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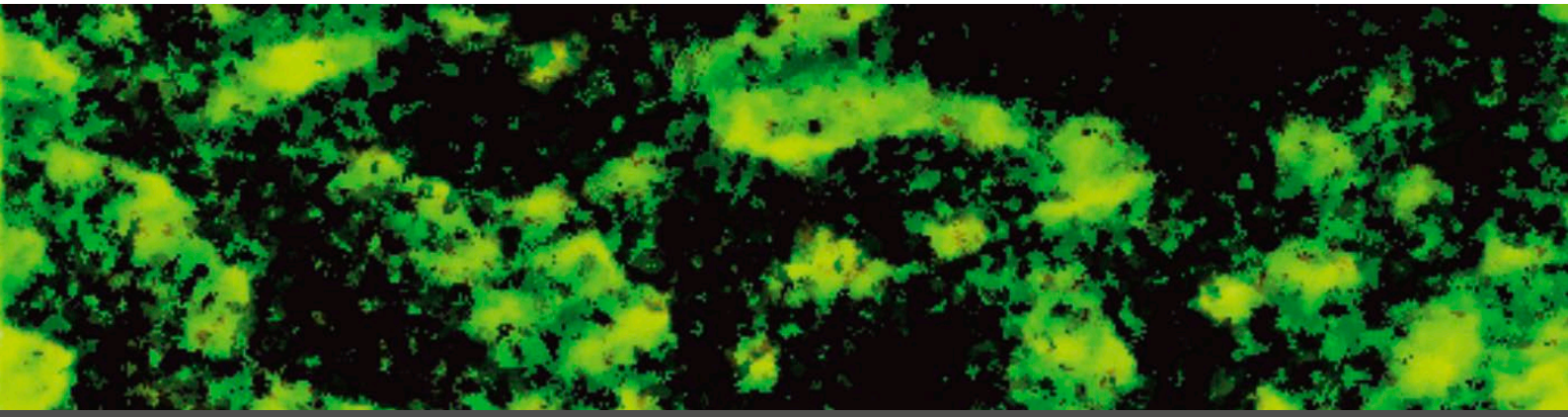
15th Symposium on Modeling and Experimental Validation of Electrochemical Energy Devices

ModVal 2018



Program

April 12–13, 2018
Aarau, Switzerland

www.modval2018.ch

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COVER PHOTO:

Elemental mapping of the surface of a proton conducting fuel cell membrane prepared by swift heavy ion beam irradiation and grafting. Green areas (sulfur) indicate ion conducting domains (diameter around 1 micron), black areas (fluorine) the insulating matrix. Related article: J. Mater. Chem. A 5 (2017) 24826 (DOI: 10.1039/c7ta07323b)

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Program

Thursday April 12th, Morning

	Session A (*Flow Batteries*) Saal 2	Plenary & Session B (*Batteries*) Saal 1
8:45	Welcome	
9:00	Plenary 1, Chair: F. Büchi **A. Kucernak** Mass transport free electrocatalysis of the oxygen and hydrogen reactions – effect of surface sites and spectator species	
9:50	Coffe Break & Poster Mounting	
	Session A1 Redox Flow Batteries Chair: L. Gubler	Session B1 Microstructure I Chair: E.J. Berg
10:20	Invited A1 **J. Noack** Current development trends and challenges for redox-flow batteries	Invited B1 **V. Wood** Understanding the Impact of Separators on Lithium Ion Battery Performance
10:50	**F. Oldenburg** Balancing Transport with Amphoteric Membranes in All-Vanadium Redox-Flow Batteries at Different Current Densities	**J. Landesfeind** Critical Analysis of Tortuosity Values obtained from Impedance Spectroscopy and X-Ray Tomographic Data
11:10	**R. Banerjee** Characterization of Carbon Felts for Vanadium Redox Flow Batteries – A Pore Network Modelling Approach	**Y. Kerdja** 3D Imaging and Multi-Scale Modeling For Positive Electrode Materials Of Lithium-Ion Batteries
11:30	**G. Shukla** A Kinetic Monte Carlo Framework for a Discrete Multiphysics Description of Semi-Solid Redox Flow Batteries	**O. Birkholz** Influence of the electrode microstructure on the effective electronic and ionic conductivity of Lithium Ion Batteries using discrete element methods
11:50	**L. Feierabend** Model Development and Simulation of Flowing Slurry Electrodes for Zinc-Air Batteries	**S. Müller** Heterogeneity of Lithium Ion Battery Electrodes and its Influence on Electrochemical Performance
12:10	Lunch & Poster Session (Foyer)	

