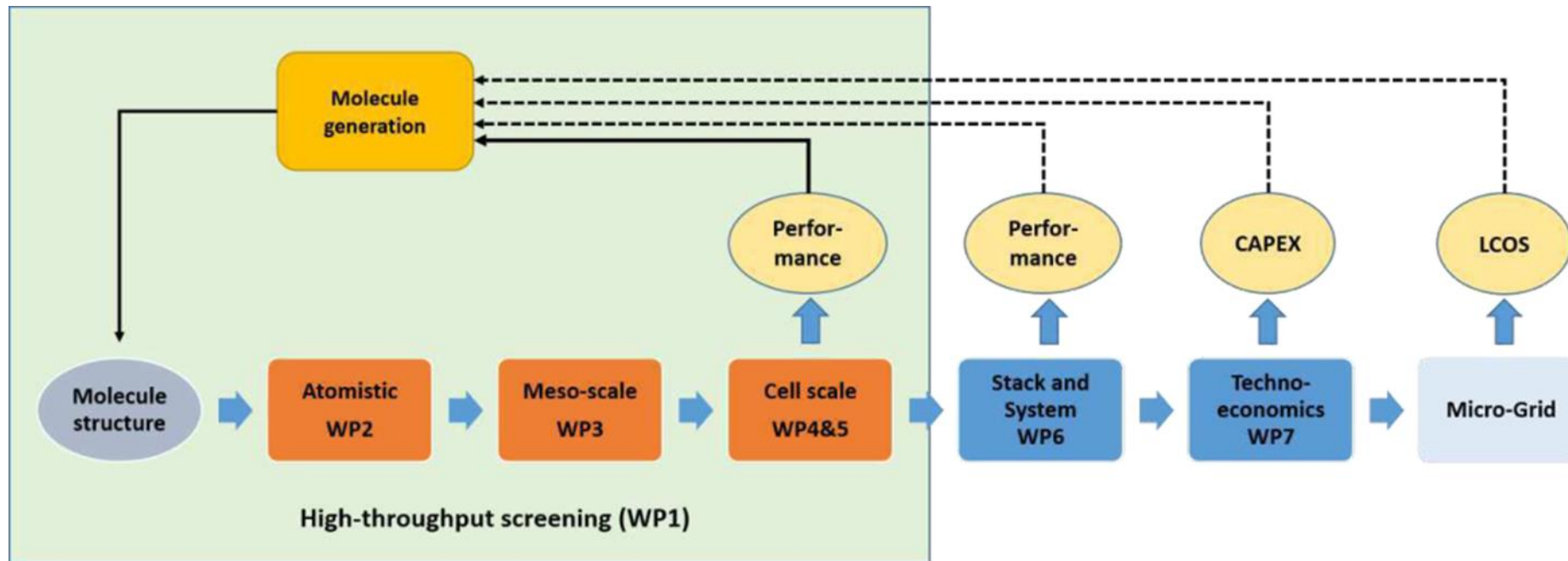
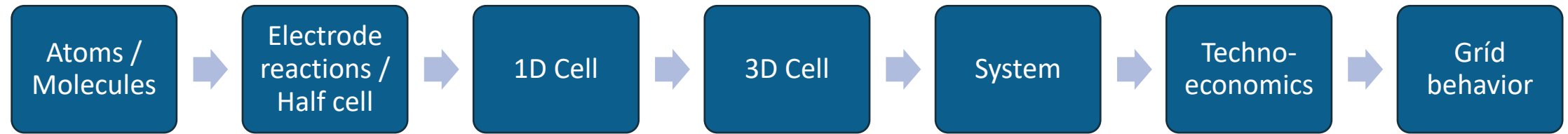
University of New South Wales (UNSW)

