31st Topical Meeting

of the International Society of Electrochemistry

15-19 May 2022
Aachen, Germany

PROGRAM

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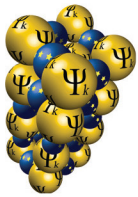

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Program of the

31st Topical Meeting of the International Society of Electrochemistry

Theory and Computation in Electrochemistry: Seeking Synergies in Methods, Materials and Systems

15-19 May 2022
Aachen, Germany

Organized by:
Division 4 Electrochemical Materials Science
Division 7 Physical Electrochemistry
ISE Region Germany

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Rebekka Tesch, *Forschungszentrum Jülich*

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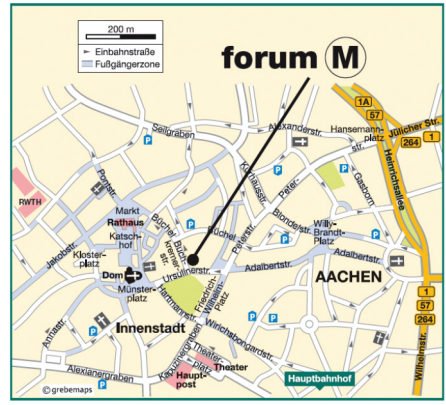
Sunday 15 May - Afternoon

Forum M

Buchkremerstraße 1-7,
52062 Aachen, Germany



15:00

Registration Open

Forum M

17:00

Opening Ceremony

Forum M

17:30 to 18:30

Opening Lecture

Forum M

Chaired by: Michael Eikerling

Marc Koper *(Leiden Institute of Chemistry, Leiden University, Leiden, Netherlands)*
Theory and modeling for the electrocatalytic reduction of CO_2

18:45 - 21:00

Welcome Reception

Forum M

Monday 16 May 2022 - Morning

Keynote

Room 1

Chaired by: Michael Eikerling

08:45 to 09:30

Alexei Kornyshev *(Chemistry, Imperial College London , London, United Kingdom)*, Joshua Edel, Anthony Kucernak, Ye Ma, Debabrata Sikdar, Michael Urbakh, Leonora Velleman, Cristian Zagar

Electrochemical photonics -tuning functionalities of optical metamaterials in real time-

S3 - Modeling functional materials: microstructure to complex electrodes

Room 1

Chaired by: Michael Eikerling

09:30 to 09:50

Qiong Cai *(Chemical and Process Engineering, University of Surrey, Guildford, United Kingdom)*, Eleftherios Andritsos, Emilia Olsson

Atomic-scale Materials Design for Energy Storage Batteries

09:50 to 10:10

Chiara Panosetti *(Theory, Fritz Haber Institute of the Max Planck Society, Berlin, Germany)*, Simon Anniés, Cristina Grosu, Christoph Scheurer

A multiscale approach to the modelling of lithium-graphite battery anodes—with a focus on approximate electronic structure

10:10 to 10:30

Artur Braun *(Functional Materials, Empa. Swiss Federal Institutes of Technology, Dübendorf, Switzerland)*, Qianli Chen, Peng Du, Maria A Gomez, Frederick G Haibach

Proton-phonon coupling and cooperative origin of proton pairdiffusivity in ceramic proton conducting membranes

10:30 to 10:50

Weihan Li *(ISEA, RWTH Aachen University, Aachen, Germany)*, Decheng Cao, Iskender Demir, Dominik Jöst, Florian Ringbeck, Dirk Uwe Sauer

Data-Driven Parameter Identification of an Electrochemical Model for Lithium-ion Batteries with Artificial Intelligence

10:50 to 11:10 **Invited**

Payam Kaghazchi *(IEK-1, FZJ, Jülich, Germany)*

Simulation of Electro-Chemo-Mechanical Effects in Microstructure of Li-based Cathode Materials

11:10 to 11:30

Coffee Break

Monday 16 May 2022 - Afternoon

S1 - Advances in first principles electrochemical methods

Room 1

Chaired by: Federico Calle-Vallejo and Mathieu Salanne

13:40 to 14:00 **Invited**

Chao Zhang *(Department of Chemistry - Ångström Laboratory, Uppsala University, Uppsala, Sweden)*

Modelling Protonic Double Layer at Metal Oxide-Electrolyte Interfaces

14:00 to 14:20

Marko Melander *(Department of Chemistry, Nanoscience Center, University of Jyväskylä, Jyväskylä, Finland)*

Grand canonical ensemble methods for electrochemistry

14:20 to 14:40

Piotr Kowalski *(IEK-13 : Theory and Computation of energy Materials, Forschungszentrum Jülich GmbH, Jülich, Germany)*

Advancements in First Principles Methods: Lessons From Integrated Theory, Simulation and Experimental Studies of Energy Materials

14:40 to 15:00

Yoshitaka Tateyama *(Center for Green Research on Energy and Environmental Materi, National Institute for Materials Science (NIMS), Tsukuba, Japan)*, Bo Gao

Standard Electrochemical Potential Analysis Based on DFT Interface Calculation: Microscopic Electrochemistry Framework

15:00 to 15:20

Alejandro D. Somoza *(Institut für Technische Thermodynamik, German Aerospace Center (DLR), Stuttgart, Germany)*, Birger Horstmann, Konstantin Lamp, Lubasch Michael, Albert J. Pool, Giorgio Silvi, Nicolas Vogt, Marina Walt

Quantum Algorithms in Electrochemistry: Atomistic and Continuous Models in Battery Research

15:20 to 15:40

Alexandra Celinda Dávila López *(Theory, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)*, Nicolas Hörmann, Thorben Eggert, Karsten Reuter

Revisiting the OH Adsorption on Pt(111) in Static Water Environments

15:40 to 16:10

Coffee Break

16:10 to 16:30 **Invited**

Kai Exner *(Theoretical Inorganic Chemistry, University Duisburg-Essen, Essen, Germany)*

A Universal Descriptor for the Screening of Catalysts for Multiple-Electron Processes: The Free-Energy Span Model in Electrocatalysis

16:30 to 16:50

Annalisa Paolone *(Istuto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, Roma, Italy)*, Sergio Brutti, Simone Di Muzio

New methods for the calculation of the electrochemical stability of ionic liquids

16:50 to 17:10

Andreas Heuer *(Physical Chemistry, University of Muenster, Muenster, Germany)*, Isidora Cekic-Laskovic, Diddo Diddens, Mariano Gruenebaum, Youssef Mabrouk, Moumita Maiti, Anand Narayanan Krishnamoorthy, Martin Winter, Christian Woelke, Peng Yan

Gaining insights on the conductivity of battery electrolytes through synergy between high-throughput experiments, data-driven analysis and computer simulations

17:10 to 17:30

Michael Busch *(Department of Chemistry and Material Science, Aalto University, Espoo, Finland)*, Elisabet Ahlberg, Kari Laasonen

How to Predict the pKa of any Compound in any Solvent

17:30 to 17:50

Chris-Kriton Skylaris *(Chemistry, University of Southampton, Southampton, United Kingdom)*, Arihant Bhandari, Jacek Dziedzic, Denis Kramer, John Owen, Chao Peng

A platform for large-scale quantum atomistic electrochemistry simulations

17:50 to 18:10

Nicolas Bergmann *(Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)*, Nicolas G. Hörmann, Karsten Reuter

Cyclic Voltammograms from First Principles

18:10 to 18:30

Nicolas Georg Hörmann *(Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)*, Nicolas Bergmann, Karsten Reuter

Cyclic Voltammograms at Applied Potential Conditions - A test for Theory?!

