

31st Topical Meeting

of the International Society of Electrochemistry

15-19 May 2022
Aachen, Germany

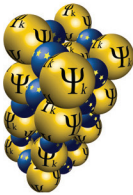
Theory and Computation in Electrochemistry:
Seeking Synergies in Methods, Materials and Systems



PROGRAM

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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



International Society of Electrochemistry
Chemin du Closelet 2
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Switzerland

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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 CO₂](#)

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 (*Istituto 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 Evolution 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 Electroquímica, Universidad 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

[O₂ 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 (*LAM - 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, Solaise, 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 MnO₂-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, Pfaffzettel, Germany*), Emmanuel Baudrin, Rocco Fornari, Alejandro Franco, Daniel Gerlach, Xinjie Guan, Jan Hamaekers, Astrid Maaß, Chris Menictas, Gael Mourouga, Hermann Nirschl, Nataliya Roznyatovskaya, Roman Schaefer, 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 Kreuer

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 Kreuer

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

Andrei Kulikovskiy (*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 Systems, 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 Process Engineering, Clausthal University of Technology, Clausthal-Zellerfeld, Germany*), Jens Osiewacz, Thomas Turek

[Understanding the limitations of electrochemical CO₂ 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

s01-001 to s01-019 *and* s02-001 to s02-027

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 Klimaforschung, 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 NaRhO₂ 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-MoS₂ 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

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 Hoffmann, Alice, *s03-002*
 Holland, Julian, *s01-006*
 Homayouni, Hooman, *s06-011*
 Hoppe, Johanna, *s02-011*
 Horstmann, Birger, (*Mon s01*)15:00, (*Wed*
s04)15:20, (*Wed s05*)16:10, *s02-015,*
s04-017
 Huang, Jun, (*Tue s02*)09:50, *s02-028, s03-*
003
 Huang, Zhipeng, (*Wed s04*)09:50
 Huefner, Lucas, *s04-007*

I

Iacob, Bogdan-Cezar, *s01-013*
 Ibragimov, Sapajan, *s01-007*
 Ivanistsev, Vladislav, *s02-012*
 Ivanov, Radoslav, (*Wed s05*)17:30

J

Jedidi, Abdesslem, *s05-001*
 Jensen, Kirsten, (*Wed s05*)17:10
 Jiang, Yiming, *s01-008*
 Jinnouchi, Ryosuke, (*Tue s02*)08:45
 Jöst, Dominik, (*Mon s03*)10:30
 Joseph, Jiju M., (*Wed s05*)17:50, *s04-014,*
s04-016
 Jovicevic, Jovan N., *s01-004*
 Ju, Hyunchul, *s06-004, s06-005*
 Junker, Mark, (*Wed s04*)14:40

K

Kadyk, Thomas, (*Thu s06*)10:10, (*Thu*
s06)10:30, *s03-011*
 Kaghazchi, Payam, (*Mon s03*)10:50, *s03-*
016
 Kajiya, Shuji, (*Tue s02*)08:45

Kanokkanchana, Kannasoot, (*Wed*
s05)18:10
 Kaplan, Dmitri, *s03-015*
 Keech, Peter, *s04-014*
 Kelder, Erik, *s04-008, s04-010*
 Kenmoe, Stephane, *s02-019*
 Kéranguévin, Gwenaëlle, (*Thu s06*)11:30
 Kiriinya, Linda, *s04-008*
 Kizilaslan, Abdulkadir, *s05-002, s06-003*
 Klüner, Thorsten, *s02-027*
 Kluge, Regina, (*Tue s02*)18:30
 Koebbing, Lukas, *s02-015*
 Kolb, Manuel, (*Tue s02*)17:10
 Kolzenberg, Lars von, *s04-017*
 Kontkanen, Outi Vilhelmiina, (*Tue*
s02)16:50, *s02-016*
 Koper, Marc, (*Sun s02*)17:30, (*Tue*
s02)13:40
 Kornyshev, Alexei, (*Mon s05*)08:45
 Korte, Carsten, *s02-008, s02-026*
 Kosek, Juraj, *s03-010, s04-003*
 Koverga, Volodymyr, *s02-012*
 Kowalski, Piotr M., (*Mon s01*)14:20,
 (*Tue s02*)14:20, *s02-005, s02-008,*
s02-009, s02-010, s02-026, s03-001,
s03-016
 Kox, Tim, *s02-019*
 Kramer, Denis, (*Mon s01*)17:30, *s01-006*
 Krewald, Vera, *s03-014*
 Krewer, Ulrike, (*Wed s04*)13:40, *s02-011,*
s06-009
 Kronberg, Rasmus, (*Tue s02*)16:30, *s04-009*
 Kucernak, Anthony, (*Mon s05*)08:45
 Kudo, Osamu, *s01-008*
 Kühnelt, Helmut, *s06-009*
 Kuhn, Yannick, (*Wed s05*)16:10
 Kulikovskiy, Andrei, (*Thu s06*)09:30
 Kunz, Ulrich, *s01-010*

