Day 3 - Thursday 22nd April 2021, morning

9:10 — **A5 Prof Dr Jun Lin** (NCEPU, Beijing) - *jun.lin@ncepu.edu.cn*
Performance improvement of nanocomposite proton exchange membranes filled with water insoluble heteropoly acid-based nanohybrids

9:45 — **A6 Dr Gregory Offer** (Imperial College London, UK) - *gregory.offer@imperial.ac.uk*
The Cell Cooling Coefficient: a new standard to define the thermal behavior of lithium-ion batteries and how to design better cells
Alastair Hales[1], Laura Bravo Diaz[1], Mohamed Waseem Marzook[1], Yan Zhao[1], Teng Zhang[3], Yatish Patel[1,2], Gregory Offer[1,2]
[1] Department of Mechanical Engineering, Imperial College London, London, United Kingdom, SW7 2AZ
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[3] Department of Mechanical Engineering, University of Surrey, Guildford, United Kingdom, GU2 7XH

10:20 — *Morning break 20'*

	B8 Battery microstructures Chair: F Röder	**C8 PEMFC Diagnostics** Chair: J Eller
10:40	**Design and manufacturing of lithium-ion battery electrodes assisted by image-based modelling** Xuekun Lu[1,2,3], Antonio Bertei[4], Marco Lagnoni[4], Kieran B O'Regan[3,5], Juyeon Park[2], Gareth Hinds[2], Emma Kendrick[3,5], Dan JL Brett[1,3], Paul R Shearing[1,3] [1]Electrochemical Innovation Lab, Department of Chemical Engineering, University College London, London, WC1E 7JE, UK - *xuekun.lu@ucl.ac.uk* [2]Natl Physical Laboratory, Hampton Rd, Teddington, Middlesex,TW11 0LW, UK [3]The Faraday Institution, Quad One, Harwell Science and Innovation Campus, Didcot, OX11 0RA, UK [4]Dptm of Civil and Industrial Engineering, University of Pisa, Pisa, 56122, Italy [5]School of Metallurgy & Materials, Univ. Birmingham, Birmingham B15 2TT, UK	**Noninvasive Determination of local Membrane Conductivity in Polymer Electrolyte Fuel Cells based on a Finite Element Model** A. Schuller[1], T. J. Schmidt[1,2], J. Eller[1] [1]Electrochemistry Laboratory, Paul Scherrer Institut, Forschungstrasse 111, 5232, Villigen PSI, Switzerland [2]Laboratory of Physical Chemistry, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093, Zürich, Switzerland *arnaud.schuller@psi.ch*
11:00	**Artificial generation of representative electrode particle architectures from microscopy data** O. Furat[1], D. P. Finegan[2] , K. Smith[2] , V. Schmidt[1] - *orkun.furat@uni-ulm.de* [1] Ulm University, Institute of Stochastics, 89069-Ulm, Germany [2] National Renewable Energy Laboratory, 80401-Golden, CO, USA	**Online Impedance Measurements as a Testing Tool** J. Scholta[1] , P. Küber[1] , H. Knaupp[1] , A. Wais[2] , A. Kabza[1] , L. Jörissen[1] [1]Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW), 89081 Ulm, Germany - *joachim.scholta@zsw-bw.de* [2]m-a-r-s Ingenieurbüro A. Wais, 89250 Senden, Germany
11:20	**The importance of passive materials in thick Li-ion battery electrodes** Tobias Knorr[1,2], Simon Hein[1,2], Benedikt Prifling[3], Matthias Neumann[3], Volker Schmidt[3], Timo Danner [1,2], Arnulf Latz[1,2,4] - *tobias.knorr@dlr.de* [1]Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Ulm, D [2]DLR, Institute of Engineering Thermodynamics, Stuttgart, Germany [3]Ulm University, Institute of Stochastics, Ulm, Germany [4]Ulm University, Institute of Electrochemistry, Ulm, Germany	**Observing Oxygen Transport in Polymer Electrolyte Water Electrolysis via operando X-ray Tomography** S. De Angelis[1], T. Schuler[1], F. Marone[2], F. N. Büchi[1] [1]Electrochemistry Laboratory, Paul Scherrer Institut, CH-5232 Villigen-PSI [2]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI *salvatore.de-angelis@psi.ch*
11:40	**Phase-field modeling of microstructure evolution in sodium-ion batteries particles of Na_xFePO_4** Tao Zhang, Marc Kamlah - *tao.zhang@kit.edu* Karlsruhe Institute of Technology, Institute for Applied Materials, 76344 Eggenstein-Leopoldshafen, Germany	**Validation of Small Angle X-ray Scattering Technique for Catalyst Layer Saturation Determination** K. Aliyah, L. Gubler, J. Eller - *aliyah.kinanti@psi.ch* Paul Scherrer Institut, Electrochemistry Laboratory, CH-5232 Villigen PSI