AUSTRALIA

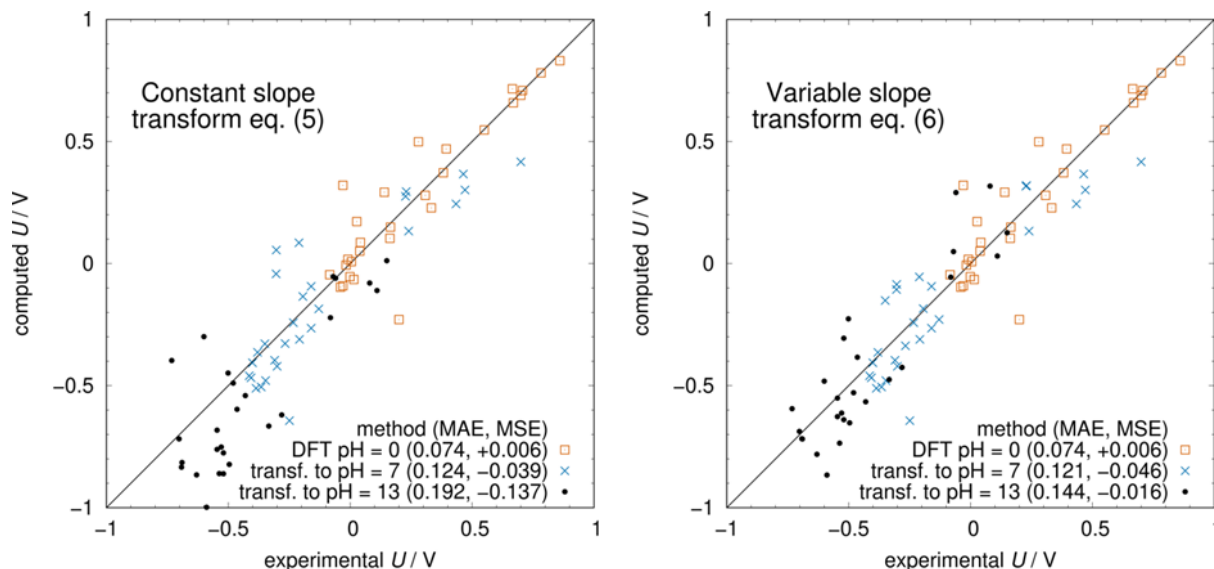




# Introduction - Approach

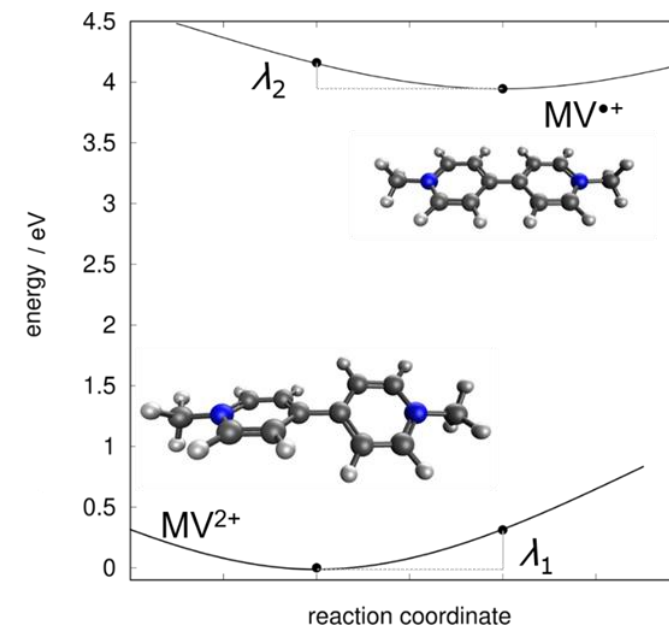


## Computed vs. experimental redox potentials



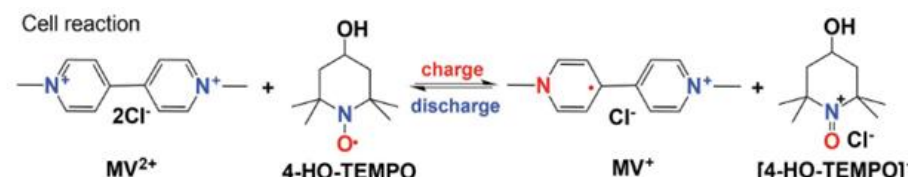
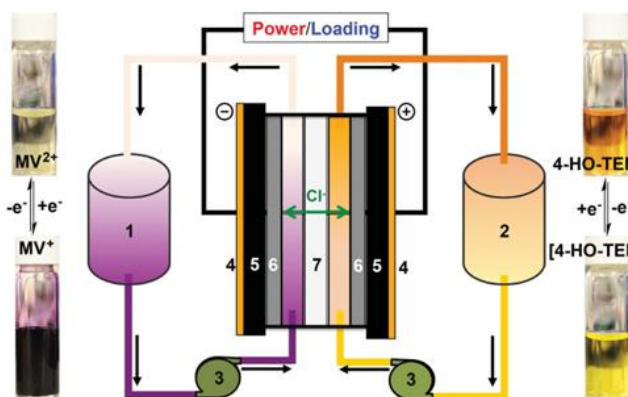
Left, transformation from pH 0 to 7 and 13 is done using the number of protons at pH=0. Right, the slope of the Pourbaix diagram is updated at every  $pK_a$ .

