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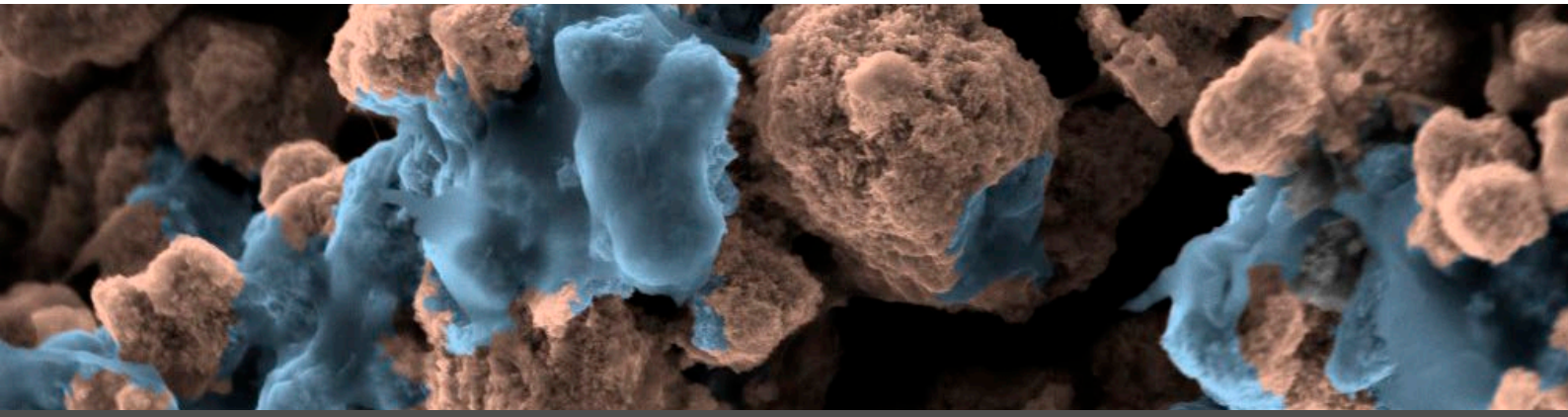
20th Symposium on Modeling and Validation of Electrochemical Energy Technologies

ModVal 2024



Program

March 13–14, 2024
Baden, Switzerland

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COVER PHOTO:

SEM image of an anode catalyst layer for a polymer electrolyte water electrolyzer cell (catalyst brown and ionomer blue).
Related article: EES Catalysis 2 (2024) 585-602 (DOI: 10.1039/D3EY00279A)

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Program

Tuesday March 12th, Evening

18:30	Registration desk opens
19:00	Welcome Get-Together with Apéro Riche (Trafo Halle 37)
21:30	Closing

Wednesday March 13th, Morning 1

8:00	Registration desk opens	
8:45	Welcome, Room 36-2	
9:00	Plenary 1, Chair: L. Gubler, Room 36-2 **U. Krewer** Electrosynthesis: Modeling Processes at Electrodes	
	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
9:50	Short Break	
10:00	Session A1: *Durability* Chair: C. Fink	Session B1: *Electrolyte* Chair: E. Knobbe
10:00	**J. Heitz** Unraveling the Influence of Ionomer on Catalyst Layer Degradation in Proton Exchange Membrane Fuel Cells: A Hierarchical Modeling Approach	**C. Schwetlik** A model for Solvation in Battery Electrolytes and analysis of Electrochemical Double Layer differential capacitance
10:20	**L. Klass** Bootcamp for Neural Networks: Boost Neural Network Training using Physical Simulation Models and Transfer Learning for Fuel Cell Operation Monitoring	**T. Ayadi** Ab initio study of the thermodynamic properties of the Li_6PS_5Cl solid electrolyte
10:40	**A. Abd El Kader** Investigating the Impact of Air Pollutants on Fuel Cell Performance and Durability: Experimental and Modelling Approaches	**B. Ruhstaller** Extracting Ion Density and Mobility - Transient Current Method Revisited
11:00	Coffee Break	