L

Laasonen, Kari, (*Mon s01*)17:10, (*Tue*
s02)16:30, *s04-009*
 Lahiri, Abhiroop, *s01-012*
 Lamp, Konstantin, (*Mon s01*)15:00
 Landstorfer, Manuel, (*Tue s02*)15:00
 Latz, Arnulf, (*Wed s04*)15:00, (*Wed*
s05)16:10, *s02-015, s03-002, s04-017*
 Lee, Jaeseung, *s06-004, s06-005*
 Lee, Yonghyuk, *s02-017*
 Legerstee, Walter, *s04-010*

Lemmermann, Torben, *s01-010*
 Li, Weihai, (*Mon s03*)10:30
 Li, Zhenyou, (*Wed s04*)15:00
 Lim, Kisung, *s06-004, s06-005*
 Lin, Yi, *s03-006*
 Löffelholz, Marco, (*Thu s06*)11:50
 Lopez Ochoa, Jesus, (*Thu s06*)09:50
 Loselli, Giulia, *s02-027*
 Luo, Xun, *s01-008*
 Lvovich, Vadim, *s03-006*
 Lyu, Dongya, *s02-027*

M

Ma, Ye, (*Mon s05*)08:45
 Maaß, Astrid, (*Wed s05*)16:30,
 (*Wed s05*)16:50
 Mabrouk, Youssef, (*Mon s01*)16:50, *s01-011*
 Maca Alaluf, Rudi Ruben, (*Wed s04*)15:00
 Maeda, Ryu, *s01-008*
 Maiti, Moumita, (*Mon s01*)16:50
 Malek, Kourosh, *s05-007*
 Manche, Alexis, *s03-007*
 Marcato, Agnese, *s04-001*
 Marchisio, Daniele, *s04-001*
 Marschall, Holger, *s04-007*
 Maschio, Lorenzo, (*Wed s04*)14:00
 Mazumder, Madhulika, *s01-012, s03-007*
 Mazúr, Petr, *s03-010, s04-003*
 Medrano-Banda, Alejandra, (*Thu s06*)11:30
 Mekazni, Dalila S., (*Tue s02*)18:10
 Melander, Marko, (*Mon s01*)14:00
 Melemed, Aaron, *s04-002*
 Menictas, Chris, (*Wed s05*)16:30
 Michael, Lubasch, (*Mon s01*)15:00
 Milenko, Karolina, *s01-013*
 Mints, Vladislav, (*Wed s05*)17:10
 Mizoguchi, Masanori, *s01-008*
 Moldovan, Rebeca, *s01-013*
 Mourouga, Gael, (*Wed s05*)16:30
 Müller, Rüdiger, (*Tue s02*)15:00

N

N. Steinmann, Stephan, *s02-001*
 Naranjo-Montoya, Oscar Andres, (*Wed*
s04)09:50
 Narayanan Krishnamoorthy, Anand, (*Mon*
s01)16:50
 Natan, Amir, *s03-015*
 Nazarenko, Michael, *s04-006*

Neophytides, Stylianos, (*Wed s04*)09:30
 Neumann, Matthias, *s03-002*
 Niroumand, Amir, *s06-011*
 Nirschl, Hermann, (*Wed s05*)16:30
 Noack, Jens, (*Wed s05*)16:30
 Noort, Tjitte, *s04-010*