Thursday April 12th, Afternoon 1

	Session A (*Conversion Devices*) Saal 2	Plenary & Session B (*Batteries*) Saal 1
13:20	Plenary 2, Chair: E.J. Berg **A. Van der Veen** Linking electrode behavior at the macro and meso scale to electronic structure	
	Session A2 Electrolysis Chair: R. Hanke-Rauschenbach	Session B2 Microstructure II Chair: V. Wood
14:20	Invited A2 **M. Carmo** Perspectives on the Research and Development of Low Temperature Water Electrolyzers	Invited B2 **V. Schmidt** Stochastic microstructure modelling of aggregate particle systems in hierarchically structured electrodes
14:50	**I. Zenyuk** *Operando* X-ray tomography and sub-second radiography for characterizing transport in polymer electrolyte membrane electrolyzer	**T. Hofmann** Electro-chemo-mechanical simulation of 3D-microstructures for lithium-ion batteries
15:10	**P. Trinke** Modelling of the supersaturation of dissolved gas in PEM electrolysis cells	**R. Morasch** Experimental Validation of Simulated Ionic Resistances in Laser-Structured Electrodes
15:30	**G. Serre** PEM water electrolysis modelling: Upscaling strategies	**T. Danner** Microstructure-Resolved Impedance Simulations for the Characterization of Li-Ion Battery Electrodes
15:50	**G. Futter** Modeling of SOECs –Physics-based Impedance Analysis of MIEC electrodes	**S. Cernak** Influence of non-spherical active material particles on the macroscopic cell performance of three-dimensional battery simulations on the microscale
16:10	Coffee Break & Poster Session (Foyer)	

Thursday April 12th, Afternoon 2

	Session A (*Conversion Devices*) Saal 2	Session B (*Batteries*) Saal 1
	Session A3 PEFC Modeling Chair: Y. Bultel	Session B3 Beyond Li-ion Chair: A. Van der Veen
16:40	**J. Fuhrmann** Robust quality preserving numerical methods for electroosmotic flows	**M. Ebadi** Modelling Lithium/Electrolyte Interfaces for Li-Metal Batteries
17:00	**J. Schumacher** An open implementation of a two-phase PEMFC model in MATLAB	**M. Bayer** Electrochemical modeling and its influence on Na-MCl_2 cell design
17:20	**M. Siegwart** Time-of-flight neutron imaging for the localization of freezing events during PEFC cold starts	**G. Bauer** Multi-scale and multi-physics simulation of all solid-state batteries
17:40	**S. Zhang** Simulation of a high temperature polymer electrolyte fuel cell short stack with OpenFuelCell	**G. Li** Modelling Space Charging in Multi-carrier Solid Electrolytes
19:30	Conference Dinner (Sorell Hotel Aarauerhof)	