12:00 — *Lunch break for 1h30'*

Thursday 22nd April 2021, afternoon

	B9 Battery modeling Chair: (H Ekström)	**C9 PEMFC H_2O management** Chair: F Büchi
13:30	**Modelling of electron-transfer kinetics in magnesium electrolytes: influence of the solvent on the battery performance** Janina Drews[1,2], Piotr Jankowski[3,4], Joachim Häcker[1], Zhenyou Li[2,5], Timo Danner[1,2],Juan Maria García Lastra[3],Tejs Vegge[3],Norbert Wagner[1],K. Andreas Friedrich[1,6], Zhirong Zhao-Karger[2,5], Maximilian Fichtner[2,5], Arnulf Latz[1,2,7] [1]DLR, Institute of Engineering Thermodynamics, Stuttgart, Germany [2]Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Ulm, D [3]Tech Univ Denmark (DTU), Dpmt Energy Conversion & Storage, Lyngby, DK [4]Warsaw University of Technology (WUT), Faculty of Chemistry, Warsaw, POL [5]KIT, Institute of Nanotechnology, Eggenstein-Leopoldshafen, Germany [6]University of Stuttgart, Institute of Energy Storage, Stuttgart, Germany [7]Univ. of Ulm, Institute of Electrochemistry, Helmholtzstraße 11, 89081 Ulm, D *janina.drews@dlr.de*	**Understanding heterogeneous wettability in PEFC catalyst layers using a structure-based model** W. Olbrich[1,2,3], T. Kadyk[1,4], U. Sauter[2], M. Eikerling[1,3,4] [1] Theory and Computation of Energy Materials (IEK-13), Institute of Energy and Climate Research, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany [2] Robert Bosch GmbH, Corporate Research, 71272 Renningen, Germany [3] Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany [4] Jülich Aachen Research Alliance, JARA Energy, 52425 Jülich, Germany *wolfgang.olbrich@de.bosch.com*
13:50	**Concentration- and field-dependent susceptibility of electrolytes** R. Müller, M. Landstorfer Weierstrass-Institute, 10117-Berlin, Germany *Ruediger.Mueller@wias-berlin.de*	**Modelling coupled porous media/free flow/drop interaction in a PEM fuel cell using a pore-net-work approach** C. Michalkowski[1], M. Veyskarami[2] , V. Schleper[1] , R. Helmig[2] [1] Robert Bosch GmbH, Corporate Research, 71272 Renningen, Germany [2] University of Stuttgart, Institute for Modelling Hydraulic and Environmental Systems (IWS), Germany *cynthia.michalkowski@de.bosch.com*
14:10	**The Role of Energy Scales for the Structure of Electrochemical Double Layers in Ionic Liquids** Birger Horstmann[1,2,3], Max Schammer[1,2] , Arnulf Latz[1,2,3] [1]Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany [2]German Aerospace Center, Pfaffenwaldring 38, 70569 Stuttgart, Germany [3]University of Ulm, Albert-Einstein-Allee 47, 89081 Ulm, Germany *birger.horstmann@dlr.de*	**Gas-evolving flow-through electrode design and experiments** J.W. Haverkort, H.Rajaei, A. Rajora [1]Delft University of Technology, 3mE, Process & Energy, 2628 CB, Delft, The Netherlands *j.w.haverkort@tudelft.nl*