O

O'Donnell, Kwang Soak, *s04-014*
 Ojha, Kasinath, (*Tue s02*)13:40
 Olbrich, Wolfgang, (*Thu s06*)10:30
 Oleinick, Alexander, *s02-023*
 Olefsky, Chen, *s03-015*
 Olsson, Emilia, (*Mon s03*)09:30
 Omranpoor, Amir Hossein, *s02-019*
 Oschinski, Hedda, *s02-020*
 Oshchepkov, Alexandr, (*Thu s06*)11:30
 Osiewicz, Jens, (*Thu s06*)11:50
 Owen, John, (*Mon s01*)17:30
 Ozaslan, Mehtap, *s02-027*

P

Panosetti, Chiara, (*Mon s03*)09:50
 Paolone, Annalisa, (*Mon s01*)16:30, *s01-003*
 Parisi, Federico, *s02-008*
 Partovi-Azar, Pouya, *s02-022*
 Pasel, Joachim, *s02-009*
 Pati, Swapan K, *s01-012, s03-007*
 Payne, Nicholas A., (*Wed s05*)17:50, *s04-*
016
 Pedersen, Jack, (*Wed s05*)17:10
 Pedersen, Pernille, *s03-008, s03-008*
 Peled, Emanuel, *s03-015*
 Peng, Chao, (*Mon s01*)17:30
 Pescara, Lars, (*Wed s04*)14:20
 Peters, Ralf, *s02-009*
 Petit, Martin, (*Wed s04*)14:00
 Pichon, Benoit, *s06-006*
 Pikma, Piret, *s02-012*
 Pilipavicius, Jurgis, *s03-017*
 Pireddu, Giovanni, (*Tue s02*)10:10, *s02-023*
 Povedic, Jaromír, *s03-010*
 Pool, Albert J., (*Mon s01*)15:00
 Prifling, Benedikt, *s03-002*

Q

Quinson, Jonathan, (*Wed s05*)17:10

R

Rabani, Ramin, *s02-024*
 Rasul, Shahid, *s05-001, s06-007*
 Razzaq, Samad, *s01-015*
 Rector, Brianna, (*Wed s05*)17:50, *s04-016*
 Reuter, Karsten, (*Mon s01*)15:20, (*Mon s01*)17:50, (*Mon s01*)18:10, (*Tue s02*)14:00, (*Tue s02*)17:50, *s02-017, s02-020*
 Richtr, Premysl, *s03-010*
 Rigos, Nireas, *s04-017*
 Rijnaarts, Huub H.M., (*Wed s04*)10:30
 Ringbeck, Florian, (*Mon s03*)10:30
 Ringe, Stefan, *s02-025 (Session 2)*
 Rodenbücher, Christian, *s02-008, s02-026*
 Röder, Fridolin, *s02-011*
 Rossmeisl, Jan, (*Wed s05*)17:10
 Rotenberg, Benjamin, (*Tue s02*)10:10
 Royer, Lisa, *s06-006*
 Roznyatovskaya, Nataliya, (*Wed s05*)16:30
 Ruhlmann, Laurent, (*Thu s06*)11:30

S

Saha, Prantik, (*Thu s06*)09:50
 Sahray, Zohar, (*Thu s04*)08:45
 Salanne, Mathieu, (*Tue s02*)17:30, *s04-002*
 Santarelli, Massimo, *s04-004*
 Santhosh, Shetty, *s04-008*
 Sauer, Dirk Uwe, (*Mon s03*)10:30, (*Wed s04*)14:40
 Sauter, Ulrich, (*Thu s06*)10:30
 Savinova, Elena, (*Thu s06*)11:30, *s06-006*
 Schaerer, Roman, (*Wed s05*)16:30
 Scheurer, Christoph, (*Mon s03*)09:50, *s02-017*
 Schmidt, Felix, *s03-011*
 Schmidt, Thorsten, (*Tue s02*)18:30
 Schmidt, Volker, *s03-002*
 Schöning, Marco, *s01-016*
 Schumacher, Juergen, (*Wed s05*)16:30
 Schuster, Rolf, *s01-016*
 Schut, Henk, *s04-010*
 Sellier, Franck, (*Wed s04*)14:00
 Senguttuvan, Premkumar, *s03-007*
 Serva, Alessandra, (*Tue s02*)17:30
 Sgroi, Mauro, (*Wed s04*)14:00
 Shacham-Diamand, Yosi, *s04-006*
 Shahzad, Rana, *s06-007*
 Shakoor, Rana, *s06-007*