Friday April 13th, Morning 1

	Session A (*Conversion Devices*) Saal 2	Plenary & Session B (*Batteries*) Saal 1
8:30	Plenary 3, Chair: L. Gubler **R. Hanke-Rauschenbach** Modeling of PEM water electrolysis: A review	
	Session A4 Catalysis Chair: J. Eller	Session B4 System & Parameter Validation Chair: P. Novák
9:30	Invited A4 **E. Fabbri** Insights into Perovskite Nano-Catalysts as Oxygen Electrodes for the Electrochemical Splitting of Water	Invited B4 **W. Bessler** End-of-life prediction of lithium-ion battery cells based on mechanistic ageing models of the graphite electrode
10:00	**R. Alink** Modeling of Cathode Catalyst Degradation in PEM Fuel Cells	**D. Howey** Parametrisation of the Single Particle Model for Lithium-ion Cells
10:20	**T. Haisch** Origin of the hysteresis between forward and reverse peak in cyclic voltammograms of the alkaline methanol electrooxidation	**S. Kosch** An efficient two-dimensional cell model for lithium-ion cells based on pseudo-spectral collocation method
10:40	**M. Lin** An integrated concentrated solar fuel generator concept utilizing a tubular solid oxide electrolysis cell as the solar absorber	**V. Laue** Is parameter estimation with a pseudo-2-dimensional battery model more than curve fitting?
11:00	Coffee Break & Poster Session (Foyer)	

Friday April 13th, Morning 2

	Session A (*Conversion Devices*) Saal 2	Session B (*Batteries*) Saal 1
	Session A5 Microstructures Chair: I. Zenyuk	Session B5 Ageing & Degradation Chair: W. Bessler
11:30	**N. Prasianakis** High performance full resolution modelling of mass transport and phase change phenomena in anode and cathode sides of PEFCs	**J. Reniers** Battery degradation modelling for optimal control of grid-connected lithium-ion batteries
11:50	**J. Yu** Simulation of Water Transport in the Stochastic Micro-structure of Polymer Electrolyte Fuel Cell Using the Lattice Boltzmann Method	**K. Darcovich** Fast mode switching effects on battery degradation
12:10	**A. Mularczyk** Convection driven droplet detachment from gas diffusion layers	**B.-X. Xu** Phase-field Modeling on Li-ion Batteries
12:30	**C. Evangelisti** New porous Nickel-doped Materials for alkaline water electrolysis	**T. Danner** Local Inhomogeneities and their Impact on Lithium Plating in Lithium-Ion Batteries
12:50	Lunch & Poster Session (Foyer)	

Friday April 13th, Afternoon

	Session A (*Conversion Devices*) Saal 2	Session B (*Batteries*) Saal 1
	Session A6 Cell Level Modeling Chair: J. Schumacher	Session B6 Ion Transport & Interfaces Chair: D. Howey
14:00	**Y. Bultel** Investigation of liquid water heterogeneities in large area PEM fuel cells using a pseudo-3D multiphysics model	**T. Zhang** A Nonlocal Species Concentration Theory: Application to Phase-separating Lithium ion Battery Cathode Particles
14:20	**C. Fink** 3D Modeling of Chemical Degradation Mechanisms in PEM Fuel Cells	**L. Blume** Non-linear Lithium-Solid Polymer Electrolyte Interface Kinetics Investigated by Millisecond Current Pulses
14:40	**A. Niroumand** Electrochemical detection of electric shorts in PEM fuel cell stacks	**J.Y. Ko** Electrochemical modeling of intercalation electrode NMC(1/3): Determination of transport and kinetic properties
15:00	**H. Grimler** Understanding limiting processes in anion-exchange membrane fuel cells	**M. El Kazzi** The Controversial Surface Reactivity of $Li_4Ti_5O_{12}$ in the Aprotic Electrolyte Disclosed with XPEEM
15:20	ModVal 2019 Announcement and Closing	

Organizing Committee

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Department of Chemistry, Uppsala University, Sweden