Wednesday March 13th, Morning 2

	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
11:30	Session A2: *Solid Oxide Fuel Cell (SOFC)* Chair: F. Büchi	Session B2: *Processing* Chair: W. Bessler
11:30	**R.K. Jeela** Multiphase-field Simulation studies on Coarsening in FIB-SEM reconstructed Ni/CGO SOFC Anodes	**B. Kellers** Systematic Workflow for Efficient Identification of Local Representative Elementary Volumes
11:50	**S. Golani** Impedance model for SOFC stacks	**M. Prasad** Influence of Passive Material Distribution and its Structural Properties on Cathode Performance
12:10	**N. Sawant** Towards SOFC modeling with the Lattice Boltzmann method	**G. Lenne** Modeling Li-ion battery electrodes accounting for microstructure properties: The Newman's model revisited
12:30	Lunch & Poster Session (Halle 37)	

Wednesday March 13th, Afternoon 1

	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
14:00	Session A3: *PEFC Water Management* Chair: M. Hanauer	Session B3: *Cathode* Chair: A. Latz
14:00	Invited A3 **J. Pauchet** Liquid water formation and transport in Membrane Electrode Assembly of PEMFC: liquid injection, vapor condensation and mixed scenario	Invited B3 **I. Castelli** Computational Workflows for an Accelerated Design of Novel Materials and Interfaces
14:30	**Y. Sun** Effect of liquid saturation transients on electrochemical impedance of PEM fuel cell	**O. Furat** Quantifying the impact of operating conditions on particle cracking in Li-ion battery cathodes, using super-resolution of SEM images and stereology
14:50	**P. Oppek** Empirical PEMFC model for local performance and resistance prediction	**S. Daubner** Investigation of nano-porous cathode particles for battery cell simulations
15:10	**L. König** Predicting the performance of real fuel cells with a fast MATLAB model	**J. Naumann** Understanding the effect of hierarchically structured cathode morphology on the performance of intercalation battery cells
15:30	Coffee Break & Poster Session (Halle 37)	

Wednesday March 13th, Afternoon 2

	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
16:00	Session A4: *Two-Phase Flow* Chair: J. Pauchet	Session B4: *Methods & Analytics* Chair: E. Ayerbe
16:00	**I. Dorner** Model-assisted Analysis of Carbon-free Silver Gas Diffusion Electrode Designs for Performance Enhancement in Electrochemical CO_2 Reduction	**E. Hagopian** Improving the Relationship between State of Charge, Charge History and Voltage Hysteresis Evolution in First Order Differential Equation Voltage Hysteresis Models
16:20	**T.C. Ma** Modeling the Interface between Transport and Catalyst Layer and its Influence on Water Electrolysis Performance	**X. Raynaud** Optimization and Parameterization of Electrochemical Systems in BattMo, the Battery Modeling Toolbox
16:40	**L. Feierabend** Numerical and Experimental Analysis of Two-phase Flow in Porous Transport Layers in Water-Electrolysis Processes	**J. Valenzuela** Parametrization of a Thermochemical-Kinetic Model for Gas Analysis of Lithium-ion Batteries
17:00	(talk canceled)	**N. Hallemans** Characterising diffusion in lithium-ion batteries from operando impedance measurements during relaxation
17:30 19:00	Poster Session with Snacks & Drinks (Halle 37)	
19:30	Conference Dinner (Trafohalle)	
22:30	Closing	

Thursday March 14th, Morning 1

9:00	Plenary 2, Chair: S. Trabesinger, Room 36-2 **A. Latz** Battery Design by Modeling and Simulation: From Particle over Electrode Structure to Cell Performance	
9:50	Short Break	
	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
10:00	Session A5: *Redox Flow Battery (RFB)* Chair: J. Schumacher	Session B5: *Lithium Plating* Chair: I. Castelli
10:00	**M. Barzegari** Topology optimization of porous electrodes for redox flow batteries using the finite element method	**S. Sahu** A continuum model for lithium plating and dendrite formation in lithium-ion batteries: formulation and validation against experiment
10:20	**R.P. Schärer** An Open-source Model for High-throughput Flow Battery Cell Performance Predictions	**M. Lagnoni** Interplay between charging and plating in graphite electrodes via phase-field modelling and operando optical microscopy
10:40	**M. Jałowiecka** Tracking CO_2 bubble flow in a direct formic acid fuel cell, numerical and experimental investigation	**N. Bless** A complementary model-based approach with electrochemical and operando microscopy experiments to unravel Li plating in Lithium-ion batteries
11:00	Coffee Break & Poster Session (Halle 37)	

