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| | **Day 1 - Tuesday 20th April 2021, morning** | |
| | **Opening Session – Invited talks** | |
| 9:00 | Welcome and Intro (J. Van herle – EPFL Valais/Wallis) | |
| 9:10 | **A1 Prof Dr Ulrike Krewer** (KIT, IAM-ET, Karlsruhe, Germany) *ulrike.krewer@kit.edu*<br>Understand Your Electrodes: Reaction Kinetic Modeling | |
| 9:45 | **A2 Dr Clemens Fink** (AVL List GmbH, 8020 Graz, Austria) *clemens.fink@avl.com*<br>PEM Fuel Cell Simulation with AVL FIRE™ – Latest Developments and Application Examples | |
| 10:20 | *Morning break 20'* | |
| | **B1 Battery modeling**<br>Chair: U Krewer | **C1 PEMFC Degradation**<br>Chair: C Fink |
| 10:40 | **Heterogenous vs Homogenous Battery Models**<br>Henrik Ekström<br>COMSOL AB, Tegnérgatan 23, 111 40 Stockholm, Sweden<br>*henrik.ekstrom@comsol.com* | **Modelling start-up in automotive PEMFC: evaluation of mitigation strategies and experimental validation**<br>E. Colombo, A. Bisello, A. Casalegno, A. Baricci<br>Politecnico di Milano, Department of Energy<br>MRT Fuel Cell & Battery Laboratory<br>via Lambruschini 4a, 20156 Milano, Italy<br>*elena.colombo@polimi.it* |
| 11:00 | **Local microstructure-induced fluctuations in Li-Ion battery: theory and simulations**<br>Igor Traskunov[1,2], Arnulf Latz[1,2,3] - *igor.traskunov@dlr.de*<br>[1]DLR, Institute of Engineering Thermodynamics, 70569 Stuttgart, Germany<br>[2]Helmholtz Institut Ulm (HIU), 89081 Ulm, Germany<br>[3]Institute of Electrochemistry, University of Ulm, 89081 Ulm, Germany | **Coupled models for PEMFC membrane degradation to bipolar plate corrosion**<br>Imen Elferjani[1,2], Benoît Ter Ovanessian[2], Bernard Normand[2], Guillaume Serre[1]<br>[1]CEA-DRT-LITEN, Grenoble, France - *imenlferjani@gmail.com*<br>[2]Université de Lyon, INSA-LYON, MATEIS UMR CNRS 5510, 69621 Villeurbanne, France |
| 11:20 | **Asymptotic Methods for the Estimation of Lithium Transport Properties in Lithium-Ion Batteries**<br>F. Brosa Planella[1,2], W.D. Widanage[1,2] - *Ferran.Brosa-Planella@warwick.ac.uk*<br>[1] WMG, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK<br>[2] The Faraday Institution, Quad One, Becquerel Avenue, Harwell Campus, Didcot, OX11 0RA | **Hydrocarbon Fuel Cell Membranes:**<br>**Can Radical Induced Damage be Repaired ?**<br>L. Gubler[1], T. De Wild[1,2], T. Nemeth[1,2], T.J. Schmidt[1,4], T. Nauser[2]<br>[1]Paul Scherrer Institut, Electrochemistry Laboratory, 5232 Villigen PSI, CH<br>[2]Laboratory of Inorganic Chemistry, ETH Zürich, 8093 Zürich, Switzerland<br>[4]Laboratory of Physical Chemistry, ETH Zürich, 8093 Zürich, Switzerland<br>*lorenz.gubler@psi.ch* |
| 11:40 | **Swelling of SiC / graphite blended electrodes: modelling and experimental measurements**<br>B. Mathieu, C. Leys, D. Vidal, W. Porcher, O. Gillia, M. Chandesris<br>Univ. Grenoble Alpes, CEA, LITEN, F-38054 Grenoble<br>*benoit.mathieu@cea.fr* | **Degradation Mechanisms of Catalyst-Layers in PEM Fuel Cells and Increase of Vehicle Life**<br>J. Trägner, M. Pollak , S. Heinke , W. Tegethoff , J. Kohler<br>TU Braunschweig, Institut für Thermodynamik, Hans-Sommer-Straße 5, 38106 Braunschweig, Germany<br>*j.traegner@tu-braunschweig.de* |
| 12:00 | *Lunch break for 1h30'* | |
| | **Tuesday 20th April 2021, afternoon** | |
| | **B2 Battery degradation**<br>Chair: | **C2 PEMFC $H_2O$ management / GDL**<br>Chair: P Boillat |