14:30	**Discerning models of phase transformation in porous graphite electrodes: insights from inverse modelling based on MRI measurements** Jose Morales Escalante[1], William Ko[1], Jamie Foster[2], Sergey Krachkovskiy[3], Gillian Goward[3], B. Protas[1] - *bprotas@mcmaster.ca* [1]McMaster University (Dept. of Math & Stats), L8S 4K1, Hamilton, ON, Canada [2]Univ. of Portsmouth (School of Math & Physics), PO1 2UP, Portsmouth, UK [3]McMaster University (Dept. of Chemistry), L8S 4K1, Hamilton, ON, Canada	**Evaporative Cooling of Polymer Electrolyte Fuel Cells – A System Level Analysis** M. Striednig[1], M. Cochet[1], P. Boillat[1,2], T.J. Schmidt[1,3], F.N. Büchi[1] [1]Electrochemistry Laboratory, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland [3]Laboratory of Physical Chemistry, ETH Zürich, 8093 Zürich, Switzerland michael.striednig@psi.ch
14:50	**Search for new electro-active organic materials: modelling routes & strategies** F. Lambert[1,2],Y. Danten[3],C. Gatti[4], C. Frayret[1,5,6] -*christine.frayret@u-picardie.fr* [1]Université de Picardie Jules Verne, Laboratoire de Réactivité et Chimie des Solides, UMR 7314 (LRCS), 15 rue Baudelocque, 80039 Amiens Cedex 1, F [2]French Environment and Energy Management Agency (ADEME) 20, avenue du Grésillé- BP 90406 49004 Angers Cedex 01, France [3] Institut des Sciences Moléculaires, UMR CNRS 5255, 33405 Talence, France [4]CNR SCITEC, CNR, Sede Via C. Golgi, 19,20133 Milano, Italy [5]Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, HUB de l'Energie, 15 rue Baudelocque, 80039 Amiens, France [6]ALISTORE-European Research Institute, FR CNRS 3104, HUB de l'Energie, 15 rue Baudelocque, 80000 Amiens, France	*free*
15:10	*Afternoon break 20'*	
	B10 Battery microstructures Chair: (G Offer)	**C10 PEMFC systems** Chair:
15:30	**Modeling heterogeneous conductive networks in porous electrode materials for batteries** F. Röder[1], O. Schmidt[2,3] - *fridolin.roeder@uni-bayreuth.de* [1]University of Bayreuth, Bavarian Center for Battery Technology (BayBatt), Universitätsstraße 30, 95447 Bayreuth, Germany [2]TU Braunschweig, Institute of Energy and Process Systems Engineering, Langer Kamp 19b, Braunschweig, Germany [3]TU Braunschweig, Battery LabFactory Braunschweig (BLB), Langer Kamp 8, 38106 Braunschweig, Germany	**Hybrid control strategy for PEM fuel cell systems optimizing efficiency and reducing degradation using artificial neural networks** M. Bahr, S. Goessling Zentrum für BrennstoffzellenTechnik GmbH, Carl-Benz-Str. 201, 47057-Duisburg, Germany
16:00	**Influence of conductivity additives and their distribution on the performance properties of lithium-ion batteries** A. Chauhan, H. Nirschl - *anshuman.chauhan@kit.edu* [1]Karlsruhe Institute of Technology, Institute of Mechanical Process Engineering and Mechanics,76131-Karlsruhe, Germany	**Predicting local transport processes in cathode catalyst layer based on overall PEMFC performance: a pore-network approach** Shahriar Alam, Ezequiel F. Medici , Kazuya Tajiri , Jeffrey S. Allen Michigan Technological University, Mechanical Engineering-Engineering Mechanics 49931 Houghton-Michigan, USA *salam2@mtu.edu*
16:20	**Stochastic 3D microstructure modeling of graphite anodes in lithium-ion batteries** B. Prifling[1], M. Ademmer[1], F. Single[2], O. Benevolenski[2], A. Hilger[3], M. Osenberg[4], I. Manke[3], V. Schmidt[1] - *benedikt.prifling@uni-ulm.de* [1] Ulm University, Institute of Stochastics, 89069-Ulm, Germany [2] SGL Carbon GmbH, 86405-Meitingen, Germany [3] Institute of Applied Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, 14109-Berlin, Germany [4] Dptm. of Materials Science and Technology, TU Berlin, 10623-Berlin, D	**Analysis and modelling of automotive Fuel Cell system** A. Grimaldi, A. Cinque, A. Baricci, A. Casalegno Politecnico di Milano, Department of Energy, MRT Fuel Cell & Battery LAB, 20156-Milan, Italy *amedeo.grimaldi@polimi.it*
16:40	**Spatially resolved simulation of cathode structures for sodium-iodine secondary batteries** F. Gerbig, S. Cernak, H. Nirschl - *felix.gerbig@kit.edu* Karlsruhe Institute of Technology, Institute of Mechanical Process Engineering and Mechanics, Straße am Forum 8, 76131 Karlsruhe, D	**An AI-Driven, Workflow-Centric Platform for Materials Discovery and Intelligence** K. Malek[1,2], Q. Wang[1], A. Malek[1], M. Eikerling[2] [1] NRC-EME, 4250 Wesbrook Mall, Vancouver, BC, V6T1W5, Canada [2] Institute of Energy and Climate Research, IEK-13: Modelling and Simulation of Energy Materials, Forschungszentrum Jülich, 52425 Jülich, Germany
17:00	*Short transition break*	
17:10	**A7 Prof. Steven C DeCaluwe** (Mech. Engineering, Colorado School of Mines, Golden, CO, USA) Experimentally-validated Simulation of Solid Electrolyte Interphase Growth and Evolution: the Impact of Detailed Chemistry Modeling - *decaluwe@mines.edu*	
17:45	**End of Programme, Day 3**	
17:50	**Closing - Announcement Modval 2022**	
18:00	**End of Symposium**	