



ModVal 2022

SCHEDULE

Day 1 - March 14, 2022

- 14:30 | Arrival
- 17:00 | Registration @ Hotel
- 19:00 | Conference Dinner @ Gutshof-Restaurant

Day 2 - March 15, 2022

- 08:00 | Welcome
- 08:15 | **Keynote: Tejs Vegge**
ML-accelerated simulations of solid-liquid interfaces in batteries and fuel cells
Eventhalle
- 09:00 | Coffee Break @ Gutshof-Foyer

I Data-Driven Battery Modeling
Chair: Tejs Vegge
Eventhalle

- 09:30 | Assessing a novel method for joint state-parameter estimation and optimal fast-charging
Dr. Nicola Courtier
- 09:50 | Bayesian Quadrature for Fast Parameter Estimation of a Lithium-ion Battery
Masaki Adachi
- 10:10 | Generation of digital twins for one- and two-layer battery electrodes containing differently sized active material particles
Dr. Matthias Neumann
- 10:30 | On Uncertainty Quantification in the Parametrization of Newman-Type Models of Lithium-Ion Batteries
Prof. Bartosz Protas
- 10:50 | Bayesian Optimization for Automated Parameterization of 1+1D Battery Cell Models
Yannick Kuhn
- 11:10 | Functional Data-Driven Framework for Fast Predictions of Mechanistic Simulations Results
Marc Duquesnoy

I PEMFC Cell & Water Management
Chair: Marc Secanell
Gutshof-Saal

- 09:30 | Investigation of Liquid Water Heterogeneities in Large Area PEM Fuel Cells using a Two-Phase Flow Multiphysics Model
Prof. Yann Bultel
- 09:50 | Representative Morphology Model for PEFC Catalyst Layer: Operando Water Saturation Determined via Small-Angle X-ray Scattering
Kinanti Aliyah
- 10:10 | Rational approximation for electrochemical systems with constant phase elements: a preliminary study
Dr. Ion Victor Gosea
- 10:30 | Rapid and Local EIS on a Segmented Fuel Cell: Combining Spatial and Temporal Resolution
Tobias Schmitt
- 10:50 | Proton Conductivity in PEFC Catalyst Layers: Imaging-Supported Modeling
Wolfgang Olbrich
- 11:10 | Assisted Cold Start of a PEMFC coupled with a Metal Hydride Reactor
Dr. Tom Gießgen

I Battery Degradation
Chair: Birger Horstmann

- 12:50 | Experimentally validated simulation of strain-induced battery aging
Dr. Ilona Glatt
- 13:10 | Simplified models for electrochemical degradation (SEI and Li plating)
Dr. Ferran Brosa Planella
- 13:30 | Simulation of a Chemo-Mechanical Model for SEI Growth on Battery Anode Particles
Dr. Fabian Castelli
- 13:50 | Li-ion battery degradation: how to model it
Dr. Simon O'Kane

I Electrolysis
Chair: Ulrich Sauter

- 12:50 | Optimal Catalyst Loading of Recombination Interlayers for PEM Water Electrolysis
Dr. Patrick Trinke
- 13:10 | Effects of the Various Serpentine Channels on Proton Exchange Membrane Water Electrolysis Cell Performance with the Large Active
Woojung Lee
- 13:30 | Analytical Multiphase Flow Modeling of Parallel Plate Electrolyzers
Dr. Aviral Rajora
- 13:50 | Modeling and simulation of an alkaline water electrolyzer
Steffen Hess
- 14:10 | Validation of a dynamic alkaline water electrolyzer model with transient experiments
Jörn Brauns

- 14:30 | Coffee Break @ Gutshof-Foyer
- 15:00 | **Keynote: David Howey**
Data-driven battery health diagnosis in real-world applications
Eventhalle

- 15:00 | **Keynote: Marc Secanell**
Transient, multi-scale, multi-phase analysis of polymer electrolyte fuel cells and electrolyzers
Gutshof-Saal

I Battery Degradation
Chair: Birger Horstmann
Eventhalle

- 15:45 | Physics-based interpretation of LIB ageing through P2D model parameters identification
Gabriele Sordi
- 16:05 | Modeling and validation of thermally and intercalation-induced thickness change of a lithium-ion pouch cell during cycling
David Schmider

I AEMFC & AEMEL
Chair: Felix Büchi
Gutshof-Saal

- 15:45 | Modeling direct ammonia anion exchange membrane fuel cells
Prof. Simon Brandon
- 16:05 | Mathematical Modelling of Anion exchange membrane based water electrolysis
Ronit Panda