## Calculation of re-organisation energies



molecule	$\lambda_1$ / eV	$\lambda_2$ / eV	$\lambda_3$ / eV
MV	0.228	0.297	0.263
EV	0.226	0.320	0.273
4-OH-TEMPO	0.496	0.462	0.479
AQS	1.485	1.601	1.543
BQDS	1.967	2.030	1.999

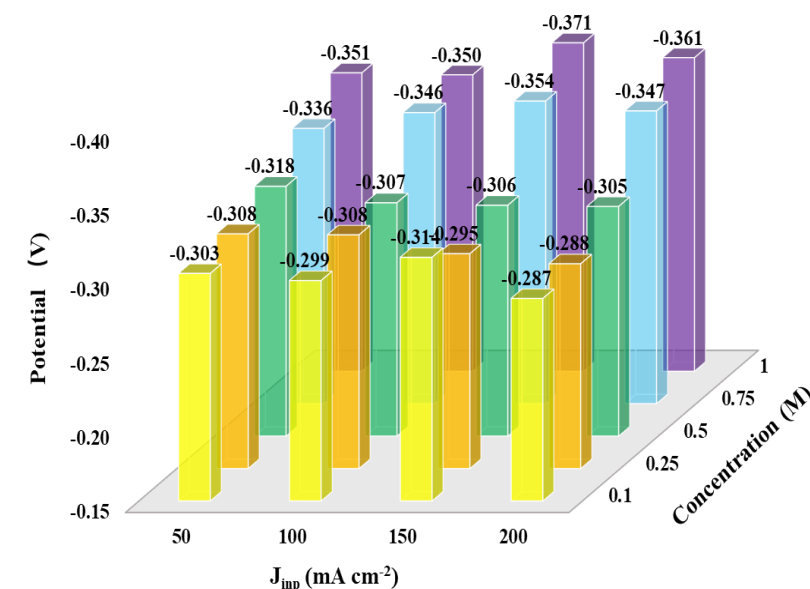
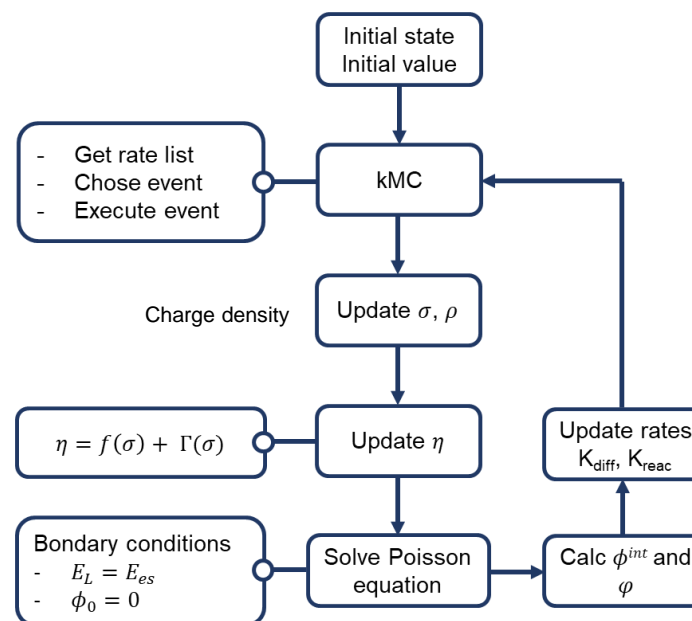
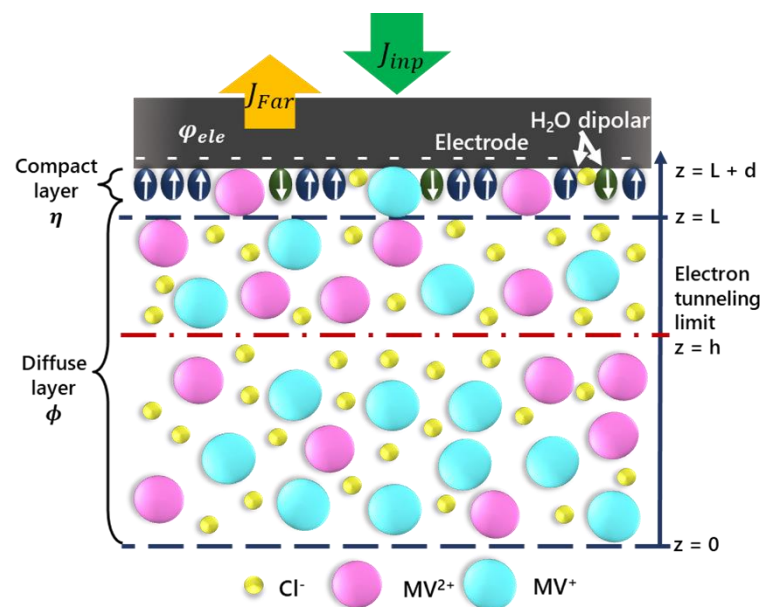
# Meso-scale modelling of the electrochemical interface



