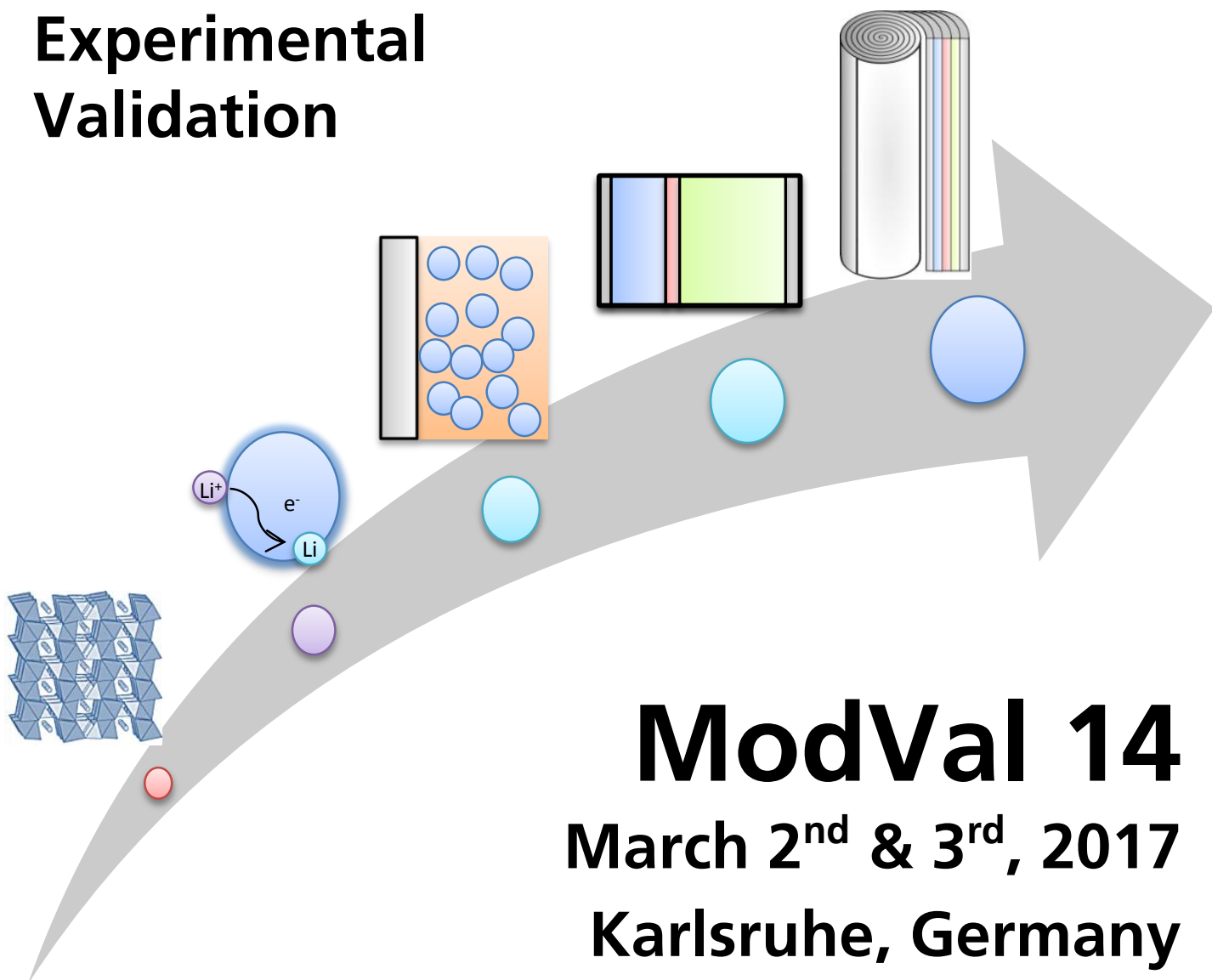


14th Symposium on Fuel Cell and Battery Modelling and Experimental Validation

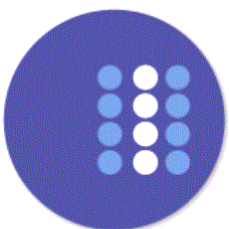


ModVal 14

March 2nd & 3rd, 2017

Karlsruhe, Germany

Conference Programme



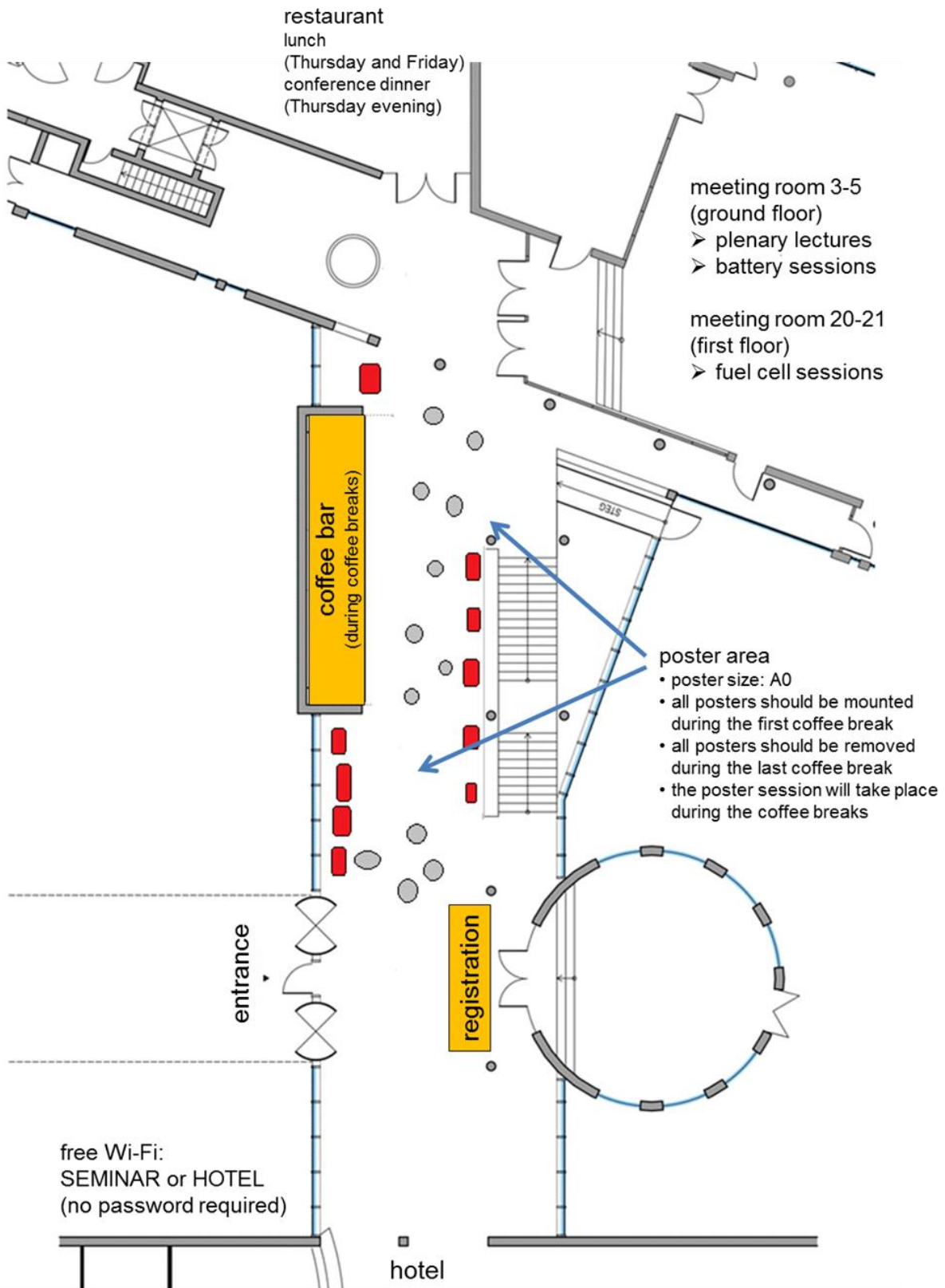
PROSOFC

