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

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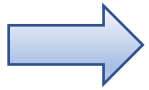
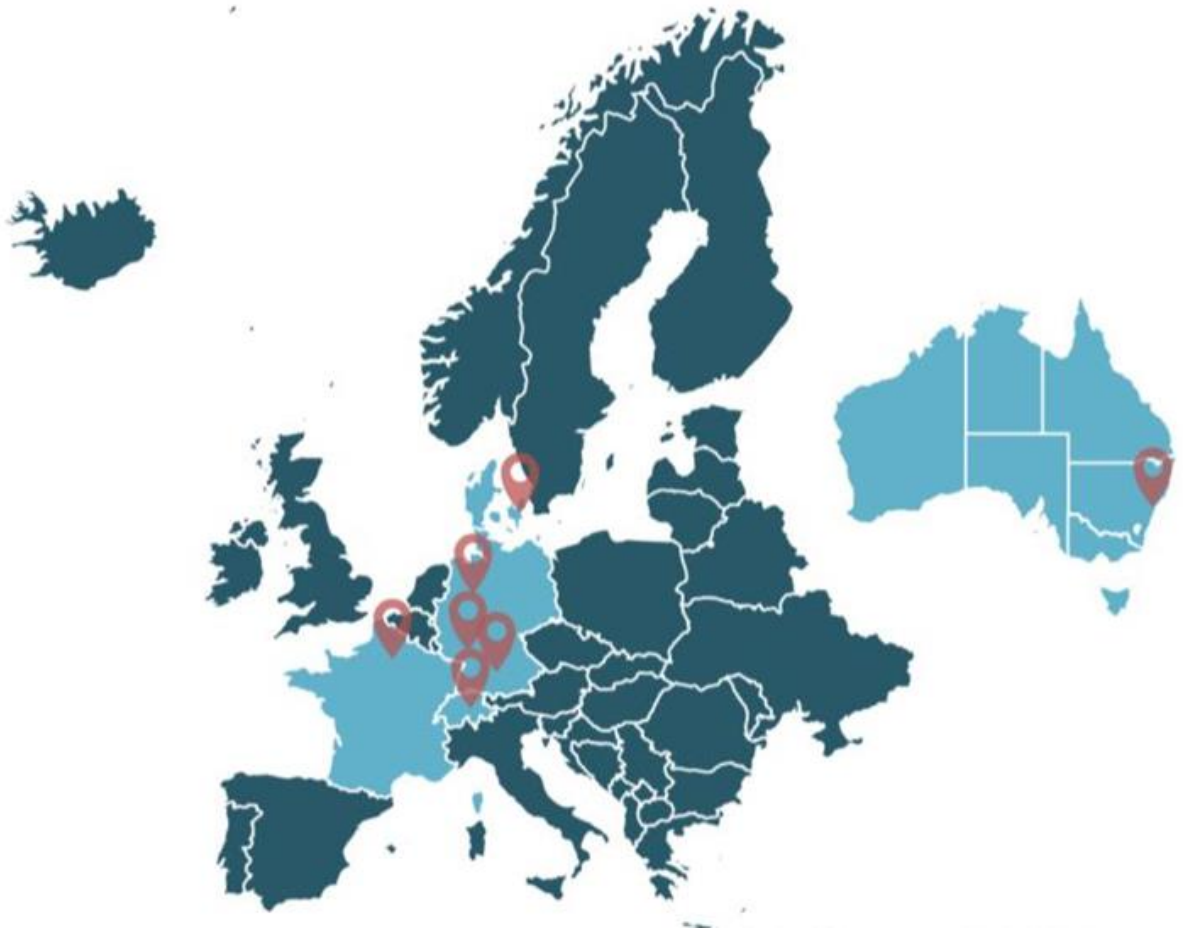
Motivation

- **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

Introduction - Partner



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Introduction - Industrial Exploitation Board