| 13:30 | **Efficient Simulation of Chemical-Mechanical Coupling in Battery Active Particles**<br>G.F. Castelli[1], L. von Kolzenberg[2,3], B. Horstmann[2,3], A. Latz[2,3,4], W. Dörfler[1]<br>[1]Karlsruhe Institute of Technology (KIT), Institute of Applied and Numerical Mathematics, 76131 Karlsruhe, Germany<br>[2]DLR, Institute of Engineering Thermodynamics, 70569 Stuttgart, Germany<br>[3]Helmholtz Institute Ulm (HIU), 89081 Ulm, Germany<br>[4]Ulm University (UUlm), 89081 Ulm, Germany<br>*fabian.castelli@kit.edu* | **The Inhomogeneous Distribution of Polytetrafluorethylene in the Gas Diffusion Layers of Polymer Electrolyte Fuel Cells**<br>D. Froning[1], U. Reimer[1], and W. Lehnert[1,2]<br>[1]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research, IEK-14: Electrochemical Process Engineering, D-52425 Jülich, Germany<br>[2]Modeling in Electrochemical Process Engineering, RWTH Aachen University, D-52056 Aachen, Germany<br>*d.froning@fz-juelich.de* |
| 13:50 | **Elucidating the species distribution during SEI formation using kinetic Monte Carlo**<br>M. Gerasimov[1], F.A. Soto[2] , J. Wagner[1] , P. B. Balbuena[2] , U. Krewer[1]<br>[1] Karlsruhe Inst. of Technology, IAM – Electrochemical Technologies, Karlsruhe, D<br>[2] Texas A&M University, Dpmt of Chemical Engineering, College Station, USA<br>*michail.gerasimov@kit.edu* | **3-D simulation of heat and water transport in PEFCs during evaporative cooling and humidification**<br>R. Herrendörfer*[1], M. Cochet[2], P. Boillat[2] J.O. Schumacher[1]<br>[1]ZHAW, Institute of Computational Physics, CH-8401 Winterthur<br>[2]Electrochemistry Laboratory, Paul Scherrer Institute, CH-5232 Villigen<br>*robert.herrendoerfer@zhaw.ch* |
| 14:10 | **A physics-based aging model for life prediction of blended anodes with Si-C composites**<br>P-F Lory[1,*], B. Mathieu[1], M. Grand-Jacques[1], S. Genies[1], M. Hubert[1], Y. Reynier[1], A. Boulineau[1], D. Thomas[1], W. Hong[2], M. Chandesris[1]<br>[1]Univ. Grenoble Alpes, CEA, LITEN, F-38054 Grenoble, France<br>[2]Samsung Electronic Inc. SAIT, South Korea<br>*Present affiliation : Automotive Cells Co. Centre R&D – 33520 Bruges - F<br>*marion.chandesris@cea.fr* | *cancelled* |
| 14:30 | *Afternoon break 20'* | |

| | B3 Redox Flow Batteries<br>Chair: | C3 Solid oxide cells microstructures<br>Chair: J Laurencin |
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| 14:50 | **Towards rigorous thermodynamics in aqueous flow batteries: measuring activity coefficients with differential scanning calorimetry**<br>Gaël Mourouga[1], Mathieu Courty[2], Emmanuel Baudrin[2], Thomas J.Schmidt[3], Jürgen O. Schumacher[1] - *mouo@zhaw.ch*<br>[1]ZHAW, Institute of Computational Physics, 8400 Winterthur, Switzerland<br>[2]Laboratoire de Réactivité et Chimie des Solides (LRCS), UMR CNRS 7374, Univ. de Picardie Jules Verne, 33 rue Saint-Leu, 80039 Amiens Cedex, France<br>[3]Paul Scherrer Institut, Energy & Environment Division, 5232 Villigen, CH | **Massive Simultaneous Cloud Computing for data driven optimization of SOFC electrodes**<br>L. Holzer[1], P. Marmet[1] , T. Hocker[1] , G. Boiger[1] , J.G. Grolig[2] , H. Bausinger[2] , A. Mai[2] , M. Fingerle[3] , J. M. Brader[4]<br>[1]Zurich University of Applied Sciences (ZHAW), Switzerland<br>[2]Hexis AG, Switzerland<br>[3]Math2Market, Germany<br>[4]University of Fribourg, Switzerland<br>*holz@zhaw.ch* |