Tuesday 17 May 2022 - Morning

Keynote

Room 1

Chaired by: Axel Groß

08:45 to 09:30

Ryosuke Jinnouchi *(Fuel Cell Research-Domain, Toyota Central R&D Labs., Inc., Nagakute, Japan)*, Naoki Hasegawa, Shuji Kajiya, Masao Shibata, Kazuma Shinozaki, Takahisa Suzuki, Shunsuke Yamakawa

Multi-scale Simulations to Identify Rate Determining Mass Transport Process in Cathode Catalyst Layer of Proton Exchange Membrane Fuel Cells

S2 - Theory and computation of interfacial and nanoscale phenomena

Room 1

Chaired by: Axel Groß

09:30 to 09:50 **Invited**

Jörg Behler *(Chemistry, Universitaet Goettingen, Goettingen, Germany)*

Investigating Solid-Liquid Interfaces Using High-Dimensional Neural Network Potentials

09:50 to 10:10

Jun Huang *(IEK-13, Forschungszentrum Jülich GmbH, Jülich, Germany)*

Three generations of density-potential functional theory for metal-solution interfaces

10:10 to 10:30

Giovanni Pireddu *(PHENIX Laboratory, Sorbonne Universite, CNRS, Paris, France)*, Giovanni Pireddu, Benjamin Rotenberg

Induced charges on metallic surfaces and their fluctuations

10:30 to 10:50

Tobias Binninger *(CPTM Department for Theoretical Chemistry, Institut Charles Gerhardt Montpellier, CNRS, Montpellier, France)*

Unified Understanding of Quantum and Classical Contributions to the Capacitance of Electrochemical Interfaces

10:50 to 11:10

Coffee Break

Tuesday 17 May 2022 - Afternoon

S2 - Theory and computation of interfacial and nanoscale phenomena

Room 1

Chaired by: Kai Exner and Chao Zhang

13:40 to 14:00

Katharina Doblhoff-Dier *(Leiden Institute of Chemistry, Leiden University, Leiden, Netherlands)*, Marc Koper, Kasinath Ojha

Pt double layer - theory meets experiment

14:00 to 14:20

Simeon Beinlich *(Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)*, Nicolas Hörmann, Karsten Reuter

Electrochemistry Standing Out - A Theoretical Evaluation of Stepped and Kinked Surface Sites

14:20 to 14:40

Rebekka Tesch *(Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich, Jülich, Germany)*, Michael H. Eikerling, Piotr M. Kowalski

Simulating the Pt(111)/Electrolyte Interface with DFT-ESM-RISM

14:40 to 15:00

Jürgen Fuhrmann *(Numerical Mathematics and Scientific Computing, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany)*

Excess chemical potential based finite Volume Schemes for Charge Transport Problems

15:00 to 15:20

Rüdiger Müller *(Thermodynamic Modeling and Analysis of Phase Transitions, Weierstrass Institute, Berlin, Germany)*, Jürgen Fuhrmann, Manuel Landstorfer

Non-equilibrium thermodynamics modeling of polycrystalline electrode | liquid electrolyte interfaces

15:20 to 15:40

Katharina Helmbrecht *(Theoretical Chemistry, University Ulm, Ulm, Germany)*, Holger Euchner, Axel Gross

Revisiting the chevrel phase: Impact of dispersion corrections on the properties of Mo6S8 for cathode applications

15:40 to 16:10

Coffee Break

16:10 to 16:30 **Invited**

Federico Calle-Vallejo *(Materials Science and Physical Chemistry, University of Barcelona, Barcelona, Spain)*

Optimizing Electrocatalysts for the Oxygen Evolution Reaction

16:30 to 16:50

Kari Laasonen *(Department of Chemistry and Materials Science, Aalto University, Aalto, Finland)*, Rasmus Kronberg

Computational Hydrogen Evolution Study on Pt(111) Using DFT Constrained MD Simulations

16:50 to 17:10

Zdenek Futera *(Faculty of Science, University of South Bohemia, Ceske Budejovice, Czech Republic)*, Denys Biriukov, Outi Vilhelmiina Kontkanen

Electric-Field Effects on Biomolecular Interfaces with Gold Electrodes

17:10 to 17:30

Manuel Kolb *(IQTC, Univ. of Barcelona, Barcelona, Spain)*, Federico Calle-Vallejo

Thermodynamic Limits for Bifunctional Oxygen Evoluation and Reduction Catalysts from Scaling Relations

17:30 to 17:50

Roxanne Berthin *(Chemistry, Sorbonne Universite, Paris, France)*, Olivier Fontaine, Mathieu Salanne, Alessandra Serva

Structure of Confined Biredox Ionic Liquid in Electrified Mesopores by Classical Molecular Dynamics

17:50 to 18:10

Thorben Eggert *(Theorie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)*, Alexandra C. Davila, Nicolas G. Hoermann, Karsten Reuter

Efficiency Through Diversity: Improving the MD Sampling of Water-Metal Interfaces

18:10 to 18:30

Enrique Herrero *(Instituto de Electroquimica, Universiad de Alicante, Alicante, Spain)*, Rosa M. Arán-Ais, Dalila S. Mekazni

On the role of adsorbed OH in the oxidation mechanisms of methanol and ethanol

18:30 to 18:50

Richard Haid *(Physics, Technical University of Munich, Garching, Germany)*, Aliaksandr Bandarenka, Federico Calle-Vallejo, Regina Kluge, Thorsten Schmidt

High-Resolution Imaging of Active Sites under Reaction Conditions for Carbon-Based Electrocatalysis

Wednesday 18 May 2022 - Morning

Keynote

Room 1

Chaired by: Birger Horstmann

08:45 to 09:30

Tejs Vegge *(Department of Energy Conversion and Storage, Technical University of Denmark, Kgs. Lyngby, Denmark)*

