

Day 2 – Wednesday 21 <sup>st</sup> April 2021, morning		
	<p><b>B4 Battery microstructures</b> Chair: V Schmidt</p>	<p><b>C4 PEMFC modeling</b> Chair: J Schumacher</p>
09:00	<p><b>Parametric 3D representation of curved grain boundaries with measurement uncertainties</b> <u>L. Petrich</u><sup>1</sup>, C.E. Krill III<sup>2</sup>, V. Schmidt<sup>1</sup> - <a href="mailto:lukas.petrich@uni-ulm.de">lukas.petrich@uni-ulm.de</a> <sup>1</sup>Ulm University, Institute of Stochastics, 89069 Ulm, Germany <sup>2</sup>Ulm University, Institute of Functional Nanosystems, 89081 Ulm, Germany</p>	<p><b>Efficient Open Source Model for PEM Fuel Cell Stacks</b> <u>L. Feierabend</u>, J. Wartmann, A. Heinzel The fuel cell research center ZBT GmbH, 47057 Duisburg, Germany University of Duisburg-Essen, Lehrstuhl Energietechnik, 47057 Duisburg, D <a href="mailto:l.feierabend@zbt.de">l.feierabend@zbt.de</a></p>
09:20	<p><b>Towards a 3D Digital Twin of Li-Ion Battery Manufacturing: from the slurry to the Electrochemical Performance</b> <u>Teo Lombardo</u><sup>1,2</sup>, Alain N. Ngandjong<sup>1,2</sup>, Emiliano N. Primo<sup>1,2</sup>, Mehdi Chouchane<sup>1,2</sup>, Abbas Shodiev<sup>1,2</sup>, Oier Arcelus<sup>1,2</sup>, Alejandro A. Franco<sup>1,2,3,4</sup> <sup>1</sup>Laboratoire de Réactivité et Chimie des Solides (LRCS), UMR CNRS 7314, Université de Picardie Jules Verne, 80039 Amiens Cedex, France <sup>2</sup>Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, Hub de l'Energie, 15, rue Baudelocque, 80039 Amiens Cedex, France <sup>3</sup>ALISTORE-European Research Institute, FR CNRS 3104, Hub de l'Energie, 15, rue Baudelocque, 80039 Amiens Cedex, France <sup>4</sup>Institut Universitaire de France, 103 Boulevard Saint Michel, 75005 Paris, F <a href="mailto:teo.lombardo@u-picardie.fr">teo.lombardo@u-picardie.fr</a>, <a href="mailto:alejandro.franco@u-picardie.fr">alejandro.franco@u-picardie.fr</a></p>	<p><b>Two-dimensional, two-phase, non-isothermal model of proton exchange membrane fuel cell</b> <u>A. Monteverde</u><sup>1</sup>, O. B. Rizvandi<sup>2</sup> <sup>1</sup>Politecnico di Torino, Department of Applied Science and Technology (DISAT), Corso Duca degli Abruzzi 24, 10129 Torino (TO), Italy <sup>2</sup>Technical University of Denmark, Department of Energy Conversion and Storage, Bygning 310, 2800 Lyngby, Denmark <a href="mailto:alessandro.monteverdevidela@polito.it">alessandro.monteverdevidela@polito.it</a></p>
09:40	<p><b>Numerical Investigations on the Influence of Particle Porosity on the Performance of Positive Lithium-Ion Battery Electrodes</b> <u>S. Cernak</u>, F. Schuerholz, M. Kespe, H. Nirschl - <a href="mailto:susanne.cernak@kit.edu">susanne.cernak@kit.edu</a> Karlsruhe Institute of Technology, Department of Chemical and Process Engineering, Institute of Mechanical Process Engineering and Mechanics, Division Process Machines, Kaiserstraße 12, 76131 Karlsruhe, Germany</p>	<p><b>Box-Jenkins Autoregressive Models for PEMFC Operating on Dynamical Conditions</b> <u>J.A. Aguilar</u>, A. Husar, J. Andrade-Cetto Inst. de Robòtica i Informàtica Industrial, CSIC-UPC, 08028-Barcelona, Spain <a href="mailto:jaguilar@iri.upc.edu">jaguilar@iri.upc.edu</a></p>