Thursday March 14th, Morning 2

	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
11:30	Session A6: *Stacks & Systems* Chair: J. Eller	Session B6: *State of Charge* Chair: F. Röder
11:30	**S. Mull** Experimental and simulative analysis of the dependence between liquid water amount and mass transfer in a planar membrane humidifier	**T. Hofmann** The ΔQ-Method: State of Health and Degradation Mode Estimation for Lithium-Ion Batteries Using a Mechanistic Model with Relaxed Voltage Points
11:50	**S. Nicolay** Model-based design of a strategy for switching stacks in a multi-stack PEM fuel cell system	**X. Gao** Predicting failure behaviors in lithium-ion batteries subjected to thermal abuse following long-term degradation
12:10	**E. Revello** Thermal Management Design and Optimization for Hydrogen-Powered Fuel Cell Systems in Aviation	**S. O'Kane** Lithium-Ion Battery Degradation: the Missing Piece in Model Validation
12:30	**Y. Fischer** Spatially Resolved Quantification of Diffusion Losses in a Segmented PEM Fuel Cell with adjustable Clamping Forces	**W. Bessler** Operando SOC and SOH diagnosis with voltage-controlled models: Application to an LFP battery pack and to smart phone batteries
12:50	Lunch & Poster Session (Halle 37)	

Thursday March 14th, Afternoon

	Session A *Conversion Devices* Room 36-3	Session B *Batteries* Room 36-2
14:00	Session A7: *Catalyst Layer* Chair: J. Herranz	Session B7: *Lithium Transport* Chair: O. Furat
14:00	Invited A7 **F.N. Büchi** The Catalyst- and Porous Transport Layer Interface: Decisive for PEWE Performance	Invited B7 **N. Marzari** What Electronic-structure Simulations Can Teach Us About Li-ion Batteries
14:30	**M.G. Justino Vaz** Effect of Model Parameters on the Performance of a PEM Fuel Cell Using a Pore-scale Catalyst Layer Model	**F. Mendez-Corbacho** Physics Informed Neural Network for solving Single Particle Model without using labeled data
14:50	**K. Gülicher** Simulation of Oxygen Diffusion and Reduction Reaction in the Cathode Catalyst Layer of a PEM Fuel Cell using Lattice Boltzmann Modeling	**M. Cornish** Modelling Dynamic Limitations of Lithium Transport in Lithium-Sulfur Batteries
15:10	**E. Tardy** Modeling Oxygen Reduction Reaction kinetics in a Gas Diffusion Electrode	**R. Pakula** Application and customization of Matlab Simscape framework for P2D simulation of batteries
15:30	**Y. Hou** Machine Learning-Assisted Optimization of Proton Exchange Membrane Fuel Cell Catalyst Layer Production Recipe	**F. Röder** Modeling of Path Dependency in Batteries
15:50	Short Break	
16:00	ModVal 2025 Announcement Room 36-2	
16:15	Poster Award & Farewell Room 36-2	

Organizing Committee

Dr. P. Boillat

Senior Scientist, Fuel Cell Systems and Diagnostics Group & Laboratory for Neutron Scattering and Imaging

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Senior Scientist, Fuel Cell Systems & Diagnostics Group