ML-accelerated simulations of solid-electrolyte interfaces in electrochemical systems

S4 - Modeling dynamic phenomena in electrochemical systems

Room 1

Chaired by: Birger Horstmann

09:30 to 09:50

Panagiotis Giotakos *(Dpt. of Chemical Engineering, University of Patras, FORTH/ICE-HT, Patras, Greece)*, Panagiotis Giotakos, Stylianos Neophytides

O_2 Reduction Mechanism, Kinetic Inertia and Energetics in HTPEMFCs

09:50 to 10:10

Yujin Tong *(Department of Physics, Universität Duisburg-Essen, Duisburg, Germany)*, Uwe Bovensiepen, Manuel Bridger, R. Kramer Campen, Zhipeng Huang, Oscar Andres Naranjo-Montoya, Alexander Tarasevitch

Vibrationally Assisted Electron Transfer Across the Metal/Aqueous Interface: a two photon photovoltage study

10:10 to 10:30

Manuel Dillenz *(Institute of Theoretical Chemistry, Ulm University, Ulm, Germany)*, Holger Euchner, Axel Groß, Mohsen Sotoudeh

Unravelling charge carrier mobility in d0-metal-based spinels

10:30 to 10:50

Amit N. Shocron *(Faculty of Mechanical Engineering, Technion, Haifa, Israel)*, P.M. Biesheuvel, Jouke E. Dykstra, Eric N. Guyes, Huub H.M. Rijnaarts, Matthew E. Suss

Enhanced Boron Removal by Capacitive Deionization

10:50 to 11:10

Coffee Break

Wednesday 18 May 2022 - Afternoon

S4 - Modeling dynamic phenomena in electrochemical systems

Room 1

Chaired by: Jun Huang

13:40 to 14:00

Florian Baakes *(IAM - Electrochemical Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany)*, Ulrike Krewer

Model-based Assessment of Species Contributions to the Thermal Runaway in Lithium-ion Batteries

14:00 to 14:20

Martin Petit *(Materials and Electrochemistry, IFP Energies nouvelles, Solaize, France)*, Andrea Bertinetti, Jerome Bikard, Gaëtan Damblanc, Vivien Esnault, Lorenzo Maschio, Franck Sellier, Mauro Sgroi, Fabrizio Silveri, Alessio Tommasi, Chen Zhao

MODALIS² project: Use of a multiscale/multiphysics approach for Gen 3b Li-ion batteries modelling in a simulation toolchain

14:20 to 14:40

Chia Qian Tong *(Department of Energy Storage System, Fraunhofer Institute for Energy Economics and Energy System, Kassel, Germany)*, Tatjana Dabrowski, Lars Pescara, Mathias Thiele

Modelling Dendrite Growth and Solid Electrolyte Interphase (SEI) Formation in Metallic Lithium Batteries

14:40 to 15:00

Mark Junker *(Institute for Power Electronics and Electrical Drives (ISEA), RWTH Aachen University, Aachen, Germany)*, Fabian Frie, Dirk Uwe Sauer

Physically Motivated Hysteresis Modelling of Non-Intercalation Active Material Blends for Anodes in Lithium-Ion Batteries

15:00 to 15:20

Janina Drews *(Institute of Engineering Thermodynamics, German Aerospace Center (DLR) Helmholtz Institute Ulm (HIU, Ulm, Germany)*, J. Alberto Blazquez, Timo Danner, Janina Drews, Maximilian Fichtner, Arnulf Latz, Zhenyou Li, Rudi Ruben Maca Alaluf, Johannes Wiedemann, Zhirong Zhao-Karger

Modelling of Magnesium Intercalation into Chevrel Phase Mo6S8

15:20 to 15:40

Niklas Herrmann *(Institute of Engineering Thermodynamics, German Aerospace Agency (DLR), Ulm, Germany)*, Birger Horstmann

Modelling Aqueous Zinc-Ion Batteries with a Novel Multi-Process Description of MnO_2-based Cathodes

15:40 to 16:10

Coffee Break

S5 - Accelerated materials development: rapid path from idea to integration

Room 1

Chaired by: Irina Zenyuk

16:10 to 16:30

Birger Horstmann *(Helmholtz-Institute Ulm, German Aerospace Center, Ulm, Germany)*, Yannick Kuhn, Arnulf Latz

Bayesian Optimization for Parameterization of Battery Cell Models

16:30 to 16:50

Jens Noack *(Applied Electrochemistry, Fraunhofer Institute for Chemical Technology, Pfinztal, Germany)*, Emmanuel Baudrin, Rocco Fornari, Alejandro Franco, Daniel Gerlach, Xinjie Guan, Jan Hamaekers, Astrid Maaß, Chris Menictas, Gael Mourouga, Hermann Nirschl, Nataliya Roznyatovskaya, Roman Schaerer, Juergen Schumacher, Maria Skyllas-Kazacos, Jakub Wlodarczyk, Amadeus Wolf, Jia Yu, Piotr de Silva

Modelling and Simulation for the Search for New Active Materials for Redox Flow Batteries - Results of the International Project SONAR

16:50 to 17:10

Astrid Maass *(Virtual Material Design, Fraunhofer Institute SCAI, Sankt Augustin, Germany)*, Niklas Dobberstein, Jan Hamaekers

SONAR-HTS: A Scale Spanning Screening Prototype for Searching Redox Materials in Organic Chemspace

17:10 to 17:30

Vladislav Mints *(Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Bern, Switzerland)*, Andy Anker, Matthias Arenz, Alexander Bagger, Kirsten Jensen, Jack Pedersen, Jonathan Quinson, Jan Rossmeisl

Exploring the relationship between HEA compositions and catalytic activity with machine learning tools

17:30 to 17:50

Vessela Tsakova *(Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria)*, Caterina Czibula, Radoslav Ivanov, Christian Teichert

Carbon Substrate-Assisted Spontaneous Noble Metals Deposition - a New Prospect for Development of Electrocatalytic Materials

17:50 to 18:10

Brianna Rector *(Chemistry, Western University, London, Canada)*, Dan Guo, Jiju M. Joseph, Nicholas A. Payne, Youn G. Shin, J. Clara Wren

Modelling Corrosion Dynamics as a Function of Solution Environments

18:10 to 18:30

Kannasoot Kanokkanchana *(Analytical Chemistry II, Ruhr University Bochum, Bochum, Germany)*, Kristina Tschulik

Electrical Modelling and Simulations of Nano Impact Electrochemical Experiments: Unraveling Experimental and Instrumentation Effects