Enerox
BUILDING ENERGY STORAGE INFRASTRUCTURE

volterion

JENA BATTERIES

sgl carbon

SCHMALZ

SCM
Software for Chemistry & Materials

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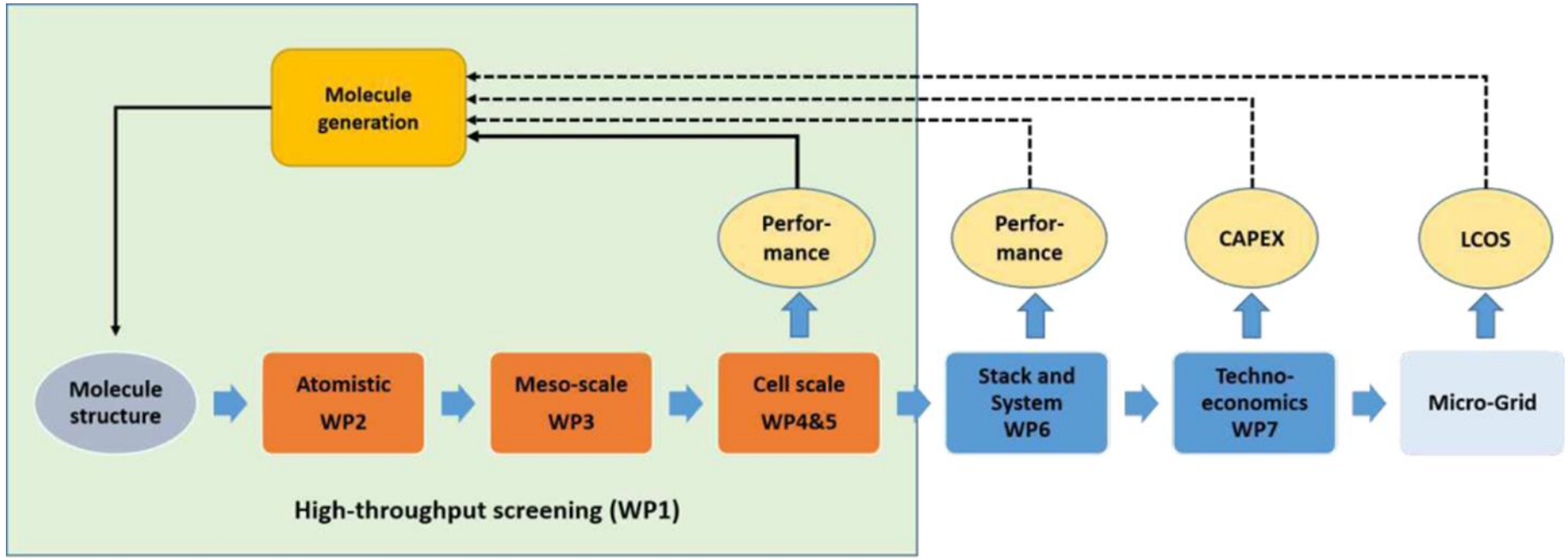
Introduction - Approach

Atoms / Molecules → Electrode reactions / Half cell → 1D Cell → 3D Cell → System → Techno-economics → Gríd behavior