Dr. Mario El Kazzi

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PD Dr. Lorenz Gubler

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Dr. Juan Herranz

Group Head, Fuel Cell Systems & Diagnostics

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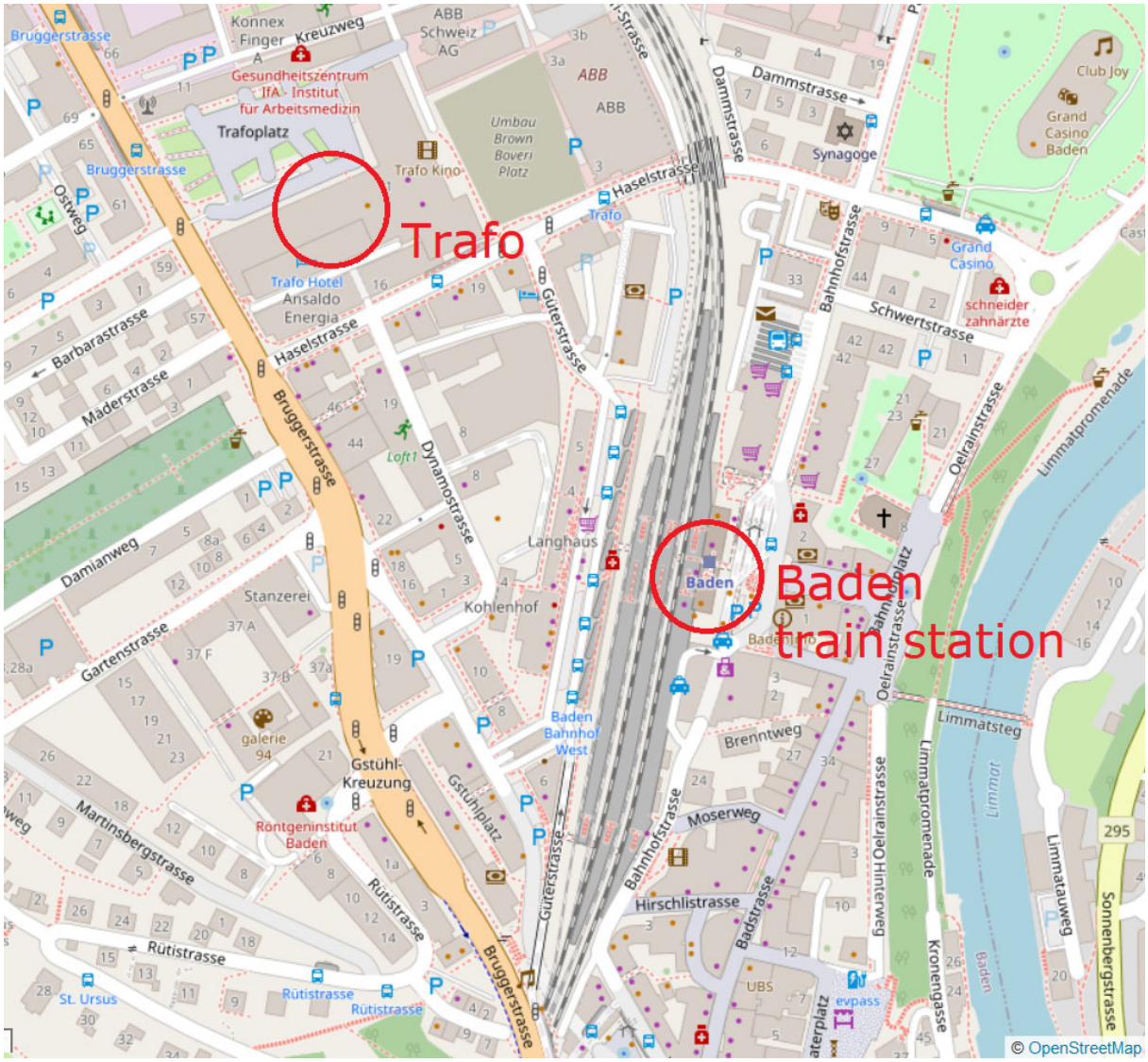
Group Head, Battery Electrodes & Cells