Thursday 19 May 2022 - Morning

Keynote

Room 1

Chaired by: Ulrike Krewer

08:45 to 09:30

Matthew Suss *(Mechanical Engineering, Technion - Israel Institute of Technology, Technion City, Haifa, Israel)*, Eric Guyes, Zohar Sahray, Amit Shocron, Rana Uwayid

Numerical Modeling Unlocks Remarkable Ion Selectivity of Capacitive Deionization

S6 - Modeling-based diagnostics of electrochemical materials and cells

Room 1

Chaired by: Ulrike Krewer

09:30 to 09:50 **Invited**

Andrei Kulikovsky *(Theory and Computation of Energy Materials, Research Centre Jülich, IEK-13, Jülich, Germany)*

Analytical impedance of two-layer oxygen transport media in a PEM fuel cell

09:50 to 10:10 **Invited**

Iryna Zenyuk *(Chemical and Biomolecular Engineering, University of California Irvine, Irvine, USA)*, Jesus Lopez Ochoa, Prantik Saha

Electric Double Layer at Polycrystalline Platinum-Electrolyte Interface Probed by Electrokinetic Streaming Current Method

10:10 to 10:30

Yufan Zhang *(IEK-13, Forschungszentrum Jülich, Jülich, Germany)*, Gerard Agravante, Michael Eikerling, Thomas Kadyk

Modelling Water Accumulation in the Cathode of a Polymer Electrolyte Fuel Cell

10:30 to 10:50

Wolfgang Olbrich *(Theory and Computation of Energy Materials (IEK-13), FZ Jülich / Robert Bosch GmbH / RWTH Aachen, Jülich, Germany)*, Michael Eikerling, Thomas Kadyk, Ulrich Sauter

Structure-Based Modeling to Rationalize the Pt Utilization in Catalyst Layers of PEM Fuel Cells

10:50 to 11:10

Coffee Break

11:10 to 11:30 **Invited**

Tanja Vidakovic-Koch *(Electrochemical Energy Conversion, Max Planck Institute for Dynamics of Complex Technical Syste, Magdeburg, Germany)*

Novel frequency response methods for process analysis / diagnosis

11:30 to 11:50

Antoine Bonnefont *(Institut de Chimie de Strasbourg, Université de Strasbourg, Strasbourg, France)*, Vasilica Badets, Glykeria Chastazeri, Gwenaëlle Kéranguéven, Alejandra Medrano-Banda, Alexandr Oshchepkov, Laurent Ruhlmann, Elena Savinova, Jing Sun, Jules Wolff

Electrocatalytic Hydrogenation of Glucose on Ni-based Electrodes: Experimental and Microkinetic Modelling Study

11:50 to 12:10

Marco Löffelholz *(Institute of Chemical and Electrochemical ProcessEngineering, Clausthal University of Technology, Clausthal-Zellerfeld, Germany)*, Jens Osiewacz, Thomas Turek

Understanding the limitations of electrochemical CO_2 reduction at silver gas diffusion electrodes: A model study

12:10 to 12:30

Elixabete Ayerbe *(Materials for Energy Unit, CIDETEC Energy Storage, San Sebastian, Spain)*, Jose Luis Gutierrez Portal, Fernando Varas

Model-based Electrolyte Diffusion Coefficient Estimation

Poster Presentations

Monday: **Session 1**
Posters of Symposia 1 and 2
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at 11:30 and 18:30

Tuesday and Wednesday: **Session 2**
Posters of Symposia 2, 3, 4, 5 and 6
s02-025
s03-001 to s03-018 *and* s04-001 to s04-019
s05-001 to s05-007 *and* s06-001 to s06-011
at 11:10

S1 - Advances in first principles electrochemical methods

s01-001

Ede Bodoki *(Analytical Chemistry, Iuliu Hatieganu University of Medicine and Pharmacy, Cluj-Napoca, Romania)*, Cosmin Farcau, Elizaveta Vereshchagina

Combining Surface Enhanced Raman Spectroscopy and Electrochemistry for Analytical Applications

s01-003

Simone Di Muzio *(Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, Rome, Italy)*, Annalisa Paolone

Theoretical investigation of the contribution of the lithium salt hydrolysis to the formation of the SEI.

s01-004

Dominic Feldhaus *(Molten salt electrolyse, IME Process Metallurgy and Metal Recycling, RWTH Aachen Uni, Aachen, Germany)*, Vesna S. Cvetkovic, Bernd Friedrich, Jovan N. Jovicevic, Natasa M. Vukicevic

The study of Nd(III) and Pr(III) electrochemical reduction in molten fluoride salts

s01-006

Julian Holland *(Faculty of Engineering and Physical Sciences, University of Southampton, Southampton, United Kingdom)*, Arihant Bhandari, Felix Hanke, Denis Kramer, Chris-Kriton Skylaris, Milman Victor

Ab-initio Study of Lithium Intercalation into a Graphite Nanoparticle

s01-007

Sapajan Ibragimov *(Chemistry and Technology of Functional Materials, Gdansk University of Technology, Gdansk, Poland)*

Cobalt III oxides: structures and redox reactions

s01-008

Yiming Jiang *(Materials science and engineering, Tokyo Institute of Technology, Yokohama, Japan)*, Tso-Fu Mark Chang, Chun-Yi Chen, Osamu Kudo, Xun Luo, Ryu Maeda, Masanori Mizoguchi, Masato Sone, Daisuke Yamane

Thermal Stability and Mechanical Property of Electrodeposited Ni-B Alloy

s01-010

Torben Lemmermann *(ICVT, TU Clausthal, Goslar, Germany)*, Maik Becker, Ulrich Kunz, Thomas Turek

In situ and in operando detection of redox reactions during vanadium transport in ion exchange membranes

s01-011

Youssef Mabrouk *(Institut für Energie-und Kilmaforschung, Forschungszentrum Jülich, Muenster, Germany)*, Diddo Diddens, Andreas Heuer

Atomic-scale modeling of battery electrolyte degradation

s01-012

Madhulika Mazumder *(New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India)*, Abhiroop Lahiri, Swapan K Pati

Mechanistic Studies of Cathodic Behaviour in $NaRhO_2$ systems : A Combined First Principles and Grand Canonical Monte Carlo Approach

s01-013

Rebeca Moldovan *(Analytical Chemistry, Iuliu Hatieganu University of Medicine and Pharmacy, Cluj-Napoca, Romania)*, Ede Bodoki, Cosmin Farcau, Bogdan-Cezar Iacob, Karolina Milenko, Elizaveta Vereshchagina

