Thursday, March 2nd, 2017		
06h30 - 09h00	**Breakfast**	
08h00 - 09h00	**Registration**	
09h00 - 09h10	**Welcome, Prof. Dr. Oliver Kraft, Vicepresident for Research of KIT**	
09h10 - 09h40	**Invited plenary talk: Prof. Jon Pharoah, Queen's University**	
09h40 - 10h10	**Invited plenary talk: Prof. Robert M. McMeeking, University of California, Santa Barbara**	
10h10 - 10h40	**Coffee break**	
10h40 - 12h20	**PEMFC I** **Chair:**	**Lithium Ion Batteries: System Aspects** **Chair:**
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	Christian Bergbreiter (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	**Lunch**	

13h50 - 15h50	**Cell and Stack Modeling** **Chair:**	**Lithium Ion Batteries: Electrodes I** **Chair:**
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): 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): Theory-based Investigation of SEI Formation
15h50 - 16h20	**Poster Session / Coffee break**	

16h20 - 18h00	**PEMFC II** **Chair:**	**Lithium Ion Batteries: Alternative Chemistries** **Chair:**
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**	

Friday, March 3rd, 2017		
06h30 - 09h00	**Breakfast**	
09h00 - 09h30	**Invited plenary talk: Prof. Aimy Bazylak, University of Toronto**	
09h30 - 10h00	**Invited plenary talk: Dr. Oleg Borodin, US Army Research Lab**	
10h00 - 10h30	**Poster Session / Coffee break**	
10h30 - 12h10	**Materials Modeling** **Chair:**	**Lithium Ion Batteries: Cell Modeling I** **Chair:**
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
12h10 - 13h40	**Lunch**	

13h40 - 15h00	**Microstructure Modeling I** **Chair:**	**Lithium Ion Batteries: Electrodes II** **Chair:**
13h40	Antonio Bertei (Imperial College): Quantification of Ni coarsening in infiltrated SOFC anodes by combining 3D tomography, impedance spectroscopy and mechanistic modelling	Timothy Flack (Cardiff University): Computational approaches to mass and ion diffusion in solids: free energies, reaction rates and overall mechanistic assessment of intercalation processes in cathode active materials
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)	Jamie M. Foster (University of Portsmouth): 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**	

15h30 - 16h50	**Microstructure Modeling II** **Chair:**	**Lithium Ion Batteries: Cell modeling II** **Chair:**
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 (UUlm): 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
16h50 - 17h00	**Closing remarks and Announcement of ModVal 2018**	