Map Baden



Conference Venue

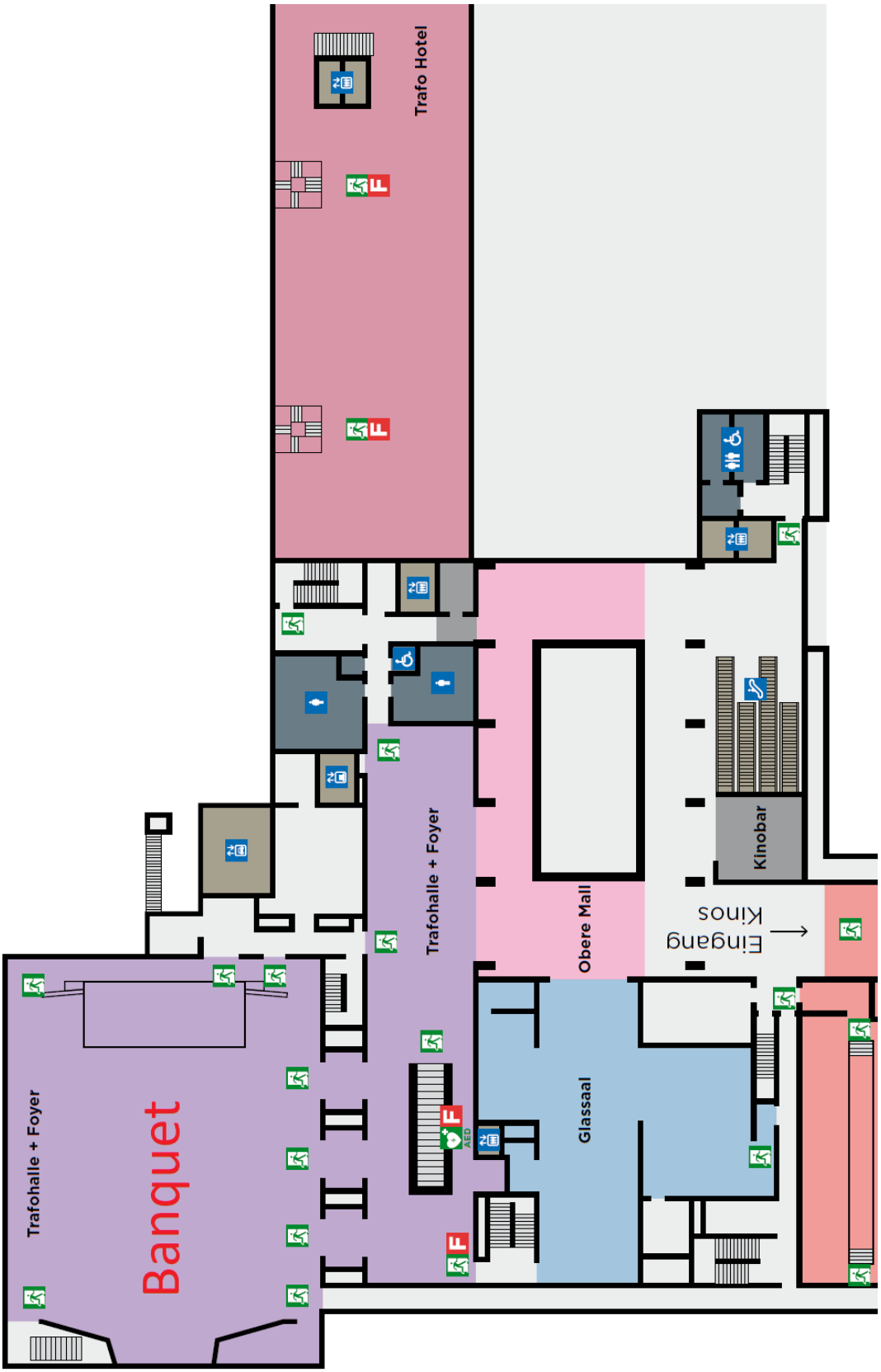
Trafo Baden
Brown Boveri Platz 1
5400 Baden

Web: www.trafobaden.ch
Phone: +41 (0)56 204 08 88

Walking distance between Trafo and Baden train station: 5 min.

Trafo Floor Plan, Ground Floor

Trafo Floor Plan, First Floor



Trafo, Venue Layout

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