EC-SERS Detection of Thiabendazole in Apple Juice Using Gold-Based Screen-Printed Electrodes

s01-015

Samad Razzaq *(Faculty of inorganic chemistry, Universität Duisburg-Essen, Essen, Germany)*, Kai S. Exner

Method to determine bifunctional index of the oxygen electrocatalysis

s01-016

Marco Schönig *(Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany)*, Rolf Schuster

Entropy changes during specific anion adsorption on Au(111)

s01-017

Margherita Buraschia (*Department of Chemistry, Imperial College, London)* Andrew Horsfield, Clotilde Cucinotta

Efficient electron open boundaries for electrochemical applications

S2 - Theory and computation of interfacial and nanoscale phenomena

s02-001

Nawras Abidi *(Department of chemistry, ENS de Lyon, Lyon 7, France)*, Audrey Bonduelle-Skrzypczak, Stephan N.Steinmann

Is Doping an efficient Strategy to activate the Basal Plane of 2H-MoS_2 for the Hydrogen Evolution Reaction?

s02-002

Binny Alangadan Davis *(Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich GmbH, Jülich, Germany)*, Michael Eikerling

Computational Study to Unravel Structure and Properties of Catalyst-Ionomer Interfaces in PEM Fuel Cells

s02-003

Tobias Binninger *(CPTM Department for Theoretical Chemistry, Institut Charles Gerhardt Montpellier, CNRS, Montpellier, France)*, Marie-Liesse Doublet

Combining Activity and Stability in the Electrocatalysis of the Oxygen Evolution Reaction on IrO_2 (110)

s02-004

Niclas Blanc *(Chair of Analytical Chemistry II, Ruhr-University Bochum, Bochum, Germany)*, Kristina Tschulik

Assessing Diffusional Mass Transport in Catalytic Single Nanoparticle Electrochemistry

s02-005

Thomas Bornhake *(Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich GmbH, Jülich, Germany)*, Oskar Cheong, Piotr M. Kowalski

A DFT study of different solvation approaches on the HCOOH/CO selectivity of CO_2 reduction reaction on Pb(100) surface

s02-006

Lars Fabian Brämer *(Chair of Analytical Chemistry II, Ruhr University Bochum, Faculty of Chemistry and Biochemistr, Bochum, Germany)*, Kristina Tschulik, Kevin Wonner

High-throughput Image Analysis for the Characterization of Individual Nanoparticle Reactivities during Electrochemical Oxidation

s02-007

Pim Broersen *(Heterogeneous Catalysis and Sustainable Chemistry, University of Amsterdam, Amsterdam, Netherlands)*

CO_2 Reduction Reactions on Non-Pristine Copper Surfaces

s02-008

Yingzhen Chen *(Institute of Energy and Climate Research, Forschungszentrum Jülich, Jülich, Germany)*, Carsten Korte, Piotr Kowalski, Federico Parisi, Christian Rodenbücher, Klaus Wippermann

Atomistic simulation of protic ionic liquid as novel fuel cell electrolytes

s02-009

Oskar Cheong *(Theory and Computation of Energy Materials (IEK-13), FZ Jülich, Jülich, Germany)*, Michael H. Eikerling, Piotr M. Kowalski

Using the Interface Force Field (IFF) to Evaluate Water Structures at Metal Surfaces: Potential and Limitations

s02-010

Oskar Cheong *(Theory and Computation of Energy Materials (IEK-13), FZ Jülich, Jülich, Germany)*, Johannes Häusler, Piotr M. Kowalski, Joachim Pasel, Ralf Peters

A Combined DFT/Experimental Study on the Ethanol Dehydrogenation Reaction on Pt-based Catalyst

s02-011

Walter Cistjakov *(Institute of Energy and Process Systems Engineering, TU Braunschweig, Braunschweig, Germany)*, Johanna Hoppe, Ulrike Krewer, Fridolin Röder

Model based Investigation of Carbon Surface Passivation in Lithium-Sulfur Battery

s02-012

Heigo Ers *(Institute of Chemistry, University of Tartu, Ravila 14a, Estonia)*, Maria Natália D.S. Cordeiro, Borja Docampo Alvarez, Vladislav Ivanistsev, Volodymyr Koverga, Piret Pikma, Iuliia Voroshylova

Studying the Characteristic Features of Interfacial Capacitance — Insights from Molecular Dynamics Simulations

s02-015

Lukas Koebbing *(German Aerospace Center, Helmholtz-Institute Ulm, Ulm, Germany)*, Birger Horstmann, Arnulf Latz

Theory and Simulation of Transport and Mechanics of a Polycrystalline SEI

s02-016

Outi Vilhelmiina Kontkanen *(Department of Physics, University of South Bohemian, Ceske Budejovice, Czech Republic)*, Denys Biriukov, Zdenek Futera

Reorganization Free Energy of Azurin on Vacuum Gold Interfaces

s02-017

Yonghyuk Lee *(Theory, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)*, Karsten Reuter, Christoph Scheurer

Stable and Cost-Efficient Core-Shell Catalysts for Enhanced Acidic Oxygen Evolution - A First Principles Approach

s02-019

Amir Hossein Omranpoor *(Theoretical Chemistry, Universität Duisburg-Essen, Essen, Germany)*, Stephane Kenmoe, Tim Kox

ab initio Molecular Dynamics Study of 2-propanol Oxidation at Co_3O_4 (001)/H_2O Interface

s02-020

Hedda Oschinski *(Fritz-Haber-Institut, Max-Planck-Gesellschaft, Berlin, Germany)*, Nicolas Hoermann, Karsten Reuter

Understanding the Interfacial Capacitance of 2D materials in Implicit Water Environment

s02-022

Pouya Partovi-Azar *(Institute for Chemistry, Martin-Luther University of Halle-Wittenberg, Halle (Saale), Germany)*

Quantum-Mechanical Characterization of Sulfur/Carbon Co-polymer Cathodes for Li-S Batteries

s02-023

Giovanni Pireddu *(Department of Chemistry, CNRS, ENS - PSL Univ., Sorbonne Univ., Paris, France)*, Christian Amatore, Alexander Oleinick, Irina Svir

Modelling Diffusion at Random Arrays: Link Between Mass Transport and Spatial Distribution of Active Sites

s02-024

Ramin Rabani *(Sustainable Chemistry, Vito, Mol, Belgium)*, Xochitl Dominguez-Benetton, Jan Fransaer

Numerical Investigation of the Precipitation of Metal Ions by the Gas-Diffusion Electrocrystallization (GDEx) Process

s02-026

Christian Rodenbuecher *(Institute of Energy and Climate Research, Forschungszentrum Jülich, Jülich, Germany)*, Yingzhen Chen, Carsten Korte, Piotr Kowalski, Klaus Wippermann