10:00	<p><b>Stochastic 3D microstructure modeling of nanoporous NMC-particles</b> <u>M. Neumann</u><sup>1</sup>, S. Wetterauer<sup>2</sup>, M. Osenberg<sup>3</sup>, A. Hilger<sup>3</sup>, A. Wagner<sup>4</sup>, N. Bohn<sup>4</sup>, J.R. Binder<sup>4</sup>, I. Manke<sup>3</sup>, T. Carraro<sup>5</sup>, V. Schmidt<sup>1</sup> - <a href="mailto:matthias.neumann@uni-ulm.de">matthias.neumann@uni-ulm.de</a> <sup>1</sup>Institute of Stochastics, Ulm University, 89069 Ulm, Germany <sup>2</sup>Institute of Applied Mathematics, Heidelberg University, 69120 Heidelberg, D <sup>3</sup>Institute of Applied Materials, Helmholtz-Zentrum Berlin, 14109 Berlin, D <sup>4</sup>Institute for Applied Materials, KIT, 76344 Eggenstein-Leopoldshafen, D <sup>5</sup>Faculty of Mech. Eng., Helmut Schmidt University, 22043 Hamburg, D</p>	<p><b>An analytical model for liquid and gas diffusion layers in electrolyzers and fuel cells</b> <u>A. Rajora</u>, J.W. Haverkort Delft University of Technology, Energy Technology, Process and Energy Laboratory, Leeghwaterstraat 39, 2628 CB, Delft, The Netherlands <a href="mailto:A.Rajora@tudelft.nl">A.Rajora@tudelft.nl</a>, <a href="mailto:J.W.Haverkort@tudelft.nl">J.W.Haverkort@tudelft.nl</a></p>
10:20	<i>Morning break 20'</i>	
10:40	<p><b>A4 Dr Mohamed Mamlouk (Univ. Newcastle, UK) - <a href="mailto:mohamed.mamlouk@newcastle.ac.uk">mohamed.mamlouk@newcastle.ac.uk</a></b> Performance and stability of radiation grafted based anion exchange membrane electrolyzers</p>	
11:15	<i>Short transition break</i>	
	<p><b>B5 Battery modeling</b> Chair: B Horstmann</p>	<p><b>C5 Water Electrolysis</b> Chair: (M Mamlouk)</p>
11:20	<p><b>Modelling of Lithium Ion Batteries with Silicon Anode and Ionic Liquid Electrolyte</b> <u>Franziska Kilchert</u><sup>1,2</sup>, Birger Horstmann<sup>1,2,3</sup>, Arnulf Latz<sup>1,2,3</sup> <sup>1</sup>Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany <sup>2</sup>German Aerospace Center, Pfaffenwaldring 38, 70569 Stuttgart, Germany <sup>3</sup>University of Ulm, Albert-Einstein-Allee 47, 89081 Ulm, Germany <a href="mailto:franziska.kilchert@dlr.de">franziska.kilchert@dlr.de</a></p>	<p><b>Pore Network Modelling of Anodic Porous Transport Layer in Electrolysers</b> <u>H. Altaf</u><sup>1,2</sup>, N. Vorhauer<sup>1</sup>, T. Vidakovic-Koch<sup>2</sup>, E. Tsotsas<sup>1</sup> <sup>1</sup>Otto von Guericke Univ., Inst. of Process Engineering, 39106 Magdeburg, D <sup>2</sup>Max Planck Institute (Dynamics of Complex Systems), 39106 Magdeburg, D <a href="mailto:haashir.altaf@ovgu.de">haashir.altaf@ovgu.de</a></p>