This conference is supported by the Seventh Framework Program, Theme SP1-JTI-FCH.2012.3.2, project PROSOFC "Production and Reliability Oriented SOFC Cell and Stack Design", grant agreement no 325278.

AkademieHotel Karlsruhe

Am Rüppurrer Schloss 40, 76199 Karlsruhe

phone: +49 721 98 98-0, <http://www.akademiehotel-karlsruhe.de>



Travel Information

Karlsruhe is located in the southwest of Germany close to the French border.

Train

Karlsruhe has hourly ICE-services in the direction of Frankfurt/Cologne and Freiburg/Basel.

Airport

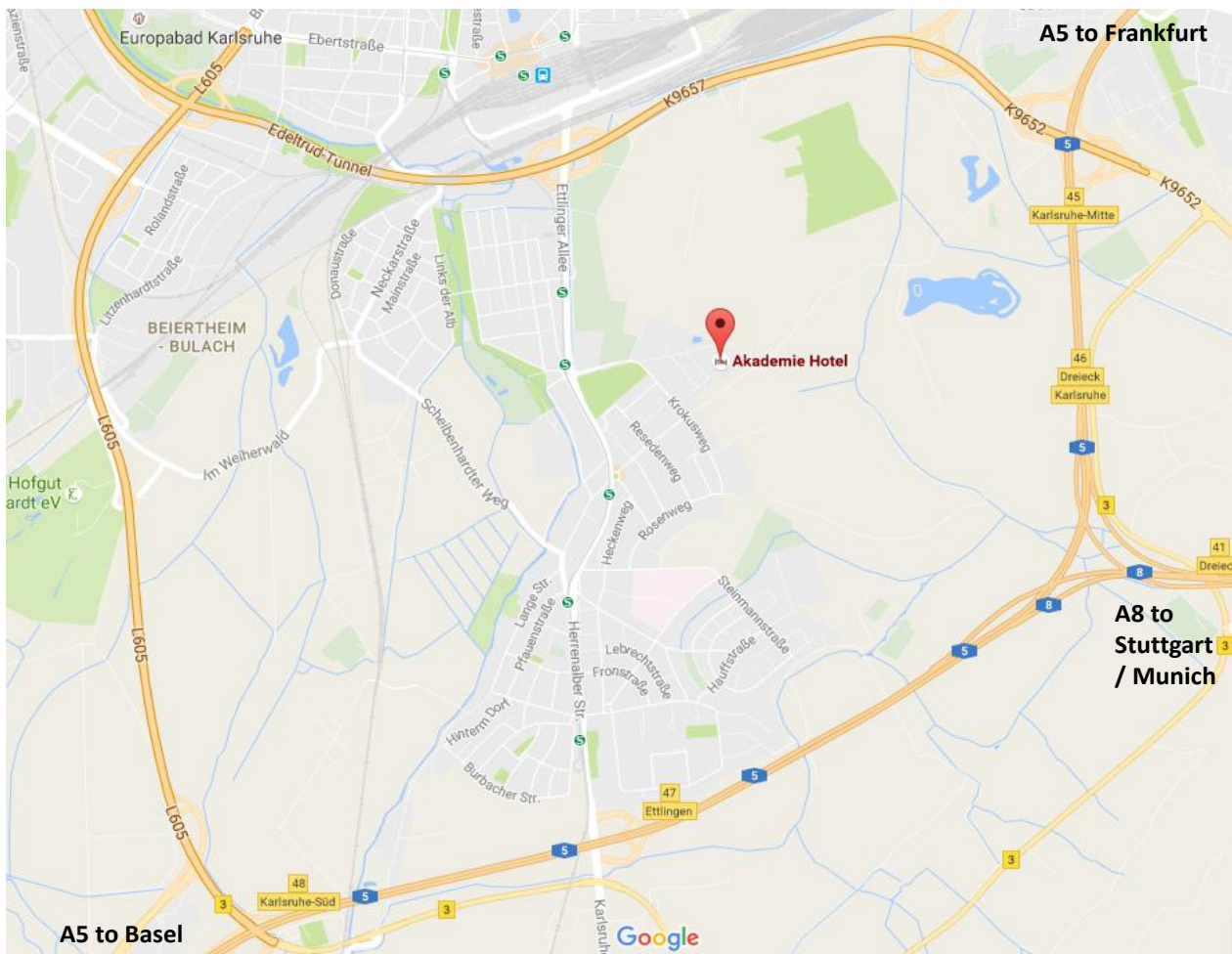
It takes about 60 minutes by train from Frankfurt- (direct ICE-connection), Stuttgart- or Strasbourg-Airport to Karlsruhe.