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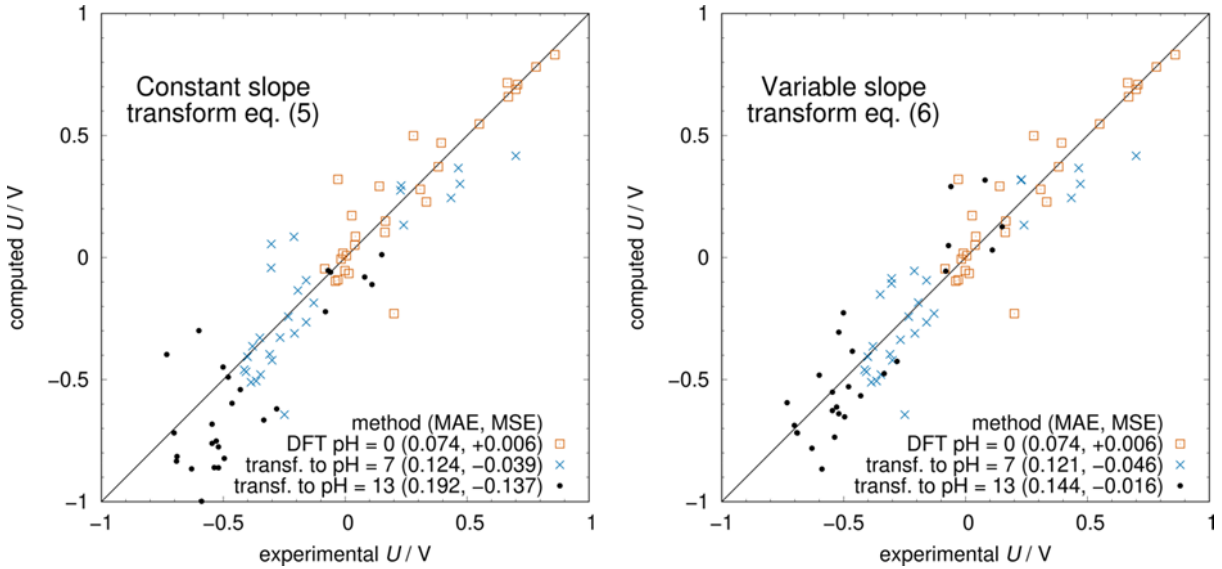
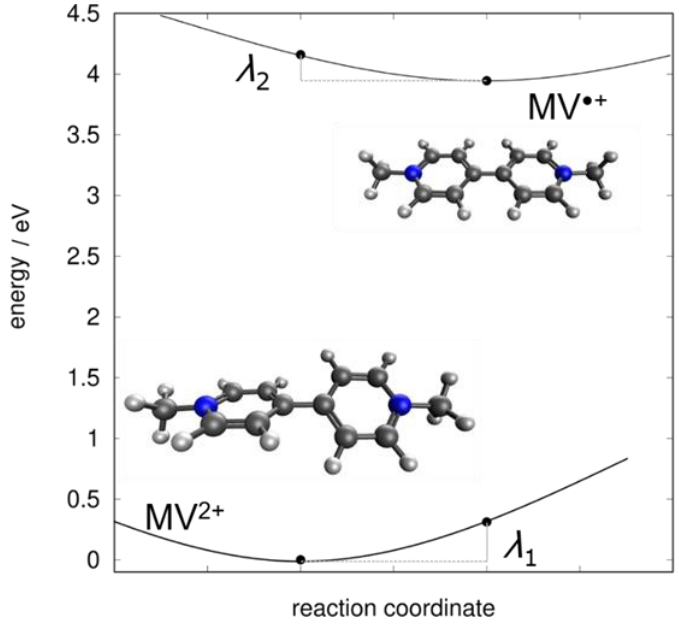
Electronic structure modelling of electroactive molecules

Computed vs. experimental redox potentials



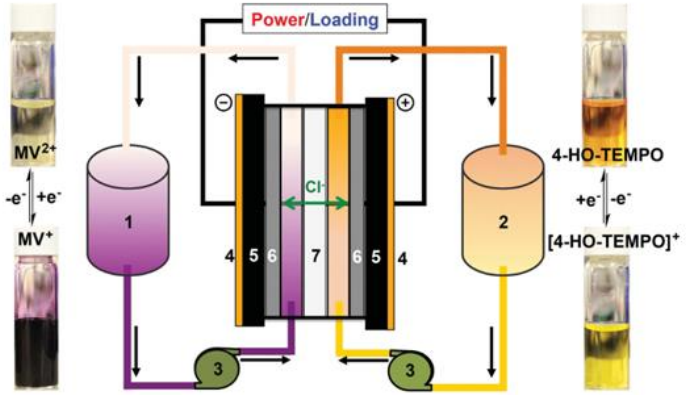
Left, transformation from pH 0 to 7 and 13 is done using the number of protons at pH=0. Right, the slope of the Pourbaix diagram is updated at every pK_a.

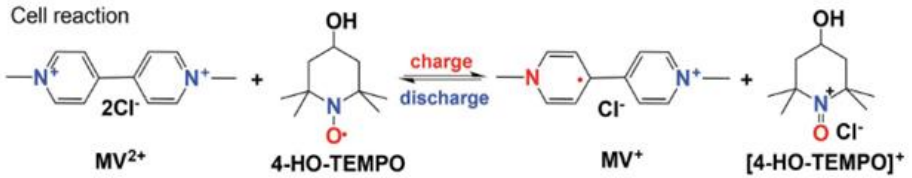
Calculation of re-organisation energies



molecule	λ_1 / eV	λ_2 / eV	λ_i / 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