11:40	<p><b>Improved performance of Li-ion battery simulations by separation of timescales</b> <u>Jan Lammel</u>, Jochen Zausch Fraunhofer Institute for Industrial Mathematics, 67663 Kaiserslautern, Germany <a href="mailto:jan.lammel@itwm.fraunhofer.de">jan.lammel@itwm.fraunhofer.de</a></p>	<p><b>Limiting current and electro-osmotic flows in alkaline water electrolysis</b> <u>J.W. Haverkort</u><sup>1</sup>, H.Rajaei Delft University of Technology, 3mE, Process &amp; Energy, 2628 CB, Delft, NL <a href="mailto:j.w.haverkort@tudelft.nl">j.w.haverkort@tudelft.nl</a></p>
12:00	<p><b>Advancing Ion Mobility in Battery Materials by Dedicated Computational Approaches</b> <u>S. Leoni</u><sup>1</sup> and B. Hou<sup>2</sup> <sup>1</sup>School of Chemistry, Cardiff University, Cardiff, CF10 3AT, UK <sup>2</sup>School of Physics and Astronomy, Cardiff University, Cardiff, CF24 3AA <a href="mailto:leonis@cf.ac.uk">leonis@cf.ac.uk</a></p>	<p><b>Closed loop energy, fuel and oxygen co-generation with a reversible photo-electrochemical device</b> <u>A. Cattry</u><sup>1</sup>, S. Tembume<sup>2</sup>, S. Haussener<sup>1</sup> <sup>1</sup>EPFL, (STI), (IGM), (LRESE), 1015-Lausanne, Switzerland <sup>2</sup>SoHHytec SA, Chemin de la Raye 13, 1024-Ecublens, Switzerland <a href="mailto:alexandre.cattry@epfl.ch">alexandre.cattry@epfl.ch</a></p>
12:20	<i>Lunch Break for 1h30'</i>	

Wednesday 21 <sup>st</sup> April 2021, afternoon		
	<p><b>B6 Battery diagnostics</b> Chair: (D Howey)</p>	<p><b>C6 Fuel Cells testing &amp; diagnostics</b> Chair: (A Friedrich)</p>
13:50	<p><b>Optimizing lithium-ion battery P2D model calibration through sensitivity analysis of physical parameters</b> G. Sordi, C. Rabissi<sup>1</sup>, A. Innocenti, A. Casalegno - <a href="mailto:gabriele.sordi@polimi.it">gabriele.sordi@polimi.it</a> Politecnico Milano, Dpt of Energy, MRT Fuel Cell&amp;Battery Lab, 20156- Milano</p>	<p><i>free</i></p>
14:10	<p><b>Cell configuration optimisation for operando Raman spectroscopy of Li-ion and Na-ion electrodes by 2D+1D electrochemical simulation</b> E.J.F. Dickinson<sup>1</sup>, T.E. Rosser<sup>1</sup>, R. Raccichini<sup>1</sup>, K. Hunter<sup>2</sup>, A.D. Searle<sup>2</sup>, C.M. Kavanagh<sup>2</sup>, P.J. Curran<sup>2</sup>, G. Hinds<sup>1</sup>, J. Park<sup>1</sup>, A.J. Wain<sup>1</sup> <sup>1</sup>National Physical Laboratory, Hampton Road, Teddington TW11 0LW, UK <sup>2</sup>Deregallera Ltd, Unit 2 De Clare Court, Pontywindy Industrial Estate, Caerphilly CF83 3HU, UK <a href="mailto:edmund.dickinson@npl.co.uk">edmund.dickinson@npl.co.uk</a></p>	<p><b>Full Factorial Characterization of PEMFC Properties in Differential Cells</b> <u>Christophe Gerling</u><sup>1,2</sup>, Matthias Hanauer<sup>1</sup>, Ulrich Berner<sup>1</sup>, K. Andreas Friedrich<sup>2,3</sup> - <a href="mailto:christophe.gerling@de.bosch.com">christophe.gerling@de.bosch.com</a> <sup>1</sup>Robert Bosch GmbH, Robert-Bosch-Campus 1, 71272 Renningen, Germany <sup>2</sup>Institute of Building Energetics, Thermal Engineering and Energy Storage (IGTE), University of Stuttgart, Keplerstraße 7, Stuttgart 70550, Germany <sup>3</sup>German Aerospace Center, Institute of Engineering Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany</p>