Car:

from Munich/Stuttgart via A8 direction Karlsruhe, change to A5 direction Basel at the motorway junction Karlsruhe and take the next exit no. 47 Karlsruhe Ettlingen

from Frankfurt (airport) via A5 direction Basel, pass the motorway junction Karlsruhe and take the next exit no. 47 Karlsruhe Ettlingen

from Basel via A5 direction Karlsruhe, leave the motorway at exit no. 47 Karlsruhe Ettlingen



Session Overview

Wednesday, March 1 st , 2017	
17h00 - 23h00	Arrival, hotel check in
19h00 - 21h00	Possibility for dinner in the hotel, 1st stay overnight

Thursday, March 2 nd , 2017	
06h30 - 09h00	Breakfast, Hotel Restaurant
08h00 - 09h00	Registration & Welcome Coffee, Hotel Lobby
Meeting Room 3 - 5	
09h00 - 09h10	Welcome, Prof. Dr. Oliver Kraft, Vicepresident for Research of KIT
09h10 - 10h10	Invited plenary talks
10h10 - 10h40	Poster mounting & Coffee Break, Hotel Lobby
	Meeting Room 20 - 21
	Meeting Room 3 - 5
10h40 - 12h20	Fuel Cells: PEMFC I
	Lithium Ion Batteries: System Aspects
12h20 - 13h50	Buffet Lunch, Hotel Restaurant
13h50 - 15h50	Fuel Cells: Cell and Stack Modeling
	Lithium Ion Batteries: Electrodes I
15h50 - 16h20	Poster Session & Coffee Break, Hotel Lobby
16h20 - 18h00	Fuel Cells: PEMFC II
	Lithium Ion Bat.: Alternative Chemistries
19h30	Conference Dinner, Hotel Restaurant

Friday, March 3 rd , 2017	
06h30 - 09h00	Breakfast, Hotel Restaurant
Meeting room 3 - 5	
09h00 - 10h00	Invited plenary talks
10h00 - 10h30	Poster Session & Coffee Break, Hotel Lobby
	Meeting Room 20 - 21
	Meeting Room 3 - 5
10h30 - 12h10	Fuel Cells: Materials Modeling
	Lithium Ion Batteries: Cell Modeling I
12h10 - 13h40	Buffet Lunch, Hotel Restaurant
13h40 - 15h00	Fuel Cells: Microstructure Modeling I
	Lithium Ion Batteries: Electrodes II
15h00 - 15h30	Coffee break, Hotel Lobby
15h30 - 16h50	Fuel Cells: Microstructure Modeling II
	Lithium Ion Batteries: Cell modeling II
Meeting room 3 - 5	
16h50 - 17h00	Closing remarks & Announcement of ModVal 2018