Nanoscale analysis of the electric double layer formed between platinum and the protic ionic liquid [Dema][TfO]

s02-027

Halil Ibrahim Sözen *(Institute of Chemistry, Carl-von-Ossietzky University of Oldenburg, Oldenburg, Germany)*, Thorsten Klüner, Giulia Loselli, Dongya Lyu, Mehtap Ozaslan, Halil Ibrahim Sözen

Ab initio design of Pt-Ir based novel bifunctional electrocatalysts for fuel cell applications

s02-028

Xinwei Zhu *(Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich, Jülich, Germany)*, Michael Eikerling, Jun Huang,

Theoretical Modeling of the Local Reaction Environment at Interfaces for Formic Acid Oxidation

s02-029

Rashid Al-Heidous (Imperial College, London, UK) *Matthew Darby, Nicholas Harrison, Clotilde Cucinotta)*

Ab Initio study of the onset of Al corrosion

S2 - Theory and computation of interfacial and nanoscale phenomena

s02-025

Stefan Ringe *(Chemistry, Korea University, Seoul, Korea)*

The importance of a charge transfer descriptor for the screening of electrocatalysts at the example of CO_2 reduction

S3 - Modeling functional materials: microstructure to complex electrodes

s03-001

Zhengda He *(Institute of Energy and Climate Research (IEK-13), Forschungszentrum Jülich, Aachen, Germany)*, Michael Eikerling, Mohammad Eslamibidgoli, Piotr Kowalski, Rebekka Tesch

Computational Investigation of Fe-doped NiOOH Electrocatalysts

s03-002

Simon Hein *(Insitut of Engineering Thermodynamics, German Aerospace Center, Ulm, Germany)*, Andreas Albrecht, Timo Danner, Emanuel Heider, Alice Hoffmann, Arnulf Latz, Matthias Neumann, Benedikt Prifling, Volker Schmidt, Margret Wohlfahrt-Mehrens

Impact of the Conductive Additive-Binder Domain in Li-ion Battery Cathodes on the Electrochemical Performance

s03-003

Jun Huang *(IEK-13, Forschungszentrum Jülich GmbH, Jülich, Germany)*

Cation overcrowding effect on the oxygen evolution reaction

s03-006

Vadim Lvovich *(Materials Chemistry and Physics, NASA, Cleveland, USA)*, John Connell, Donald Dornbusch, Yi Lin, Rocco Viggiano, Vesselin Yamakov

Computationally Guided Development of Components for High Energy Density Solid-State Lithium-Sulfur Batteries

s03-007

Madhulika Mazumder *(New Chemistry Unit (NCU), Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India)*, Nabadyuti Barman, Raphaele J Clement, Subham Ghosh, Raynald Giovine, Eliovardo Gonzalez-Correa, Alexis Manche, Swapan K Pati, Premkumar Senguttuvan, Aryan Zaveri

Elucidating the Impact of Mg Substitution on the Properties of NASICON-$Na_{3+y}V2\text{-}yMg_y(PO_4)_3$ Cathodes

s03-008

Pernille Pedersen *(Department of Energy Conversion and Storage, Technical University of Denmark, Kgs Lyngby, Denmark)*, Thomas Bligaard, Heine Hansen, Pernille Pedersen, Tejs Vegge

Atomic scale modelling of TMDC electrocatalysts for CO_2RR

s03-010

Premysl Richtr *(Department of Chemical Engineering, University of Chemistry and Technology Prague, Prague, Czech Republic)*, Martin Bures, David Gráf, Juraj Kosek, Petr Mazúr, Jaromír Pocedic

Influence of turbulence promoters on zinc electrodeposition in alkaline zinc-air flow battery

s03-011

Felix Schmidt *(Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich, Jülich, Germany)*, Michael Eikerling, Thomas Kadyk

Structure-based Modeling of Degradation in Solid Oxide Cells

s03-012

Devesh Kumar Singh *(Chemistry, Banaras Hindu University, Varanasi, India)*, Vellaichamy Ganesan

Improved kinetics and selectivity of the oxygen reduction facilitated by iron phthalocyanine integrated carbon nanotubes: Energetics of the key intermediate

s03-013

Sukanya Sinha *(Department of Energy Conversion and Strorage, Technical University of Denmark, Kongens Lyngby, Denmark)*, Heine Hansen, Tejs Vegge

Exploring Transition Metal Based Catalysts for Oxygen Reduction Reaction: A DFT Study

s03-014

Young-Joon Song *(Institute for Theoretical Physics, Goethe University, Frankfurt am Main, Germany)*, Charlotte Gallenkamp, Vera Krewald, Roser Valení

Effect of Graphene Sheets on Chlorinated Iron Porphyrin

s03-015

Polina Tereshchuk *(Mechanical Engineering, Nuclear Research Center - Negev, Beer-Sheva, Israel)*, Dmitri Kaplan, Amir Natan, Chen Olewsky, Emanuel Peled, Meital Shviro

Study of Ruthenium Contamination Effect on Oxygen Reduction Activity of Platinum-based Fuel Cells Cathode Catalyst

s03-016

Yin-Ying Ting *(Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich GmbH, Jülich, Germany)*, Payam Kaghazchi, Piotr M. Kowalski

Computation of High Entropy, Mixed Transition Metal Oxide Cathode Materials

s03-017

Linas Vilciauskas *(Chemical Engineering and Technologies, Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania)*, Denis Gryaznov, Jurgis Pilipavicius, Gustautas Snarskis

From Computational Modeling to Experimental Understanding of NASICON Materials for Electrochemical Energy Storage

S4 - Modeling dynamic phenomena in electrochemical systems

s04-001

Luca Banetta *(Applied Science and Technology, Politecnico di Torino, Torino, Italy)*, Gianluca Boccardo, Silvia Bodoardo, Graziano Frungieri, Agnese Marcato, Daniele Marchisio, Daniele Versaci

Computational Modelling of the Solid Electrolyte Interface (SEI) in Lithium-Ion Batteries and Its Impact on Long-Term Battery Aging.

s04-002

Sheng Bi *(Physico-chimie des Electrolytes et Nanosystèmes Interfaciau, Sorbonne Universite, Paris, France)*, Betar Gallant, Aaron Melemed, Mathieu Salanne, Dhyllan Skiba

Molecular Understanding of Ion Association in Borohydride-Based Electrolytes

s04-003

Martin Bures *(Department of chemical engineering, University of chemistry and technology, Prague 6 Dejvice, Czech Republic)*, Jiri Charvát, Juraj Kosek, Petr Mazur, Milos Svoboda, Zbynek Tomiska, Alexandr Zubov

