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

Fact Sheet

Project Information

SONAR

Grant agreement ID: 875489

DOI
10.3030/875489

Funded under
SOCIETAL CHALLENGES - Secure, clean and efficient energy

Total cost
€ 2 820 535

EU contribution
€ 2 385 985

Start date
1 January 2020

End date
31 December 2023

Coordinated by
FRAUNHOFER GESELLSCHAFT ZUR FORDERUNG DER ANGEWANDTEN FORSCHUNG EV

Germany

Project description

Energising redox flow batteries

SONAR will develop a framework for the simulation-based screening of electroactive materials for aqueous and nonaqueous organic redox flow batteries (RFBs). It will adopt a multiscale modelling paradigm, in which simulation methods at different physical scales will be further advanced and linked by combining physics- and data-based modelling. SONAR will develop a screening framework to determine levelized cost of storage, starting from the automatic generation of candidate structures for the electroactive material, then iterating through molecular-, electrochemical interface-,
porous electrodes-, cell-, stack-, system- and techno-economic-level models. To increase the throughput of the screening, SONAR will exploit advanced data integration, analysis and machine-learning techniques, drawing on the growing amount of data produced during the project. Project results are expected to reduce the cost and time-to-market of redox flow batteries, thus strengthening the competitiveness of the EU battery industry.

**Objective**

SONAR will develop a framework for the simulation-based screening of electroactive materials for aqueous and nonaqueous organic redox flow batteries (RFBs). It will adopt a multiscale modelling paradigm, in which simulation methods at different physical scales will be further advanced and linked by combining physics- and database modelling. Competing energy storage technologies are only comparable when using the levelized-cost-of-storage (LCOS) as a global metric, accounting for the complex interrelations between factors like CAPEX, lifetime and performance. SONAR will thus develop a screening framework to determine LCOS, starting from the automatic generation of candidate structures for the electroactive material, then iterating through molecular-, electrochemical interface-, porous electrodes-, cell-, stack-, system- and techno-economic-level models. For the iterative traversal of the different scales, exclusion criteria like solubility, standard potentials and kinetics will be defined, and the results for individual candidates will be stored in a database for further processing. To increase the throughput of the screening, SONAR will exploit advanced data integration, analysis and machine-learning techniques, drawing on the growing amount of data produced during the project. The models will be validated e.g. by comparison with measurements of redox potentials for known chemistries, or measurement data of RFB half-cells and lab-sized test cells. SONAR will work closely with industrial partners (incl. JenaBatteries, Volterion) to ensure the commercial viability of the results. The models will be exploited individually and in a comprehensive screening service offered by Fraunhofer SCAI, facilitating the rapid assessment of the technical and economic potential of a new technology in its earliest development stages. This will reduce the cost and time-to-market, thus strengthening the competitiveness of the EU’s battery industry in the emerging field of organic RFBs.

**Fields of science**

natural sciences &gt; chemical sciences &gt; electrochemistry &gt; electric batteries

**Programme(s)**
H2020-EU.3.3. - SOCIETAL CHALLENGES - Secure, clean and efficient energy

H2020-EU.3.3.4. - A single, smart European electricity grid

**Topic(s)**

LC-BAT-3-2019 - Modelling and simulation for Redox Flow Battery development

**Call for proposal**

H2020-LC-BAT-2019-2020

See other projects for this call

**Sub call**

H2020-LC-BAT-2019

**Funding Scheme**

RIA - Research and Innovation action

**Coordinator**

FRAUNHOFER GESELLSCHAFT ZUR FORDERUNG DER ANGEWANDTEN FORSCHUNG EV

Net EU contribution

€ 918 900,00

Address

Hansastrasse 27c
80686 Munchen
Germany

Region

Bayern > Oberbayern > München, Kreisfreie Stadt

Activity type

Research Organisations

Links

Contact the organisation  Website
<table>
<thead>
<tr>
<th>Organisation Name</th>
<th>Country</th>
<th>EU Contribution</th>
<th>Address</th>
<th>Region</th>
</tr>
</thead>
<tbody>
<tr>
<td>DANMARKS TEKNISKE UNIVERSITET</td>
<td>Denmark</td>
<td>€ 392,335.00</td>
<td>Anker Engelundsvej 1 Bygning 101 A 2800 Kgs Lyngby</td>
<td>Danmark &gt; Hovedstaden &gt; Københavns omegn</td>
</tr>
<tr>
<td>CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS</td>
<td>France</td>
<td>€ 220,200.00</td>
<td>Rue Michel Ange 3 75794 Paris</td>
<td>Ile-de-France &gt; Ile-de-France &gt; Paris</td>
</tr>
</tbody>
</table>
THIRD-PARTY

UNIVERSITE DE PICARDIE JULES VERNE
France
Net EU contribution
€ 136,350,00
Address
Chemin Du Thil
80025 Amiens
Region
Hauts-de-France > Picardie > Somme
Activity type
Higher or Secondary Education Establishments

ZURCHER HOCHSCHULE FUR ANGEWANDTE WISSENSCHAFTEN
Switzerland
Net EU contribution
€ 390,700,00
Address
Gertrudstrasse 15
8401 Winterthur
KARLSRUHER INSTITUT FUER TECHNOLOGIE

Germany

Net EU contribution

€ 327 500,00

Address

Kaiserstrasse 12
76131 Karlsruhe

Region

Baden-Württemberg > Karlsruhe > Karlsruhe, Stadtkreis

Activity type

Higher or Secondary Education Establishments

Links

Contact the organisation  
Website  
Participation in EU R&I programmes  
H2020 collaboration network

Non-EU contribution

€ 0,00

UNIVERSITY OF NEW SOUTH WALES

Australia

Net EU contribution

€ 0,00

Address

Anzac Parade
2052 Sydney
Activity type
Higher or Secondary Education Establishments

Links
Contact the organisation Website Participation in EU R&I programmes H2020 collaboration network

Non-EU contribution
€ 434 550,00

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