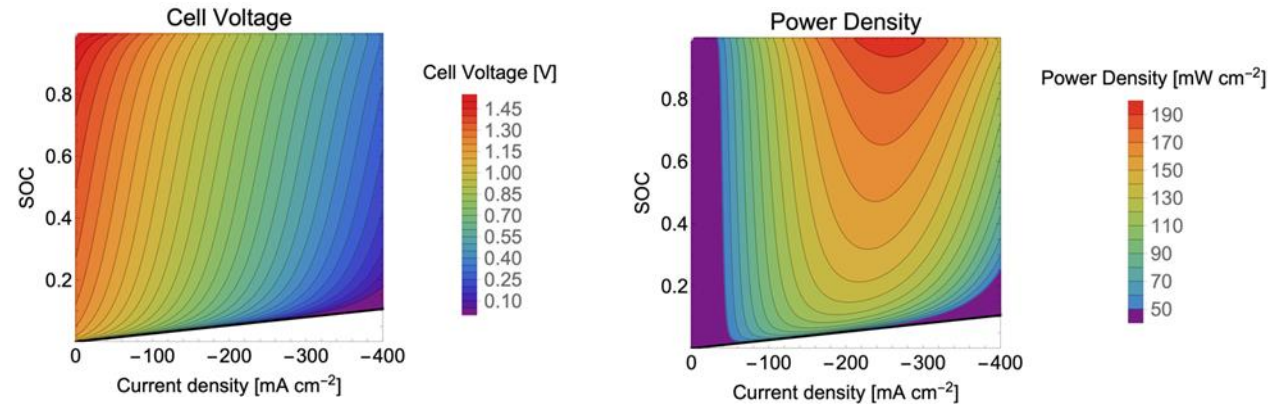
Consideration of

- Motion
- Electron transfer
- Adsorption/ desorption
- Dimerisation

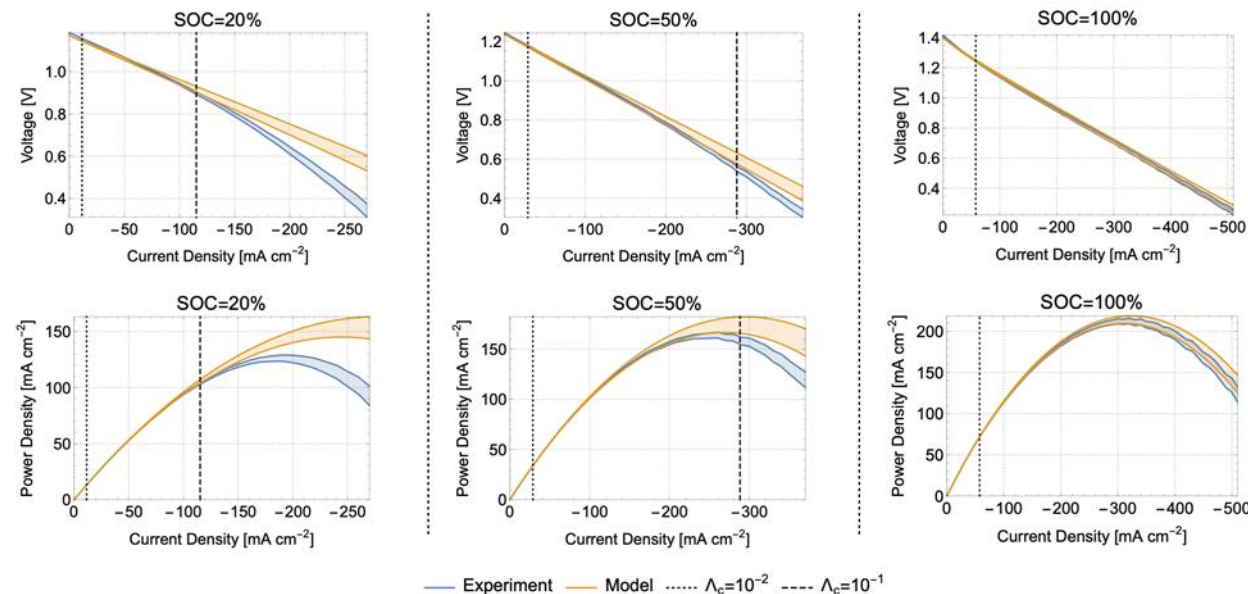
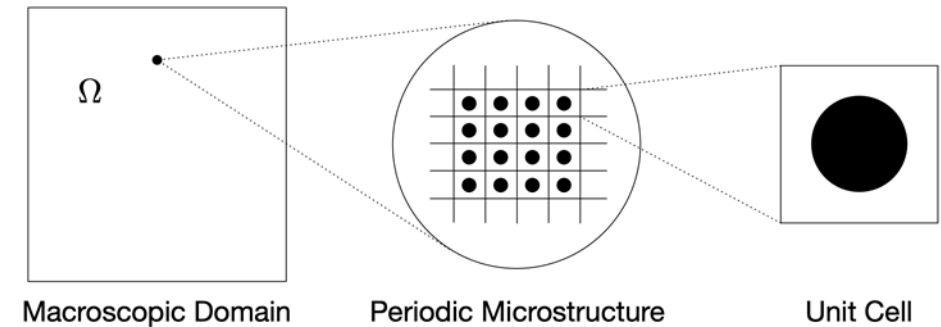
-> Calculation of electrode potential  $\phi$



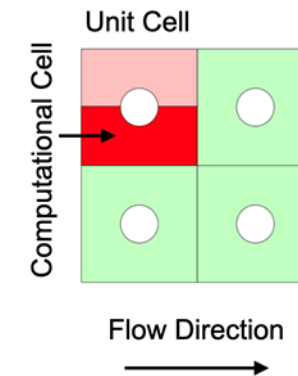
# Bridging the scales: connection of electrochemical double layer properties, porous media flow and continuum modelling of RFBs



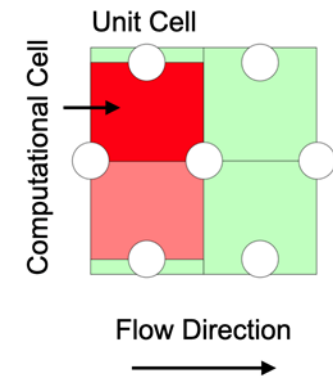
- Development of a 0D-U-I-SOC cell model
- Simulations based on MV/TMA-TEMPO