Predicting properties of carbon felt electrodes by mathematical modelling and μ-computed tomography

s04-004

Davide Dessantis *(Department of Energy, Politecnico di Torino, Torino, Italy)*, Julia Amici, Piera Di Prima, Domenico Ferrero, Carlotta Francia, Massimo Santarelli, Sabrina Trano, Daniele Versaci

Modelling of lithium-ion battery with sulfide-based solid-state electrolyte

s04-006

Tali Dotan *(Department of Physical Electronics, Faculty of Engineering, Tel Aviv University, Tel Avin, Israel)*, Michael Nazarenko, Yosi Shacham-Diamand

Modeling of Redox Cycling Amplification Under Flow in an Interdigitated Microelectrodes Array

s04-007

Lucas Huefner *(Ernst-Berl-Institute, TU Darmstadt, Darmstadt, Germany)*, Bastian J. M. Etzold, Holger Marschall

Development of a Co-Simulation Concept for Investigation of Multiphase Transport in Polymer Electrolyte Membrane Fuel Cells

s04-008

Lindah Kiriinya *(Radiation Science and Technology, Delft University of Technology, Delft, Netherlands)*, Shibabrata Basak, Erik Kelder, Shetty Santhosh

Molecular Dynamics Simulation of Alginate Polymer Electrolyte

s04-009

Rasmus Kronberg *(SR-COMP, CSC - IT Center for Science, Espoo, Finland)*, Kari Laasonen

Interfacial Dynamics of Water Self-Ions and Electrochemical Hydrogen Evolution from Density Functional Theory Simulations

s04-010

Walter Legerstee *(Storage of electrochemical energy, Delft University of Technology, Delft, Netherlands)*, Erik Kelder, Tjitte Noort, Henk Schut

Analysis of Degradation Processes in Porous Silicon as a result of Lithiation and De-lithiation with Positron Annihilation Spectroscopy

s04-014

Kwang Soak O'Donnell *(Chemistry, Western University, London, Canada)*, Mehran Behazin, Jiju Joseph, Peter Keech, Youn Gyeong Shin, Jungsook Clara Wren

The Effect of H_2O_2 on the Corrosion Dynamics of Carbon Steel in Small Volume Stagnant Solutions

s04-016

Brianna Rector *(Chemistry, Western University, London, Canada)*, Dan Guo, Jiju M. Joseph, Nicholas A. Payne, Youn G. Shin, J. Clara Wren

Re-Examining the Current-Potential Relationship in Corrosion Systems

s04-017

Nireas Rigos *(Institute of Engineering Thermodynamics, German Aerospace Center (DLR), Stuttgart, Germany)*, Timo Danner, Simon Hein, Birger Horstmann, Lars von Kolzenberg, Arnulf Latz

Interplay of Degradation Phenomena during Fast Charging: Li plating and SEI Growth

S5 - Accelerated materials development: rapid path from idea to integration

s05-001

Ian Brewis *(Faculty of Engineering and Environment, Northumbria University, Newcastle, United Kingdom)*, Abdesslem Jedidi, Shahid Rasul

Designing the Multi-Metallic Electrocatalytic Interfaces for CO_2 Reduction to C_3 Products

s05-002

Mustafa Celik *(Metallurgical & Materials Engineering, Sakarya University, Sakarya, Turkey)*, Hatem Akbulut, Tugrul Cetinkaya, Abdulkadir Kizilaslan, Mahmud Tokur

Crystallization Kinetics of Li7P3S11 Solid Electrolytes

s05-003

Manuel Corva *(Analytical Chemistry II, Ruhr University Bochum, Bochum, Germany)*, Niclas Blanc, Christoph Bondue, Kristina Tschulik

Differential Tafel Analysis: a Quick and Robust Benchmark to Inspect Charge-transfer in Electrocatalysis

s05-007

Fabian Tipp *(Institute of Energy and Climate Research, Forschungszentrum Jülich, Jülich, Germany)*, Michael Eikerling, Mohammad Eslamibidgoli, Kourosh Malek

AI-guided Inverse-design of Anion Exchange Membranes to Achieve High Alkaline Stability

S6 - Modeling-based diagnostics of electrochemical materials and cells

s06-003

Mustafa Celik *(Metallurgical & Materials Engineering, Sakarya, Turkey)*, Hatem Akbulut, Tugrul Cetinkaya, Abdulkadir Kizilaslan

Effect of Ceramic Fillers for Li-Air Battery Gel Polymer Electrolytes: Experimental and Density Functional Theory Investigation

s06-004

Jaeseung Lee *(Mechanical engineering, Inha university, Incheon, Korea)*, Alam Afroz, Jaeyoo Choi, Seonggu Heo, Hyunchul Ju, Kisung Lim, Soobin Yoon

Numerical Analysis of Bubble effect in Alkaline Water Electrolysis with Eulerian Multi-phase Model

s06-005

Kisung Lim *(Department of Mechanical Engineering, Inha University, Incheon, Korea)*, Seungbeen Choe, Jaeyoo Choi, Hyunchul Ju, Jaeseung Lee

Multi-variate optimization of passive air-cooled fuel cell system in consideration of effects of GDL compression and intrusion

s06-006

Lisa Royer *(heterogeneous catalysis, ICPEES - Strasbourg university , strasbourg, France)*, Antoine Bonnefont, Thierry Dintzer, Benoit Pichon, Elena Savinova

Experimental Investigation and Modelling of the Electrochemical Properties of Cobalt Iron Oxide Core-Shell Nanoparticle Multilayers

s06-007

Rana Shahzad *(Mechanical and Construction Engineering, Northumbria University , Newcastle Upon Tyne and Wear, United Kingdom)*, Adam Cosheril, Shahid Rasul, Rana Shakoor

Theoretical and experimental insights for designing composite materials by additive manufacturing for battery thermal management systems

s06-008

Amit N. Shocron *(Faculty of Mechanical Engineering, Technion, Haifa, Israel)*, Daniel Alfisi, Arunchander Asokan, Robert Gloukhovski, Matthew E. Suss

Characterizing High Power Density Flow Battery Electrodes via Impedance Spectroscopy

s06-009

Somayeh Toghyani *(Institute for Applied Materials - Electrochemical Technology, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany)*, Florian Baakes, Walter Cistjakov, Ulrike Krewer, Helmut Kühnelt, Ningxin Zhang

Model-based identification of high energy density solid-state lithium-ion batteries with hybrid electrolytes

s06-011

Qingxin Zhang *(Chemistry, Simon Fraser University/Greenlight Innovation, Burnaby, Canada)*, Michael Eikerling, Byron Gates, Hooman Homayouni, Amir Niroumand