- 16:30 | Poster Session
- 19:00 | Conference Dinner @ Gutshof-Restaurant

Day 3 - March 16, 2022

- 08:15 | **Keynote: Momo Safari**
Formulation, design, and characterization of NMC porous electrodes: a model-assisted approach
Eventhalle
- 08:15 | **Keynote: Andrea Baricci**
Modelling voltage loss in polymer electrolyte membrane fuel cells after catalyst layer degradation
Gutshof-Saal

I Battery Fundamentals
Chair: Momo Safari
Eventhalle

- 09:30 | Concentration and Velocity Profiles in a Polymeric Lithium-ion Battery Electrolyte
Prof. Hans-Georg Steinrück
- 09:50 | Validity of solid-state Li+ diffusion coefficient estimation by electrochemical approaches for lithium-ion batteries
Zeyang Geng
- 10:10 | Modelling the Transport of Secondary Carriers in a Solid Lithium-Ion Conductor
Dr. Guanchen Li
- 10:30 | A system identification approach to estimate lithium-ion battery entropy coefficients
Dr. Dhammika Widanage
- 10:50 | Entropy measurements of Li and Na battery materials
Dr. Michael Mercer
- 11:10 | Nonlinear Frequency Response Analysis – a Modelling Assessment for Li-ion Batteries
Hoon Seng Chan

I SOFC & SOEC
Chair: Yann Bultel
Gutshof-Saal

- 09:30 | Towards a Solid Oxide Fuel Cell microstructure evolution model calibrated using long-term performance experiment data
Dr. Tomasz Prokop
- 09:50 | Segmented cell testing for local performance and degradation investigation in reversible operation
Dr. Hamza Moussaoui
- 10:10 | Optimization of MIEC-based SOFC anodes by Digital Microstructure Design (DMD)
Philip Marmet
- 10:30 | Capacitance of the blocking YSZ|Au electrode
Dr. Petr Vágner
- 10:50 | Modelling and experimental investigation of a reversible SOC using Total Harmonic Distortion Analysis as an advanced online monitoring tool
Gerald Hammerschmid
- 11:10 | Optimizing innovative Power-to-Methane plant concepts with integrated SOEC module via multi-scale modelling
Lukas Wehrle

I 3D Battery Modeling
Chair: Timo Danner

- 12:50 | Modelling inhomogeneous degradation in lithium-ion batteries: the effect of thermal gradients
Dr. Shen Li
- 13:10 | Performing Fully-Coupled Electrochemical-Thermal Simulations of Cylindrical Cell Jelly Rolls in 3D
Dr. Simon Clark
- 13:30 | 3D microstructure characterization of polymer-based battery electrodes by statistical image analysis based on synchrotron tomography
Marten Ademmer
- 13:50 | Microstructure-resolved modelling of solid-state batteries: The importance of anisotropy and secondary phases in the composite cathode
Moritz Clausnitzer
- 14:10 | A Computational Approach for 3D Resolved Electro-Chemo-Mechanical Analysis of ASSB Including Contact Effects
Christoph Schmidt

I Redox Flow Batteries
Chair: Roswitha Zeis

- 12:50 | 3D printed electrodes for redox flow batteries
Dr. Jonas Hereijgers
- 13:10 | Modelling and Simulation for the Search for New Active Materials for Redox Flow Batteries - Results of the International Project SONAR
Prof. Jens Noack
- 13:30 | Non-solvent Induced Phase Separation: A Versatile Synthetic Method for High Performance Redox Flow Battery Electrodes
Prof. Antoni Forner-Cuenca
- 13:50 | In situ and in operando detection of redox reactions during vanadium transport in ion exchange membranes
Torben Lemmermann
- 14:10 | Pore-scale resolved 3D simulation of aqueous organic flow batteries
Amadeus Wolf

I Lithium Intercalation
Chair: David Howey
Eventhalle

- 14:45 | Current Constriction at the Li|Li7La3Zr2O12 Interface
Janis Kevin Eckhardt
- 15:05 | Linear stability analysis of a graphite multi-layer phase field model
Antoine Cordoba
- 15:25 | Compensatory measures to overcome performance limitations of recycled Li-ion battery materials
Marco Lagnoni
- 15:45 | A guideline to the time-adaptive reduced order modelling of lithium-ion cells
Eduardo Jané
- 16:05 | Development and Verification of a Method to efficiently solve Discontinuous Thermal Transport Models
Oliver Queisser