Dr. Felix N. Büchi

Head Fuel Cell Systems and Diagnostics Group, Paul Scherrer Institut

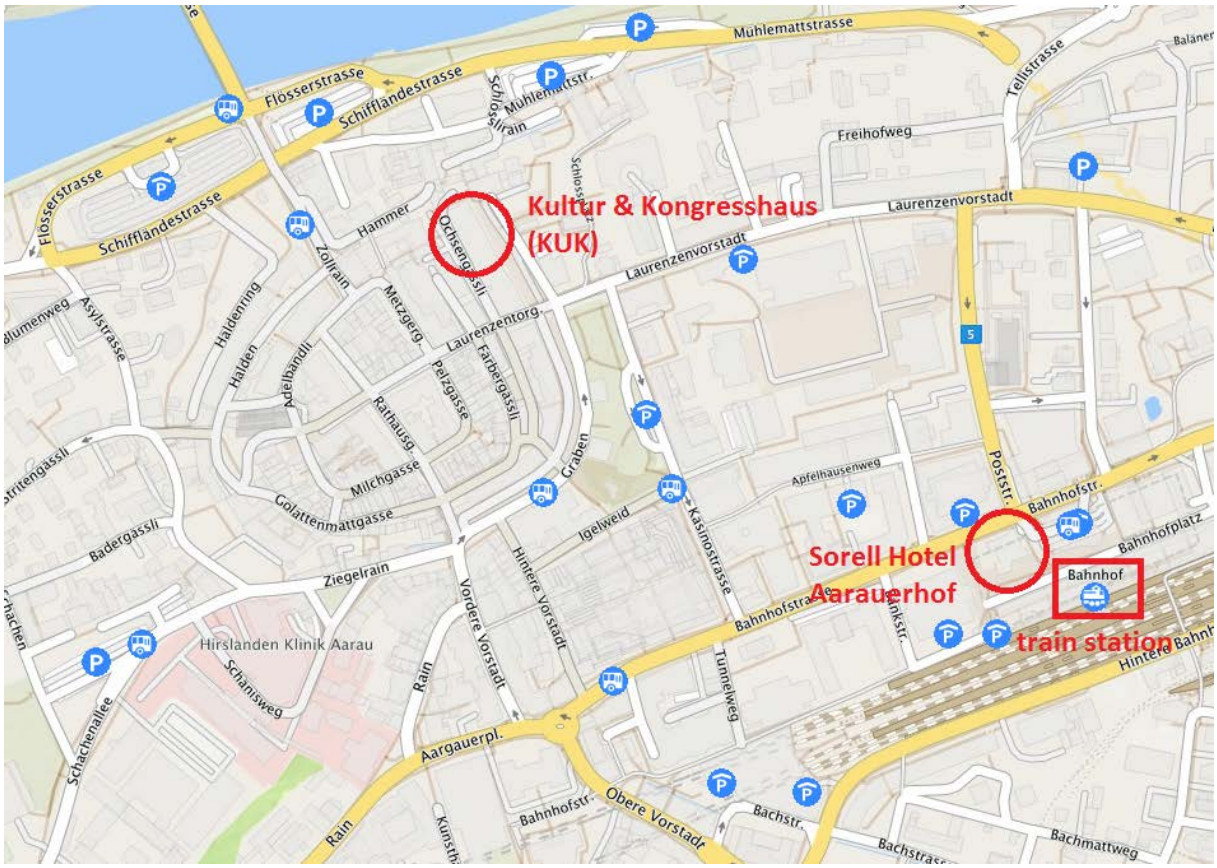
Dr. Jens Eller

Senior Scientist, Fuel Cell Systems and Diagnostics Group, Paul Scherrer Institut

Dr. Lorenz Gubler

Head Membranes and Electrochemical Cells Group, Paul Scherrer Institut

Map Aarau



Conference Venue

Kultur & Kongresshaus (KUK) Aarau
Schlossplatz 9
5000 Aarau

Web: www.kuk-aarau.ch
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Conference Dinner (Thursday, April 12, 19:30)