14:30	<p><b>Physicochemical SEI model for cell diagnosis with C-rate and EIS data</b> D. Witt<sup>1,2,3</sup>, F. Röder<sup>4</sup>, U. Krewer<sup>2</sup> - <a href="mailto:d.witt@tu-braunschweig.de">d.witt@tu-braunschweig.de</a> <sup>1</sup>TU Braunschweig, Institute of Energy and Process Systems Engineering, 38106-Braunschweig, Germany <sup>2</sup>Karlsruhe Institute of Technology, Institute for Applied Materials – Electrochemical Technologies, 76131-Karlsruhe, Germany <sup>3</sup>Battery LabFactory Braunschweig, 38106-Braunschweig, Germany <sup>4</sup>University of Bayreuth, Electrical Energy Systems, 95447-Bayreuth, Germany</p>	<p><b>Distribution of voltage and current density in JRC ZEROVCELL: a single cell testing hardware for PEM fuel cells</b> T. Bednarek European Commission, Joint Research Centre (JRC), Directorate C Energy Transport and Climate, The Netherlands <a href="mailto:Tomasz.Bednarek@ec.europa.eu">Tomasz.Bednarek@ec.europa.eu</a></p>
14:50	<p><b>Early degradation identification of lithium-ion batteries via thermal diagnostics</b> Jie Lin, H.N. Chu, C.W. Monroe, D.A. Howey University of Oxford, Department of Engineering Science, OX1 3PJ, Oxford, United Kingdom <a href="mailto:jie.lin@eng.ox.ac.uk">jie.lin@eng.ox.ac.uk</a></p>	<p><b>Voltage drop study of a SOFC stack at low currents and flows</b> M. Serra<sup>1</sup>, H. Renaudineau<sup>3</sup>, A. Husar<sup>1</sup>, R. Costa-Castelló<sup>1</sup>, L. Bernadet<sup>2</sup>, M. Torrell<sup>2</sup> - <a href="mailto:maria.serra@upc.edu">maria.serra@upc.edu</a> <sup>1</sup>Inst de Robòtica i Informàtica Industrial, CSIC-UPC, 08028-Barcelona, Spain <sup>2</sup>Inst de Recerca en Energia de Catalunya, 08930-Sant Adrià del Besòs, Spain <sup>3</sup>Univ Técnica Federico Santa María (Electronics Eng. Dep.), Valparaiso, Chile</p>
15:10	<i>Afternoon break 20'</i>	
	<p><b>B7 Battery thermal behaviour</b> Chair: E Dickinson</p>	<p><b>C7 Solid Oxide Electrolysis</b> Chair: J Van herle</p>
15:30	<p><b>Thermal Control Platform: building better temperature control for battery model parameterisation</b> E.V. Brouillet<sup>1</sup>, D.J. Auger<sup>2</sup>, B. Edwards<sup>1</sup>, A. Hales<sup>3</sup>, J. Kay<sup>1</sup>, S. Mores<sup>1</sup>, G. Offer<sup>3</sup>, Z. Zhihuo<sup>2</sup> <sup>1</sup>Thermal Hazard Technology, MK11SW, Bletchley, UK <sup>2</sup>Cranfield Univ, Advanced Vehicle Engineering Centre, MK430AL Cranfield, UK <sup>3</sup>Imperial College London, Dpt. of Mechanical Engineering, SW72AZ, UK <a href="mailto:etienne@thtuk.com">etienne@thtuk.com</a></p>	<p><b>Optimizing the performance of solid oxide electrolysis cells and stacks for Power-to-Gas applications</b> <u>L. Wehrle</u><sup>1</sup>, D. Schmider<sup>1,2</sup>, J. Dailly<sup>2</sup>, A. Banerjee<sup>3</sup>, O. Deutschmann<sup>1</sup> <sup>1</sup>Karlsruhe Institute of Technology (KIT), Institute for Chemical Technology and Polymer Chemistry (ITCP), 76131 Karlsruhe, Germany <sup>2</sup>European Institute for Energy Research (EIFER), 76131 Karlsruhe, Germany <sup>3</sup>University of Twente, Faculty of Science and Technology, Catalytic Processes and Materials, 7522 NB Enschede, the Netherlands <a href="mailto:lukas.wehrle@kit.edu">lukas.wehrle@kit.edu</a></p>