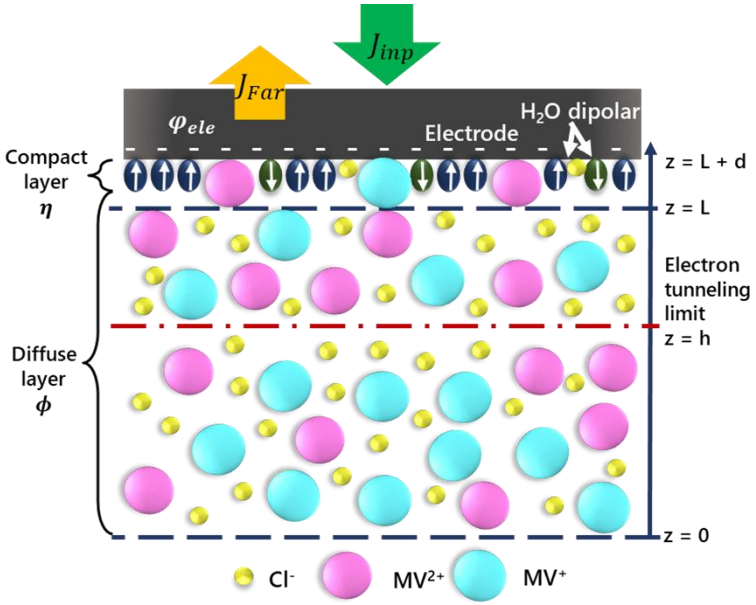
Meso-scale modelling of the electrochemical interface

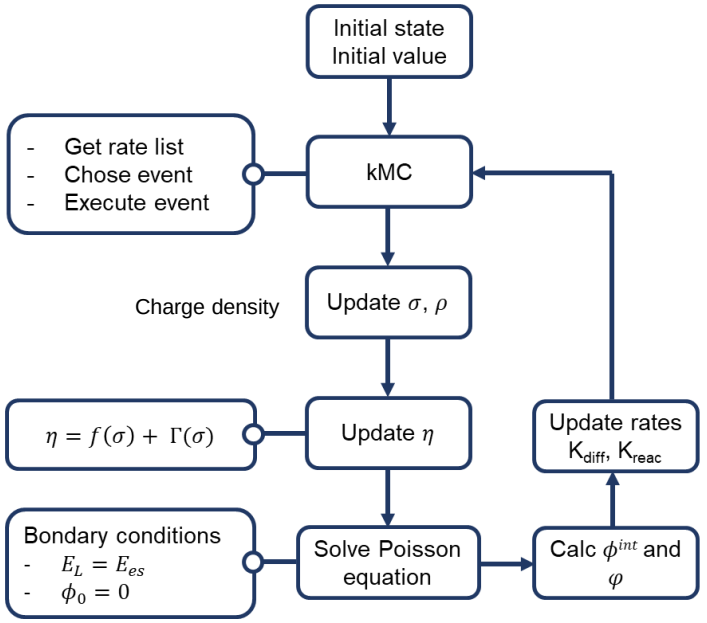


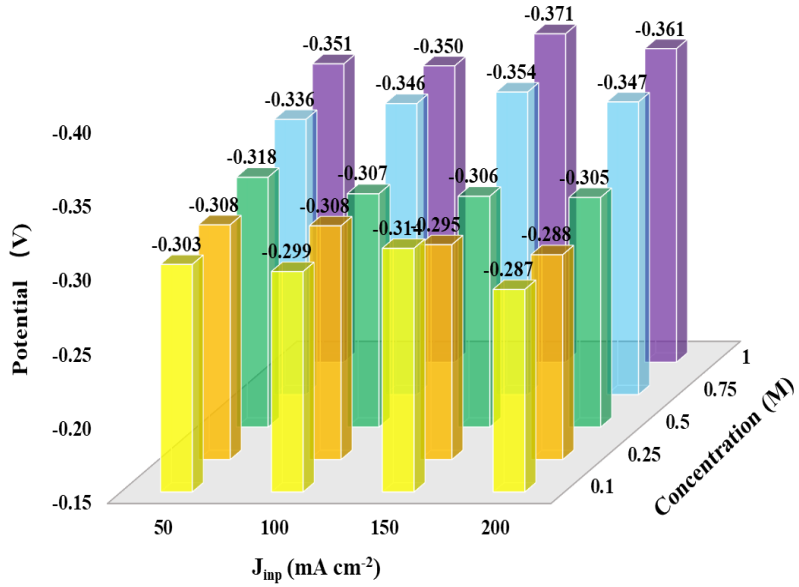


Consideration of
- Motion
- Electron transfer
- Adsorption/ desorption
- Dimerisation