Sorell Hotel Aarauerhof
Bahnhofplatz 2
5000 Aarau

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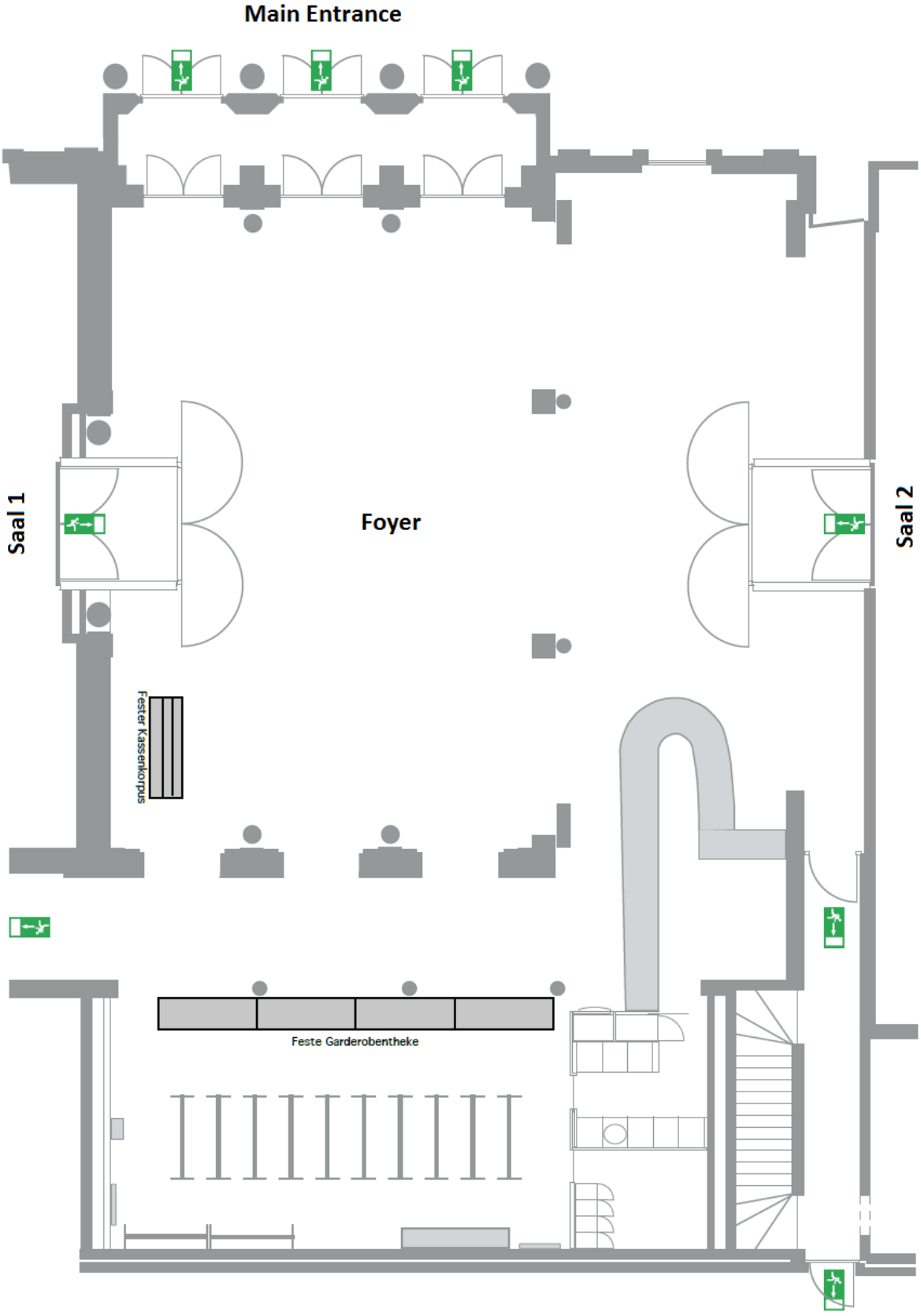
Phone: +41 (0)62 837 83 00

Walking distance between KUK and Sorell Hotel Aarauerhof: 10 min.

KUK Floor Plan



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