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

Wyniki

Informacje na temat projektu

SONAR

Identyfikator umowy o grant: 875489

Strona internetowa projektu

DOI
10.3030/875489

Projekt został zamknięty

Data podpisania przez KE
10 Października 2019

Data rozpoczęcia
1 Stycznia 2020

Data zakończenia
31 Grudnia 2023

Finansowanie w ramach
SOCIETAL CHALLENGES - Secure, clean and efficient energy

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Koordynowany przez
FRAUNHOFER GESELLSCHAFT ZUR FORDERUNG DER ANGEWANDTEN FORSCHUNG EV
Niemcy

CORDIS oferuje możliwość skorzystania z odnośników do publicznie dostępnych publikacji i rezultatów projektów realizowanych w ramach programów ramowych HORYZONT.

Odnośniki do rezultatów i publikacji związanych z poszczególnymi projektami 7PR, a także odnośniki do niektórych konkretnych kategorii wyników, takich jak zbiory danych i oprogramowanie, są dynamicznie pobierane z systemu OpenAIRE.

Rezultaty

Dokumenty, raporty (8)

Tutorials and public workshops

Workshop tutorials and report on workshops on the functionality and usage of the new work-flows and models, including feedback from consultations with the Industrial Exploitation Board. (Task 8.3)

Scaling strategies 3

Dissipative particle dynamics or Lattice Boltzmann approach coupled to kMC (Task 3.5)

Scaling strategies 1

Mean field model derived from kMC simulation Task 35

Optimized Techno-Economical model

Optimized mathematical model for the specific needs of organic redox flow batteries with different active materials Addition of further variable parameters and dependencies especially the integration of an optimized battery model Task 71

Upgraded kMC model

Upgrade of preexisting kMC code in Python programming language. Adaptation to organic based redox flow systems. (Task 3.1)

Scaling strategies 2

Hybrid model coupling mean field with kMC approach (Task 3.5)

Simplified model of the electrochemical double layer

Model of the electrochemical double layer without spatial resolution modelabbreviation DLM that is computationally less expensive than the kMC model of Task 31 Task 42

Use cases

Report on use cases, demonstrating the performance of new models and work-flows for dissemination and exploitation purposes (Task 8.3)

Inne (5)

Database with DFT results for data-driven models

For a large set of redox-active molecules, the electronic structure parameters needed to train and validate machine-leraning models will be calculated and

stored in an accessible database format. The precise content of the database will depend on the specific requirements of the model, but will include redox potentials, solvation free energies, and any potential desriptors derived from electronic structure calculations. (Task 2.2)

1D single cell performance model

One-dimensional continuum-scale RFB model (RFB-OS-1D) to simulate the driving potentials and fluxes of mass and charge in the through-plane direction of the cell assembly. A manuscript including the model description is submitted to a scientific journal. The source code of the model is included in the article submission. (Task 4.1)

kMC software deposit in GitHub

Release of kMC code in python programming language. This code will be parallelized (Task 3.1-3.8)

Numerical upscaling of the EDL model

One-dimensional RFB model (RFB-SCSM-1D) that is suitable for computer-based material screening, where details of cell components (membrane, porous electrodes) are described in interaction with the properties of new redox couples. (Task 4.3)

Database with calculated parameters for kMC simulations

For selected redox-active molecules, a database with parameters needed for performing kinetic Monte Carlo simulations will be generated. It will include reaction rates calculated from first principles for e.g. chemical and electrochemical degradation reactions, or heteregenous electron transfer reactions. (Task 2.3)

Witryny, zgłoszenia patentowe, filmy wideo itp. (1)

Public dissemination

This report will cover all dissemination activities carried out during the project, in accordance with the dissemination plan (D8.2) (Task 8.2 and 8.6)

Publikacje

Artykuły recenzowane (9)

Rapid Prescreening of Organic Compounds for Redox Flow Batteries: A Graph Convolutional Network for Predicting Reaction Enthalpies from SMILES

Autorzy: James Barker, Laura-Sophie Berg, Jan Hamaekers, Astrid Maass
Opublikowane w: Batteries & Supercaps, 2021, ISSN 2566-6223
Wydawca: Wiley-VCH GmbH
DOI: 10.1002/batt.202100059

Optimization of the microstructure of carbon felt electrodes by applying the lattice Boltzmann method and Bayesian optimizer

Autorzy: Yu J, Duquesnoy M, Liu C, Franco AA
Opublikowane w: Journal of Power Sources Journal of Power Sources, 2023, ISSN 1873-2755
Wydawca: Elsevier
DOI: 10.1016/j.jpowsour.2023.233182

A Three-Dimensional Hydraulic Stack Model for Redox Flow Batteries Considering Porosity Variations in Porous Felt Electrodes and Bypass Flow in Side Gaps

Autorzy: X. Guan, M. Skyllas-Kazacos, and C. Menictas
Opublikowane w: Batteries, 2023, ISSN 2313-0105
Wydawca: MDPI
DOI: 10.3390/batteries9070359

A Multiscale Flow Battery Modeling Approach Using Mass Transfer Coefficients

Autorzy: Amadeus Wolf, Emmanuel Baudrin, Hermann Nirschl
Opublikowane w: Energy Technology, Numer Volume 11, Numer 7, 2023, ISSN 2194-4296
Wydawca: Wiley
DOI: 10.1002/ente.202300175

A Computational Protocol Combining DFT and Cheminformatics for Prediction of pH-Dependent Redox Potentials