-> Calculation of electrode potential φ







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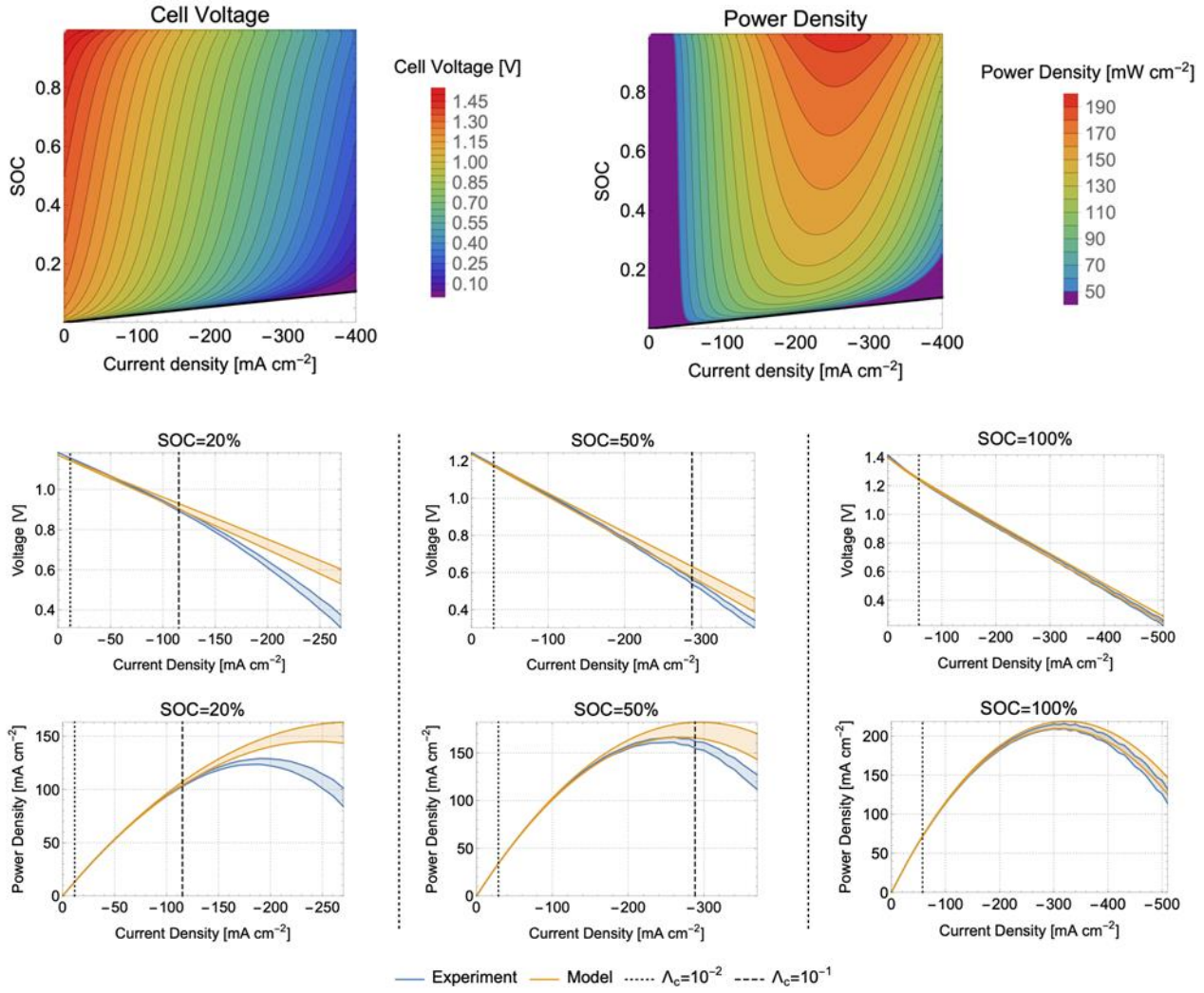
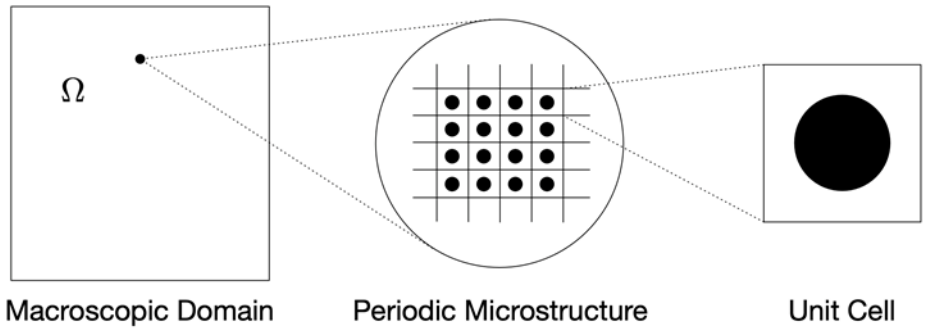