Conference Program

Thursday, March 2 nd , 2017		
06h30 - 09h00	Breakfast, Hotel Restaurant	
08h00 - 09h00	Registration & Welcome Coffee, Hotel Lobby	
Meeting Room 3 - 5		
09h00 - 09h10	Welcome, Prof. Dr. Oliver Kraft, Vicepresident for Research of KIT	
09h10 - 09h40	Invited plenary talk: Prof. Jon Pharoah, Queen's University: The Eternal Golden Braid: Modelling and Experiment	
09h40 - 10h10	Invited plenary talk: Prof. Robert M. McMeeking, University of California, Santa Barbara: The Generation of Stress and Fracture in the Storage Particles of Lithium-Ion Batteries	
10h10 - 10h40	Poster mounting & Coffee Break, Hotel Lobby	
	Meeting Room 20 - 21	Meeting Room 3 - 5
10h40 - 12h20	Fuel Cells: PEMFC I Chairs: Steven Beale (FZJ) Jürgen Schumacher (ZHAW)	Lithium Ion Batteries: System Aspects Chairs: Oleg Borodin (U.S. Army Research Lab.) Dong Kyu Kim (KIST Europe)
10h40	Martin Andersson (Lund University / FZJ): Volume-of-Fluid Modeling in Microscale Channels relevant for PEFCs	Marco Heinrich (PTB/TUBS): Ageing induced changes of charge distributions in a LIB analysed by correlating EIS simulations and experiments
11h00	Ivan Pivac (University of Split): Modeling of inductive phenomena at low frequencies in electrochemical impedance spectroscopy of PEM fuel cell	Kotub Uddin (University of Warwick): The impact EV power electronics on battery degradation
11h20	Guillaume Serre (CEA (Grenoble)): A multi-physic PEM Electrolyzer code for cell design optimization	Carlos Ziebert (KIT): Challenges for electrochemical and thermal characterization of Li-ion cells to improve parametrization for modelling
11h40	Denis Kramer (University of Southampton): Enhanced ORR Electrocatalysts Through Electronic Metal-Support Interactions between Pt and Boron Carbide	Nan Lin (TUBS): Parameter Sensitivity Study of a 3D Multiphysics Model of Large-format Li-ion Batteries
12h00	Matthias Messerschmidt (ZSW): CFD Modelling as a Validated Tool to Understand and Develop PEMFCs	Johannes Sturm (TUM): Modelling the Electrochemical-Thermal Behaviour of Cylindrical Lithium-Ion Cells during Internal Short Circuit Scenarios
12h20 - 13h50	Buffet Lunch, Hotel Restaurant	