Electrochemical Pressure Impedance Spectroscopy for Polymer Electrolyte Fuel Cells via Back-Pressure Control

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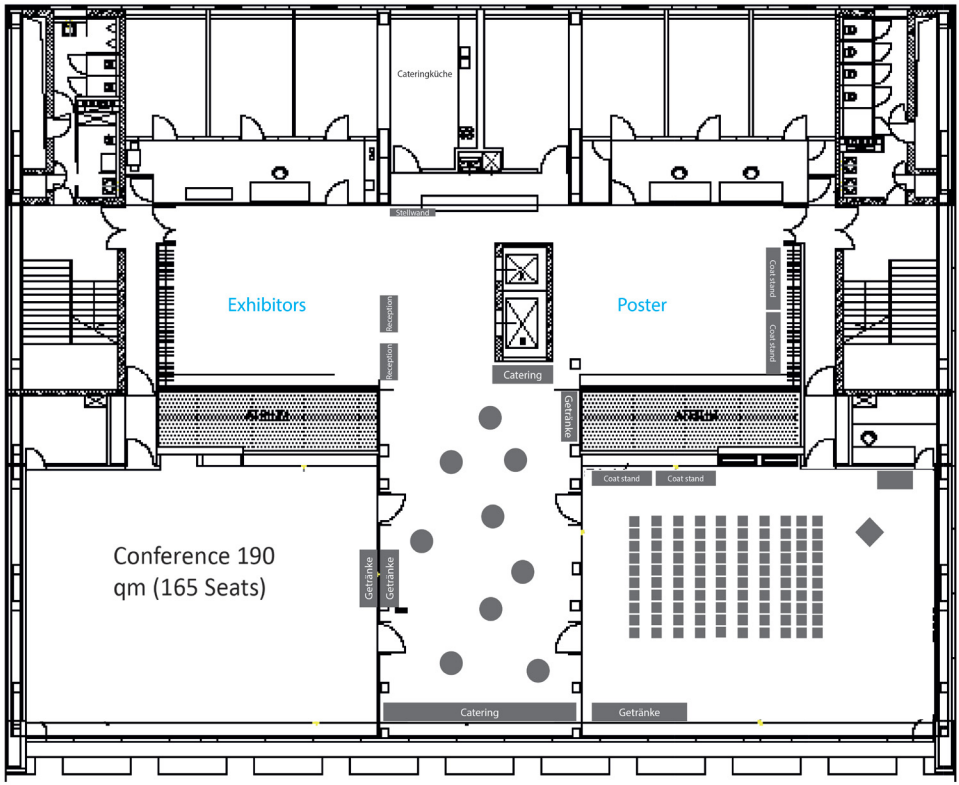

RWTH AACHEN UNIVERSITY

Super C building on the inner-city campus

6th Floor (6.OG, top level)

RWTH Aachen University, Germany

Templergraben 57, 52062 Aachen, Germany

31st Topical Meeting of the International Society of Electrochemistry
Conference Schedule

	SUNDAY 15	MONDAY 16	TUESDAY 17	WEDNESDAY 18	THURSDAY 19
08:45-09:30		Keynote: **Alexei Kornyshev**	Keynote: **Ryosuke Jinnouchi**	Keynote: **Tejs Vegge**	Keynote: **Matthew Suss**
09:30-09:50		Qiong Cai	Invited: **Jörg Behler**	Panagiotis Giotakos	Invited: **Andrei Kulikovsky**
09:50-10:10		Chiara Panosetti	Jun Huang	Yujin Tong	Invited: **Iryna Zenyuk**
10:10-10:30		Artur Braun	Giovanni Pireddu	Manuel Dillenz	Yufan Zhang
10:30-10:50		Weihan Li	Tobias Binninger	Amit N. Shocron	Wolfgang Olbrich
10:50-11:10		Invited: **Payam Kaghazchi**	Coffee break	Coffee break	Coffee break
11:10-11:30		Coffee break	**Poster Session 2** symposia 3, 4, 5 & 6	**Poster Session 2** symposia 3, 4, 5 & 6	Invited: **Tanja Vidakovic-Koch**
11:30-11:50		**Poster Session 1** symposia 1 & 2			Antoine Bonnefont
11:50-12:10					Marco Löffelholz
12:10-12:20					Elixabete Ayerbe
12:20-12:40					Closing Ceremony
12:40-14:40		**Lunch** : 12:30-13:40	**Lunch** : 12:20-13:40	**Lunch** : 12:20-13:40	**Lunch** : 12:20-13:40
13:40-14:00		Invited: **Chao Zhang**	Katharina Doblhoff-Dier	Florian Baakes	
14:00-14:20		Marko Melander	Simeon Beinlich	Martin Petit	
14:20-14:40		Piotr Kowalski	Rebekka Tesch	Chia Qian Tong	
14:40-15:00		Yoshitaka Tateyama	Jürgen Fuhrmann	Mark Junker	
15:00	Registration Open	Alejandro D. Somoza	Rüdiger Müller	Janina Drews	
15:20-15:40		Alexandra Celinda Dávila-López	Katharina Helmbrecht	Niklas Herrmann	
15:40-16:10		Coffee break	Coffee break	Coffee break	**City tour** : 16:00
16:10-16:30		Invited: **Kai Exner**	Invited: **Federico Calle-Vallejo**	Birger Horstmann	
16:30-16:50		Annalisa Paolone	Kari Laasonen	Jens Noack	
16:50-17:10		Andreas Heuer	Zdenek Futera	Astrid Maass	
17:00-17:30	Opening Ceremony	Michael Busch	Manuel Kolb	Vladislav Mints	
17:10-17:30		Chris-Kriton Skylaris	Roxanne Berthin	Vessela Tsakova	
17:30-18:30	Opening Lecture: **Marc Koper**	Nicolas Bergmann	Thorbern Eggert	Brianna Rector	
17:50-18:10		Nicolas Georg Hörmann	Enrique Herreo	Kannasoot Kanokkanchana	
18:10-18:30			Richard Haid		
18:30-18:50		**Poster Session 1** symposia 1 & 2			
18:45-21:00	Welcome Reception				
18:50-19:10					
19:10-19:30				**bus depart** : 19:00 / **return** : 22:45	
19:30-19:50				**Banquet** : 19:30	

S1 - Advances in first principles electrochemical methods

S2 - Theory and computation of interfacial and nanoscale phenomena

S3 - Modeling functional materials: microstructure to complex electrodes

S4 - Modeling dynamic phenomena in electrochemical systems

S5 - Accelerated materials development: rapid path from idea to integration

S6 - Modeling-based diagnostics of electrochemical materials and cells