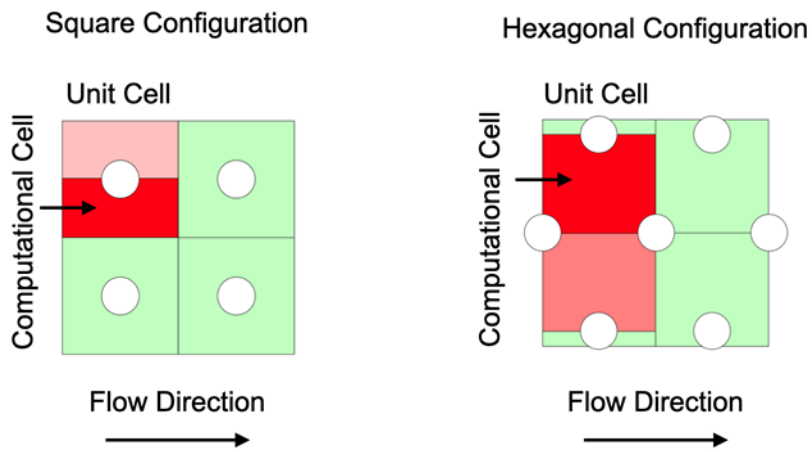
Bridging the scales: connection of electrochemical double layer properties, porous media flow and continuum modelling of RFBs