Autorzy: Rocco Peter Fornari, Piotr de Silva
Opublikowane w: Molecules, Numer 14203049, 2021, ISSN 1420-3049
Wydawca: Multidisciplinary Digital Publishing Institute (MDPI)
DOI: 10.3390/molecules26133978

Physics-based 0D-U-I-SoC cell performance model for aqueous organic redox flow batteries

Autorzy: GaelMourouga, Roman P.Schaerer, XianYang, TobiasJanoschka, Thomas J.Schmidt, Juergen O.Schumacher
Opublikowane w: Electrochimica Acta, Numer 00134686, 2022, ISSN 0013-4686
Wydawca: Pergamon Press Ltd.
DOI: 10.1016/j.electacta.2022.140185

Techno-Economic Optimization of Flow Batteries Using the Optimization Potential to Prioritize Different Optimization Possibilities

Autorzy: Daniel Gerlach, Jens Noack, Katharina Bischof, Chloé Le Boulch, Sabine Trupp
Opublikowane w: Journal of The Electrochemical Society, Numer Volume 170, Number 6, 2023, ISSN 0013-4651
Wydawca: Electrochemical Society, Inc.
DOI: 10.1149/1945-7111/acdda0

Upscaling of Reactive Mass Transport through Porous Electrodes in Aqueous Flow Batteries

Autorzy: Jakub K. Wlodarczyk, Roman P. Schärer, K. Andreas Friedrich and Jürgen O. Schumacher
Opublikowane w: Journal of The Electrochemical Society, Numer 171, 2024, Strona(/y) 020544, ISSN 1945-7111
Wydawca: The Electrochemical Society by IOP Publishing Limited
DOI: 10.1149/1945-7111/ad258e

Gaining Insight into the Electrochemical Interface Dynamics in an Organic Redox Flow Battery with a Kinetic Monte Carlo Approach

Autorzy: Jia Yu, Garima Shukla, Rocco Peter Fornari, Oler Arcelus, Abbos Shodiev, Piotr de Silva, Alejandro A. Franco
Opublikowane w: Small, Numer 16136810, 2022, Strona(/y) 2107720, ISSN 1613-6810
Wydawca: Wiley - V C H Verlag GmbbH & Co.
DOI: 10.1002/smll.202107720

Materiały z konferencji (3)

Techno-economic comparison of different organic flow batteries based on experimental data versus a vanadium flow battery

Autorzy: Daniel Gerlach, Katharina Bischof, Chloé Le Boulch, Jens Noack, Nataliya Roznyatovskaya, Maria Skyllas-Kazacos, Karsten Pinkwart
Opublikowane w: IFBF Conference Papers, Numer annual, 2023, Strona(/y) 38, ISBN 978-1-9162004-3-2
Wydawca: IFBF

A three-dimensional hydraulic model for flow battery stack design optimisation

Autorzy: Xinjie Guan, Maria Skyllas-Kazacos, Chris Menictas, Jens Noack
Opublikowane w: IFBF conference papers, Numer annual, 2023, Strona(/y) 42, ISBN 978-1-9162004-3-2
Wydawca: IFBF 2023

Pore-scale resolved 3D Simulations of aqueous organic flow batteries
Autorzy: Amadeus Wolf, Hermann Nirschl
Opublikowane w: IFBF conference papers, Numer annual, 2022, Strona(/y) 88
Wydawca: IFBF

Zbiory danych

Zbiory danych za pośrednictwem OpenAIRE (2)

heat of hydrogenation for diverse organic compounds -- experimental and calculated data for 166 unique reactions
Autorzy: Maass, Astrid
Opublikowane w: Zenodo

SONAR -- experimental redox potentials for organic compounds undergoing 2-electron/2-proton transfer reactions
Autorzy: Maass, Astrid
Opublikowane w: Zenodo

Oprogramowanie

Oprogramowanie za pośrednictwem OpenAIRE (1)

Code for publication Mourouga et al. 2022 "Estimation of activity coefficients for aqueous organic redox-flow batteries: Theoretical basis and equations"
Autorzy: Mourouga, Gaël; Chery, Déborah; Baudrin, Emmanuel; Randriamahazaka, Hyacinthe; Schmidt, Thomas J.; Juergen O. Schumacher
Wydawca: Zenodo
DOI: 10.5281/zenodo.6926800; 10.5281/zenodo.6926799

Pozostałe produkty badawcze

Pozostałe produkty badawcze dostępne przez OpenAire (3)

Upscaling of reactive mass transport through porous electrodes in aqueous flow batteries

Autorzy: Wlodarczyk, Jakub Karol; Schärer, Roman Pascal; Friedrich, Andreas; Schumacher, Jürgen
Opublikowane w: IOP Publishing

Physics-based 0D-U-I-SoC cell performance model for aqueous organic redox flow batteries

Autorzy: Mourouga, Gaël; Schärer, Roman P.; Yang, Xian; Janoschka, Tobias; Schmidt, Thomas J.; Schumacher, Jürgen O.
Opublikowane w: Elsevier BV

Estimation of activity coefficients for aqueous organic redox flow batteries : theoretical basis and equations

Autorzy: Mourouga, Gaël; Chery, Déborah; Baudrin, Emmanuel; Randriamahazaka, Hyacinthe; Schmidt, Thomas J.; Schumacher, Juergen O.
Opublikowane w: Cell Press

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