Thursday, March 2 nd , 2017		
	Meeting Room 20 - 21	Meeting Room 3 - 5
13h50 - 15h50	Fuel Cells: Cell and Stack Modeling Chairs: Aimy Bazylak (University of Toronto) Guillaume Serre (CEA)	Lithium Ion Batteries: Electrodes I Chairs: Bob McMeeking (UCSB) Thomas Carraro (Uni Heidelberg)
13h50	Steven Beale (FZJ): Stability Issues for Three Dimensional Fuel Cell Models	Tobias Hofmann (FHG ITWM): Stress simulation of phase-separating cathode materials
14h10	Denis Gryaznov (University of Latvia): First principles calculations of perovskite cathode materials for protonic ceramic fuel cells	Peter Stein (TUD): Mechanically coupled modeling of ionic transport and electrochemical reactions in Li-ion battery electrodes
14h30	Peter Urthaler (AVL): 3D Modeling of HT-PEMFC and Validation on an Industrial Cell	Yixiang Gan (University of Sydney): Universality of the Emergent Scaling in Finite Random Binary Percolation Networks
14h50	Thomas Strohbach (Sunfire): Homogenized 3D SOC model and validation	Georg Bauer (BMW): Modeling of mechanical effects in lithium ion batteries
15h10	Shidong Zhang (FZJ): An Open-source Code for High Temperature Polymer-electrolyte Fuel Cells	Timo Danner (DLR, HIU): Thick electrodes for Li-Ion batteries: A model based analysis
15h30	Roman Kodým (University of Chemistry and Technology Prague): Concept of 3D Mathematical Modeling of HT PEM FC Stack Degradation and Single Cell Model Experiments	Fabian Single (DLR, HIU): Theory-based Investigation of SEI Formation
15h50 - 16h20	Poster Session & Coffee Break, Hotel Lobby	
16h20 - 18h00	Fuel Cells: PEMFC II Chairs: Peter Urthaler (AVL) Felix Büchi (PSI)	Lithium Ion Bat.: Alternative Chemistries Chairs: Carlos Ziebert (KIT) Bartosz Protas (McMaster University)
16h20	Georg Futter (DLR): A Physics-based Model for PEMFCs: Process Identification from EIS Simulation	Wolfgang Bessler (HS Offenburg): Electrochemical pressure impedance spectroscopy (EPIS): A promising tool for model parameterization and validation
16h40	Tasleem Muzaffar (Simon Fraser University): Water Phenomena in PEFC Catalyst Layers as the Origin of the Pt Loading Effect: A Modelling Study	Tobias Gerber (FHG ICT): Measurement method for locally resolved current density measurements in redox flow cells and stacks
17h00	Sven-Joachim Kimmerle (Universitaet der Bundeswehr Muenchen): Mathematical Modelling of Hydrogen Nanobubbles in PEM Electrolysers	Dong Kyu Kim (KIST Europe): Investigation of mass transport through Nafion® 115 in the vanadium redox flow battery
17h20	Jürgen Schumacher (ZHAW): Influence of pore-scale material properties on the performance of proton exchange membrane fuel cells	Ismail Celik (West Virginia University): Modeling of porous media effects on transport processes in sodium sulfur batteries
17h40	Victoria Manzi-Orezzoli (PSI): Towards Patterned Wettability in Gas Diffusion Media for PEFCs	Manik Mayur (HS Offenburg): Two-dimensional multiphysics simulation of Li-air button cells for electrolyte choice and electrode design
19h30	Conference Dinner, Hotel Restaurant	

Friday, March 3 rd , 2017		
06h30 - 09h00	Breakfast, Hotel Restaurant	
Meeting room 3 - 5		
09h00 - 10h00	Invited plenary talks	
09h00 - 09h30	Invited plenary talk: Prof. Aimy Bazylak, University of Toronto: Modeling and validation for designing porous materials for PEM fuel cells and electrolyzers	
09h30 - 10h00	Invited plenary talk: Dr. Oleg Borodin, US Army Research Lab: Modelling Lithium Battery Electrolytes and Solid Electrolytes Interphases	
10h00 - 10h30	Poster Session & Coffee Break, Hotel Lobby	
	Meeting Room 20 - 21	Meeting Room 3 - 5
10h30 - 12h10	Fuel Cells: Materials Modeling Chairs: Andreas Häffelin (Bosch) Adrien Lamibrac (PSI)	Lithium Ion Batteries: Cell Modeling I Chairs: Wolfgang Bessler (HS Offenburg) Clemens Guhke (WIAS)
10h30	Eugene Kotomin (MPI-FKF): Large scale first principles modeling of non-stoichiometric complex perovskites for fuel cell applications	Thomas Carraro (UHD): On the charging behavior of a multi-radii Newman-type battery model
10h50	Bolahaga Randrianarizafy (CEA Grenoble): Cathodic carbon corrosion: from a 1D-model to a full 2D-model	Markus Ganser (Bosch): A Fully Coupled Electro-Chemo-Mechanical Model for Ion Transport in Solid Electrolytes at Large Strains
11h10	Julian Szász (KIT): Secondary Phases at Cathode/Electrolyte Interfaces	Michael Kespe (KIT): Numerical simulation and optimization of lithium-ion batteries on the microscale
11h30	Felix Büchi (PSI): Evaporation of water from gas diffusion layers	Christian Merdon (WIAS): A novel concept for the discretisation of the coupled Nernst-Planck-Poisson-Navier-Stokes system
11h50	Fabio Greco (EPFL): Parameter estimation of the elastic and creep properties of Ni-YSZ anode based on four-point bending measurements	Teng Zhang (Imperial College): Understanding the performance bottleneck in Li-S batteries: a model-informed approach