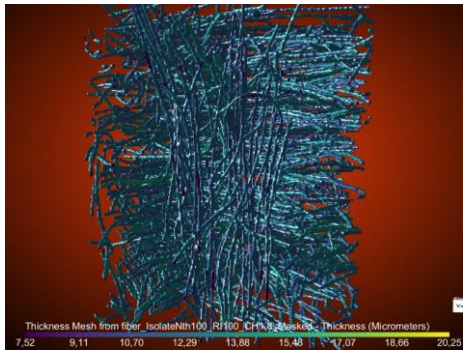
- **Development of a 0D-U-I-SOC cell model**
- **Simulations based on MV/TMA-TEMPO**

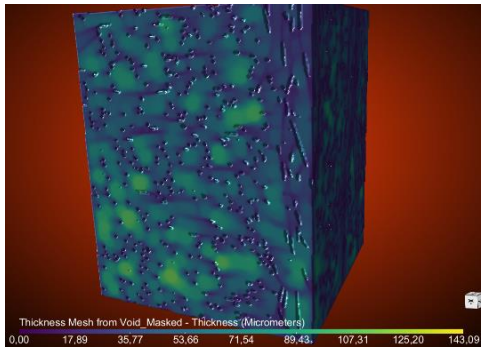


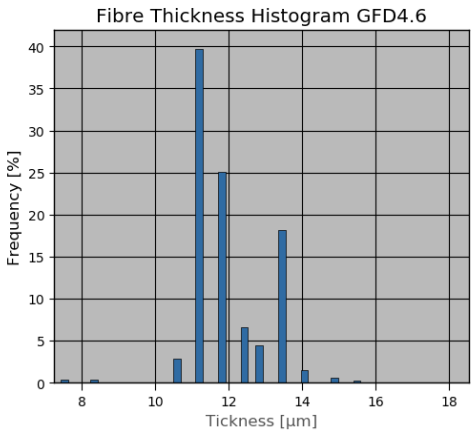


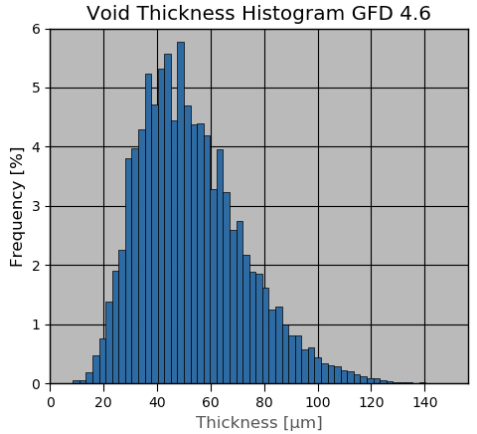
Cell performance simulation and cell design optimisation

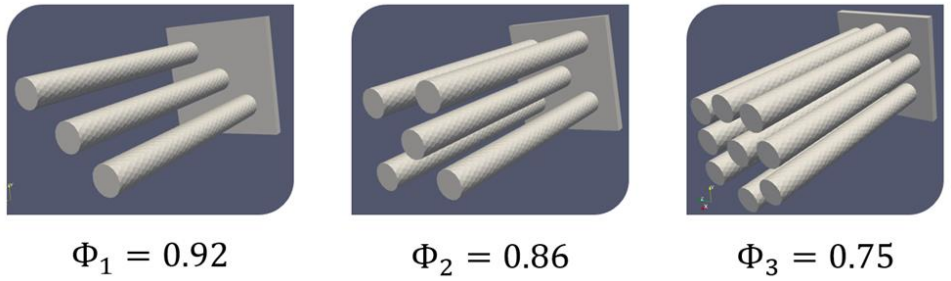
Micro Computer Tomography for electrode digitalisation

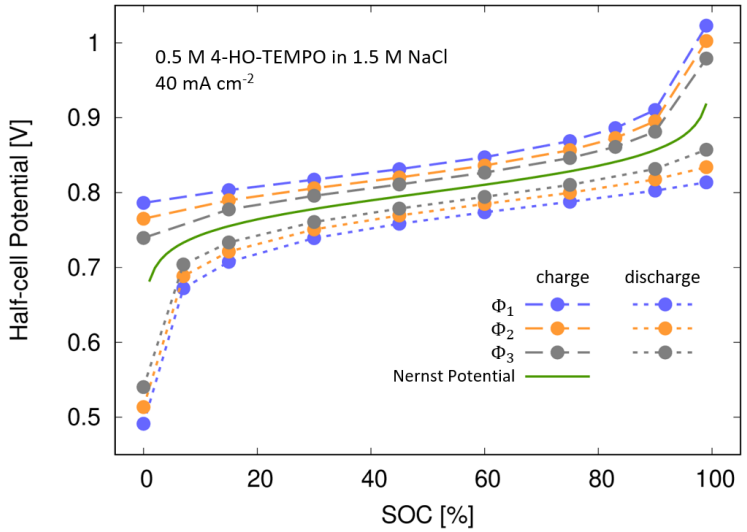












Different colours indicate different porosities. Dashed lines represent the charging process and dotted lines represent the discharging process. The simulations assume a constant supply of electrolyte