Square Configuration

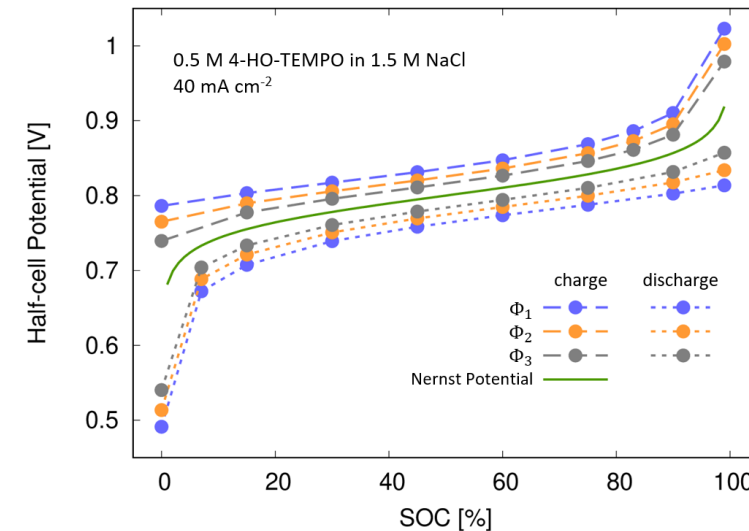
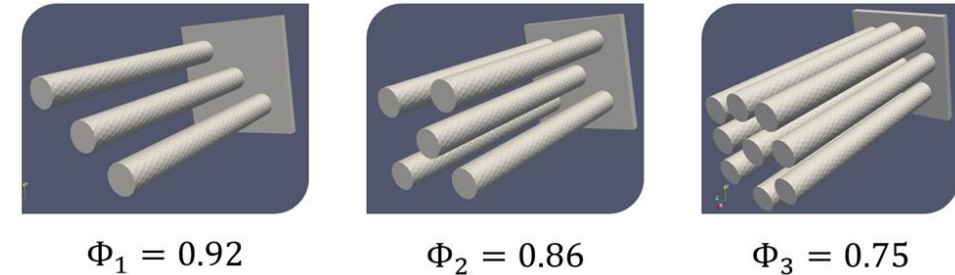
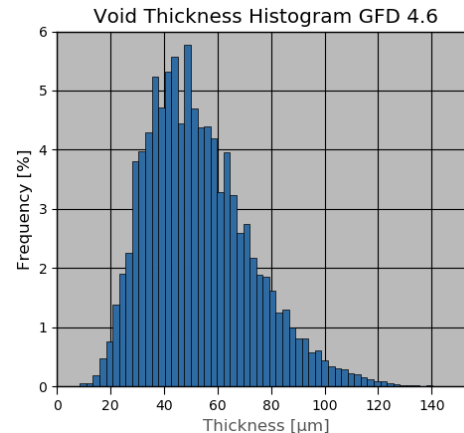
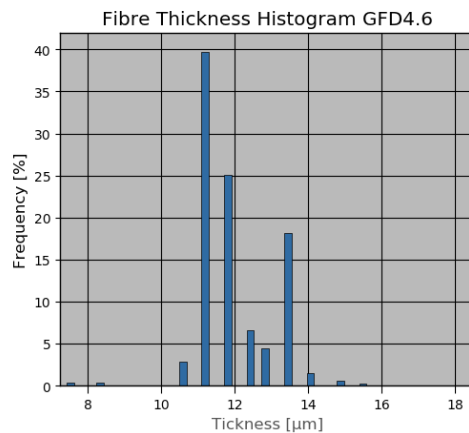
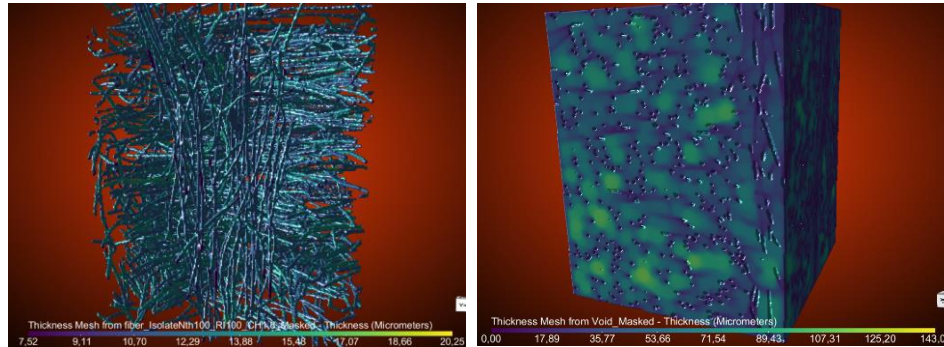