| 15:10 | **Effects of the diffusive mixing and self-discharge reactions in membraneless redox flow batteries**<br>Santiago E. Ibáñez León[1], Alberto E. Quintero[3], Pablo A. García-Salaberri[2], Jesús Palma[1], Rebeca Marcilla[1], Paula Navalpotro[1], Marcos Vera[2]<br>[1]Electrochemical Processes Unit, IMDEA Energy Institute, Avda. Ramón de La Sagra 3, 28935, Móstoles, Spain - *santiago.ibanez@imdea.org*<br>[2]Fluid Mechanics Dep., Univ. Carlos III de Madrid, 28911, Leganés, Spain.<br>[3]Micro Electrochemical Technologies, Federico Cantero Villamil, 2-B, 28935, Móstoles, Spain | **3-D morphology-based modeling of Ni-YSZ electrodes microstructural evolution in solid oxide cells**<br>Hamza Moussaoui[1], Arata Nakajo[1], Giorgio Rinaldi[1], Maxime Hubert[2], Jérôme Laurencin[2], Jan Van herle[1]<br>[1]Group of Energy Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland<br>[2]Univ. Grenoble Alpes, CEA/LITEN, 17 rue des Martyrs, 38054, Grenoble, F<br>*hamza.moussaoui@epfl.ch* |
| 15:30 | **Thermodynamics and diffusional mass transport problems in concentrated electrolytes – an application in $H_2/Br_2$ redox flow battery simulations**<br>Jakub Wlodarczyk[1], Norman Baltes[2], Andreas Friedrich[3], J. O. Schumacher[1]<br>[1]ZHAW, Institute of Computational Physics, 8401 Winterthur, Switzerland<br>[2]Fraunhofer Institute for Chemical Technology, Joseph-von-Fraunhofer-Strasse 7, 76327 Pfinztal, Germany - *jakub.wlodarczyk@zhaw.ch*<br>[3]German Aerospace Center, Institute of Engineering Thermodynamics, Electrochemical Energy Technology, Pfaffenwaldring 38-40, 70569 Stuttgart, D | **Generalized Nernst-Planck-Poisson Model of Solid Oxide YSZ\|LSM\|$O_2$ Electrode Interface**<br>P. Vágner[1], V. Miloš[2,3], D. Budáč[3], M. Carda[3], M. Paidar[3], J. Fuhrmann[1], K. Bouzek[3] - *petr.vagner@wias-berlin.de*<br>[1]Weierstrass Institute for Applied Analysis and Stochastics, 10117-Berlin, D<br>[2]Mathematical Institute, Charles University, 12116-Prague, Czechia<br>[3]Department of Inorganic Technology, University of Chemistry and Technology, 16628-Prague, Czechia |
| 15:50 | **How pillar electrodes enhance redox flow batteries**<br>M. De Rop , J. Hereijgers ,T. Breugelmans<br>University of Antwerp, Faculty of Applied Engineering<br>Applied Electrochemistry and Catalysis (ELCAT)<br>2610-Wilrijk, Belgium | **Model based optimization of CGO anodes**<br>P. Marmet[1], L. Holzer[1], J.G. Grolig[2], H. Bausinger[2], A. Mai[2], J. M. Brader[3], T. Hocker[1] - *mame@zhaw.ch*<br>[1]ZHAW, Inst. of Computational Physics, 8400, Winterthur, Switzerland<br>[2]Hexis AG, CH-8404 Winterthur, Switzerland<br>[3]University of Fribourg, Department of Physics, CH-1700 Fribourg, Switzerland |
| 16:10 | **Multiphysics modelling of vanadium redox flow batteries**<br>V. Muñoz[1]*, S. Berling[2], P.A. García-Salaberri[1], S.E. Ibañez[1], E. García[2], J. Palma[2], M. Vera[1] - *vamunozp@ing.uc3m.es*<br>[1]Universidad Carlos III de Madrid, Department of Thermal and Fluid Mechanics Engineering, 28911-Leganés, Spain<br>[2]IMDEA Energía, Unit of Electrochemical Processes, 28935-Móstoles, Spain | *free* |
| 16:30 | *Short transition break* | |
| 16:40 | **A3 Dr Jérôme Laurencin** (CEA, Grenoble) *jerome.laurencin@cea.fr*<br>Impact of Microstructure and Reaction Mechanisms on Solid Oxide Cell Performances and Degradation<br>E. Effori[1], F. Monaco[1], H. Moussaoui[1], M. Hubert[1], D. Ferreira Sanchez[2], P. Cloetens[3], J. Laurencin[1] - *jerome.laurencin@cea.fr*<br>[1]Univ. Grenoble Alpes, CEA/LITEN, F-38054 Grenoble, France<br>[2]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland<br>[3]European Synchrotron Radiation Facility (ESRF), 38000, Grenoble, France | |
| 17:15 | **End of Programme, Day 1** | |