Framework for high-volume pre-selection, data integration and design

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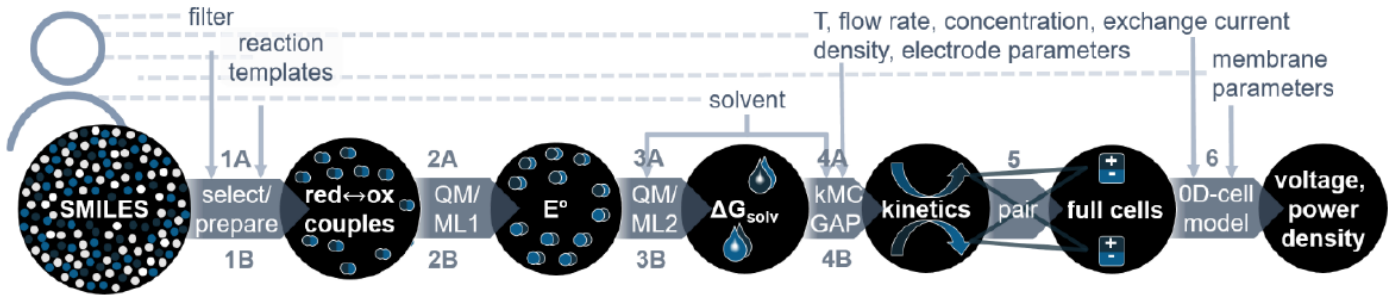
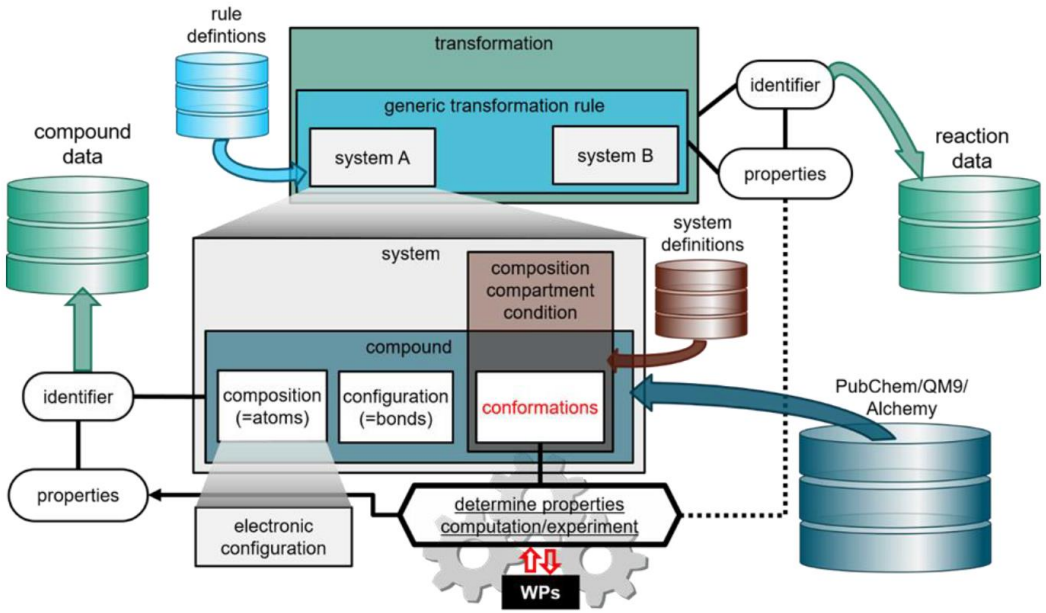
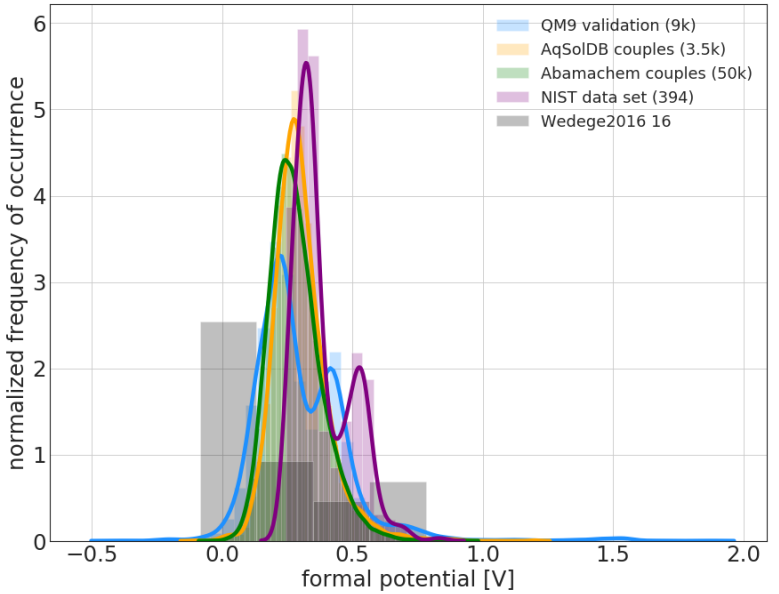
Data flow



Data management



Calculated formal potentials vs. databases



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