Hexagonal Configuration



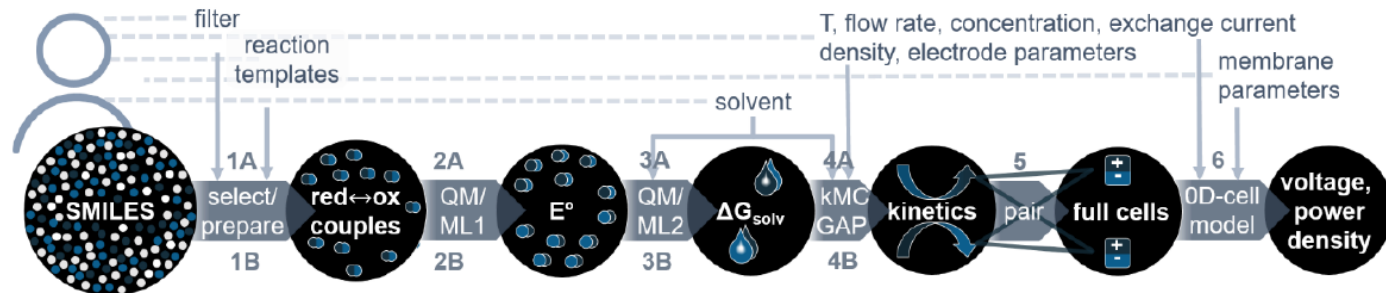


## Micro Computer Tomography for electrode digitalisation

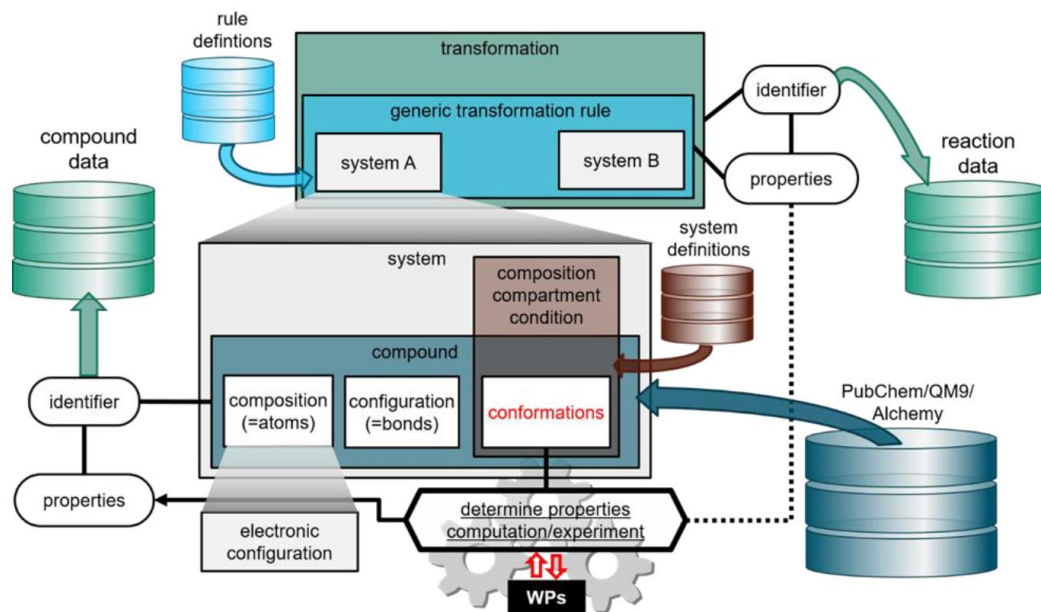


Different colours indicate different porosities. Dashed lines represent the charging process and dotted lines represent the discharging process. The simulations assume a constant supply of electrolyte

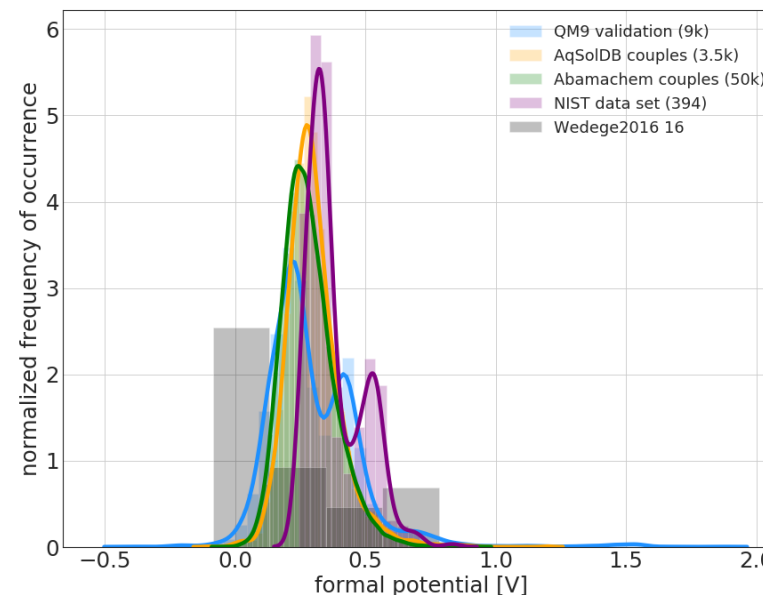
## Data flow



## Data management



## Calculated formal potentials vs. databases



# Thank you for your attention!



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## Contact

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