Friday, March 3 rd , 2017		
12h10 - 13h40	Buffet Lunch, Hotel Restaurant	
	Meeting Room 20 - 21	Meeting Room 3 - 5
13h40 - 15h00	Fuel Cells: Microstructure Modeling I Chairs: Lorenz Holzer (ZHAW) Eugene Kotomin (MPI-FKF)	Lithium Ion Batteries: Electrodes II Chairs: Peter Stein (TUD) Hermann Nirschl (KIT)
13h40	Antonio Bertei (Imperial College): Quantification of Ni coarsening in infiltrated SOFC anodes by combining 3D tomography, impedance spectroscopy and mechanistic modelling	Reiner Mönig (KIT): Measurements of Stress and Strain in Electrode Materials of Lithium-Ion Batteries
14h00	Henrik Ekström (Comsol / KTH): A model for analysis of the porous nickel electrode polarization in the molten carbonate electrolysis cell	Herman Lemmens (ThermoFisher Scientific): Battery electrode imaging in 3D: Field of View or Resolution ?
14h20	Jochen Joos (KIT): Microstructure Modelling of Porous Cathodes for Solid Oxide Fuel Cells (SOFCs)	Bartosz Protas (McMaster University): Mathematical Model of Binder Distribution During Drying of Lithium-Ion Battery Electrodes
14h40	Roswitha Zeis (HIU): Pore network modelling of phosphoric acid distribution in high temperature PEM fuel cells	Janina Costard (KIT): Combined Impedance Study (EIS) and microstructure analysis (FIB/SEM) of intercalation electrodes: Determination of charge transfer parameters
15h00 - 15h30	Coffee break, Hotel Lobby	
15h30 - 16h50	Fuel Cells: Microstructure Modeling II Chairs: Antonio Bertei (Imperial College) Jochen Joos (KIT)	Lithium Ion Batteries: Cell modeling II Chairs: Jochen Zausch (FHG-IWTM) Reiner Mönig (KIT)
15h30	Lorenz Holzer (ZHAW): Microstructure limitations for relative permeability and liquid drainage in fibrous GDL (PEFC): The importance of the 'short range effect'	Andrea Falconi (Renault): Transient Lithium Ion Battery Behavior Simulations Through Electrochemical Modelling
15h50	Marie-Dominique Baum (DLR): Analysis of local heterogeneities and their effect on DMFC performance with a physical 2D cell model	Johannes Landesfeind (TUM): Parameters Controlling the Fast-Charging Limitations for Lithium Ion Batteries and their Temperature Dependence
16h10	Hamza Moussaoui (CEA Grenoble): 3D morphological modeling and validation for optimization of SOCs electrode microstructures	Jonas Keil (TUM): Modeling capacity fade due to SEI formation in Li-ion cells validated by neutron diffraction data
16h30	Matthias Neumann (UUIm): Big data for microstructure-property relationships: a case study of predicting effective conductivities	Bartosz Protas (McMaster University): Inverse Modelling Approach to Determine Material Properties of Electrolytes: Effects of Faradaic Convection
Meeting room 3 - 5		
16h50 - 17h00	Closing remarks & Announcement of ModVal 2018	