I PEMFC Microstructure & Degradation
Chair: Andrea Baricci
Gutshof-Saal

- 14:45 | Macroscopic simulation of 1000 PEMFC ageing cycles
Dr. Guillaume Serre
- 15:05 | Modeling of platinum oxides formation and reduction: a performance model for O2 reduction reaction
Florent Vandenberghe
- 15:25 | High-fidelity pore-level simulation of the flow in the channel and GDL of a micro-PEFC
Seyyed Khatoonabadi
- 15:45 | Predicting optimal catalyst layer microstructures in low Pt loading PEMFCs
Corey Randall
- 16:05 | Automating Image Analysis for Electrochemical Materials Characterization with Deep Learning
André Colliard Granero

- 16:30 | Concluding Remarks and Announcement of ModVal19 @ Eventhalle
- 16:45 | End



Supporting Partners

Sponsors & Exhibitors

Batteries

I Battery Fundamentals

- B1.1** | A Geometry-corrected Pore Network Model for the Electrolyte Filling of Batteries
Benjamin Kellers
- B1.2** | Why do we observe a momentum flow in eNMR measurements?
Franziska Kilchert
- B1.3** | Analysis of Nonlinear Features in the Machine Learning-based Modeling of Lithium-Ion Batteries
Joachim Schaeffer
- B1.4** | Simulative Analysis of Efficiently Computed Chemical-Mechanical Coupled Contact Problems for Battery Active Particles
Raphael Schoof
- B1.5** | Solvation Behaviour in Electrochemical Double Layers: Modeling Solvation Energy
Constantin Schwetlick
- B1.6** | Incorporating Transport Effects in Coatings and Grain Boundaries into a Monolithically Coupled Electrochemistry-Mechanics Model for ASSB
Stephan Sinzig

I Battery Cell Models

- B3.1** | Prediction of Reversible Lithium Plating with a Pseudo-3D Lithium-Ion Battery Model
Dr. Serena Carelli
- B3.2** | Investigating sodium-iodine battery cathodes using EIS simulations
Felix Gerbig
- B3.3** | A Multi-Process Cathode Model for MnO₂-based Aqueous Zinc-Ion Batteries
Niklas Herrmann
- B3.4** | Lithium-ion cell optimisation using a time-adaptive reduced order model
Ruth Medeiros
- B3.5** | Full parametrization of commercial 18650 battery cell for physics-based modelling
Bhawna Rana
- B3.6** | Reduction of battery module equivalent circuit models using a distribution of time constants analysis
Tom R ther
- B3.7** | Parameterization of Lithium-Ion Batteries: Differences and Similarities between High Energy and High Power Cylindrical Cells
Christina Schmitt
- B3.8** | A new continuum model of Metal-Sulfurized Polyacrylonitrile (SPAN) batteries
Esther Kezia Simanjuntak
- B3.9** | Conceptual design of solid-state electrode for eVTOL urban air mobility
Dr. Somayeh Toghiani
- B3.10** | From Particle-Scale Information to Cell Performance
Johannes Wiedemann

I Battery Degradation

- B2.1** | Degradation and State Estimation of Li-Ion Batteries in Satellite Applications
Linda Bolay
- B2.2** | Coupled modeling of the thermal, electrical and aging behavior of Li-ion battery cells
Lisa Cloos
- B2.3** | Modeling and Simulation of Transport, Interfaces and Mechanics inside the SEI
Lukas K bbing
- B2.4** | Towards physically interpretable neural ODEs with an example for SEI formation
Srivatsan Ramasubramanian
- B2.5** | An Efficient Numerical Solver for SEI Degradation in Li-Ion Batteries
Falco Schneider
- B2.6** | Chemical Thermal Runaway Modelling of Lithium Ion Batteries for Prediction of Heat and Gas Generation
Niklas Weber