15:50	<p><b>Multi-scale modelling for the security of lithium-ion batteries</b> Ridha Omrani, Didier Buzon, Philippe Azais University Grenoble Alpes, CEA-LITEN, F-38054 Grenoble, France <a href="mailto:ridha.omrani@cea.fr">ridha.omrani@cea.fr</a></p>	<p><b>Modeling of Solid Oxide Electrolysis Stacks under High-Pressure Operation</b> <u>O. B. Rizvandi</u>, H. L. Frandsen - <a href="mailto:obari@dtu.dk">obari@dtu.dk</a> Department of Energy Conversion and Storage, Technical University of Denmark (DTU), Build- ing 310, Fysikvej, DK-2800 Lyngby, Denmark</p>
16:10	<p><b>Multi-scale modelling of Li-ion batteries: simulating outbreak of the thermal runaway</b> T. Katrašnik, I. Mele, K. Želič University of Ljubljana, Faculty of Mechanical Engineering, Laboratory for Internal Combustion Engines and Electromobility, 1000-Ljubljana, Slovenia <a href="mailto:tomaz.katrasnik@fs.uni-lj.si">tomaz.katrasnik@fs.uni-lj.si</a></p>	<p><b>Solar-Integrated High-Temperature Electrolysis Reactor Operating With Concentrated Irradiation</b> Clemens Suter<sup>1</sup>, Meng Lin<sup>1,2</sup>, <u>Sophia Haussener</u><sup>1</sup> - <a href="mailto:sophia.haussener@epfl.ch">sophia.haussener@epfl.ch</a> <sup>1</sup>Laboratory of Renewable Energy Science and Engineering, STI, EPFL, 1015-Lausanne, Switzerland <sup>2</sup>Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, China</p>
16:30	<p><b>Simulating power tool battery packs: a case study with practical relevance</b> V. Steinbauer, V. Knoblauch - <a href="mailto:veit.steinbauer@hs-aalen.de">veit.steinbauer@hs-aalen.de</a> Aalen University, Materials Research Institute (IMFAA), Battery Research Group, 73430 Aalen, Germany</p>	<p><b>Transient CFD Simulation of Reversible SOC Operation in a 3D Stripe Model</b> <u>S. Herrmann</u>, T. Van Lo, H. Spliethoff Technical University of Munich, Chair for Energy Systems, 85748, Germany <a href="mailto:stephan.herrmann@tum.de">stephan.herrmann@tum.de</a></p>
16:50	<p><b>Low Temperature Batteries for Deep Space Missions</b> <u>Lukas Lehnert</u><sup>1,2,3</sup>, Birger Horstmann<sup>1,2,3</sup>, Arnulf Latz<sup>1,2,3</sup> <sup>1</sup>Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany <sup>2</sup>German Aerospace Center, Pfaffenwaldring 38, 70569 Stuttgart, Germany <sup>3</sup>University of Ulm, Albert-Einstein-Allee 47, 89081 Ulm, Germany <a href="mailto:lukas.lehnert@dlr.de">lukas.lehnert@dlr.de</a></p>	<p><b>Numerical analysis of lock-in thermography applied to solid oxide cells</b> Guillaume Jeanmonod, Jan Van herle Group of Energy Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland <a href="mailto:guillaume.jeanmonod@epfl.ch">guillaume.jeanmonod@epfl.ch</a></p>
17:10	<b>End of Programme, Day 2</b>	