I Battery Electrode Models

- B4.1** | Simulation of Li-Plating in Si/Graphite Composite Electrodes
Lioba Boveleth
- B4.2** | The Effect of Mechanical Cycling on the Electronic Conductivity of Composite Electrodes
Thimo Brendel
- B4.3** | Influence of Carbon Binder Domain on the Performance of Lithium-Ion Batteries: Impact of Size and Fractal Dimension
Anshuman Chauhan
- B4.4** | Methods from machine learning for the structural analysis of Li-ion electrode particles
Orkun Furat
- B4.5** | Binder identification in granular and fibrous energy material scans
Dr. Ilona Glatt
- B4.6** |
- B4.7** | Modelling of Laser Structured Electrodes
Dr. Franz Pichler
- B4.8** | Modelling Lithium Flow from Power-Law Creep in 2D
Albert Pool
- B4.9** | Effect of a Heterogeneous Distribution of the Conductive Additives and Binder Domain on the Impedances of Lithium-Ion Battery Electrodes
Mrudula Prasad
- B4.10** | Reconstruction of the carbon-binder domain in Li-ion battery cathodes and its influence on the electrochemical performance
Benedikt Prifling
- B4.11** | Particle based computation of mechanics in granular multiphase electrodes
Alexandra Wahn

Fuel Cells, Electrolysis & Redox Flow

I Fuel Cells

- F.1** | Control of hybrid PEM fuel cell system reducing degradation based on Reinforcement Learning
Matthias Bahr
- F.2** | Distribution of current density across the active area of the JRC ZEROCELL single cell PEM fuel cell testing hardware
Dr. Tomasz Bednarek
- F.3** | In-situ estimation of effective diffusion coefficients in PEMFC
Rémi Bligny
- F.4** | Evaluation of different system configurations for a heavy duty PEM fuel cell system model
Joscha Böhm
- F.5** | Fault detection and identification for Polymer Electrolyte Membrane Fuel Cell
Prof. Yann Bultel
- F.6** | Performance degradation of Proton Exchange Membrane Fuel Cells under Repeated Compression for the Maintenance
Bogeun Choi
- F.7** | Investigation of Water Cluster and Droplet Interactions in PEFC using Operando XTM
Tim Dörenkamp
- F.8** | Multiphase and Pore Scale Modeling on Catalyst Layer of High-temperature Polymer Electrolyte Membrane Fuel cell
Kangjun Duan
- F.9** | Machine Learning in Dynamic Fuel Cell Modeling
Dieter Froning

- F.10** | Impedance-Based, Multi-physical DC-Performance-Model for a PEMFC Stack
Tobias Goosmann
- F.11** | 2-D + 1-D PEM fuel cell model for fuel cell system simulations
Dr. Sönke Gößling
- F.12** | Model-based investigation of PEMFC ageing under realistic automotive conditions
Amedeo Grimaldi
- F.13** | Simulating the Cathode Catalyst Layer of a PEM Fuel Cell using Lattice Boltzmann Modelling
Konrad Gülicher
- F.14** |
- F.15** | Monte Carlo simulation of electrical and thermal conductivity for highly filled compo-site in fuel cells
André Kayser
- F.16** | Application of Loewner framework for data-driven modeling of electrochemical energy technologies
Bansidhar Patel
- F.17** | The impacts of GDL contact angle on the water management of the PEMFC: 3D simulation and optimization using artificial neural networks
Hossein Pourrahmani
- F.18** | Unravelling the Water Distribution in the Cathode of a Polymer Electrolyte Fuel Cell
Yufan Zhang

I Electrolysis

- E.1** | Water management in gas-fed CO₂ reduction devices with bipolar membranes
Matthieu Dessiex
- E.2** | TFFA model for electrochemical CO₂ reduction at silver gas diffusion electrodes
Marco Löffelholz
- E.3** | Elucidating the Effect of Electro-Osmotic Drag on H₂ Crossover at High Current Densities in PEM Water Electrolysis
Agate Martin

- E.4** | A Scaling Analysis for Bubble Plumes in Gas Evolving Electrodes
Aviral Rajora
- E.5** | Simulation-aided Prototyping of Photo-electrochemical (PEC) Cell Design
Carmen Tenholt
- E.6** | Quantifying Water Transport Limitations in Bipolar Membrane Electrolysis in Dependence of Membrane Thickness
Oskar Weiland

I Redox Flow Batteries

- R.1** | Kinetics of Oxygen Evolution Reaction in Soluble Lead Flow Batteries
Miji Joy
- R.2** | Detailed Model of a Vanadium Flow Battery Including Separator Crossover and Electrolyte Composition Changes
Alexander Kubicka
- R.3** | Reactive Transport in Porous Electrodes: From Pore-scale to Macroscale Descriptions
Dr. Roman Schärer

- R.4** | The mass transfer effects of pulsating flow in redox flow batteries
Renée De Wolf
- R.5** | Performance evaluation of vanadium redox flow battery: An effect of pre-treatment and porosity of carbon felt electrode
Anand Kumar Tripathi