Shibata, Masao, (*Tue s02*)08:45
 Shin, Youn Gyeong, (*Wed s05*)17:50, *s04-016, s04-014*
 Shinozaki, Kazuma, (*Tue s02*)08:45
 Shocron, Amit, (*Wed s04*)10:30, (*Thu s04*)08:45, *s06-008*
 Shviro, Meital, *s03-015*
 Sikdar, Debabrata, (*Mon s05*)08:45
 Silveri, Fabrizio, (*Wed s04*)14:00
 Silvi, Giorgio, (*Mon s01*)15:00
 Singh, Devesh Kumar, *s03-012*
 Sinha, Sukanya, *s03-013*
 Skiba, Dhyllan, *s04-002*
 Skylaris, Chris-Kriton, (*Mon s01*)17:30, *s01-006*
 Skyllas-Kazacos, Maria, (*Wed s05*)16:30
 Snarskis, Gustautas, *s03-017*
 Sözen, Halil Ibrahim, *s02-027, s02-027*
 Somoza, Alejandro D., (*Mon s01*)15:00
 Sone, Masato, *s01-008*
 Song, Young-Joon, *s03-014*
 Sotoudeh, Mohsen, (*Mon s03*)10:10
 Sun, Jing, (*Thu s06*)11:30
 Suss, Matthew, (*Wed s04*)10:30, (*Thu s04*)08:45, *s06-008*
 Takahisa, (*Tue s02*)08:45
 Svir, Irina, *s02-023*
 Svoboda, Milos, *s04-003*

T

Tarasevitch, Alexander, (*Wed s04*)09:50
 Tateyama, Yoshitaka, (*Mon s01*)14:40
 Teichert, Christian, (*Wed s05*)17:30
 Tereshchuk, Polina, *s03-015*
 Tesch, Rebekka, (*Tue s02*)14:20, *s03-001*
 Thiele, Mathias, (*Wed s04*)14:20
 Ting, Yin-Ying, *s03-016*
 Tipp, Fabian, *s05-007*
 Toghyani, Somayeh, *s06-009*
 Tokur, Mahmud, *s05-002*
 Tomiska, Zbynek, *s04-003*
 Tommasi, Alessio, (*Wed s04*)14:00
 Tong, Chia Qian, (*Wed s04*)14:20
 Tong, Yujin, (*Wed s04*)09:50
 Trano, Sabrina, *s04-004*
 Tsakova, Vessela, (*Wed s05*)17:30
 Tschulik, Kristina, (*Wed s05*)18:10, *s02-004, s02-006, s05-003*
 Turek, Thomas, (*Thu s06*)11:50, *s01-010*

U

Urbakh, Michael, (*Mon s05*)08:45
Uwayid, Rana, (*Thu s04*)08:45

V

Valení, Roser, *s03-014*
Varas, Fernando, (*Thu s06*)12:10
Vegge, Tejs, (*Wed s04*)08:45, *s03-008*, *s03-013*
Velleman, Leonora, (*Mon s05*)08:45
Vereshchagina, Elizaveta, *s01-001*, *s01-013*
Versaci, Daniele, *s04-001*, *s04-004*
Victor, Milman, *s01-006*
Vidakovic-Koch, Tanja, (*Thu s06*)11:10
Viggiano, Rocco, *s03-006*
Vilciauskas, Linas, *s03-017*
Vogt, Nicolas, (*Mon s01*)15:00
Voroshylova, Iuliia, *s02-012*
Vukicevic, Natasa M., *s01-004*

W

Walt, Marina, (*Mon s01*)15:00
Wiedemann, Johannes, (*Wed s04*)15:00
Winter, Martin, (*Mon s01*)16:50
Wippermann, Klaus, *s02-008*, *s02-026*
Wlodarczyk, Jakub, (*Wed s05*)16:30
Woelke, Christian, (*Mon s01*)16:50
Wohlfahrt-Mehrens, Margret, *s03-002*
Wolf, Amadeus, (*Wed s05*)16:30
Wolff, Jules, (*Thu s06*)11:30
Wonner, Kevin, *s02-006*
Wren, Jungsook Clara, (*Wed s05*)17:50,
s04-014, *s04-016*

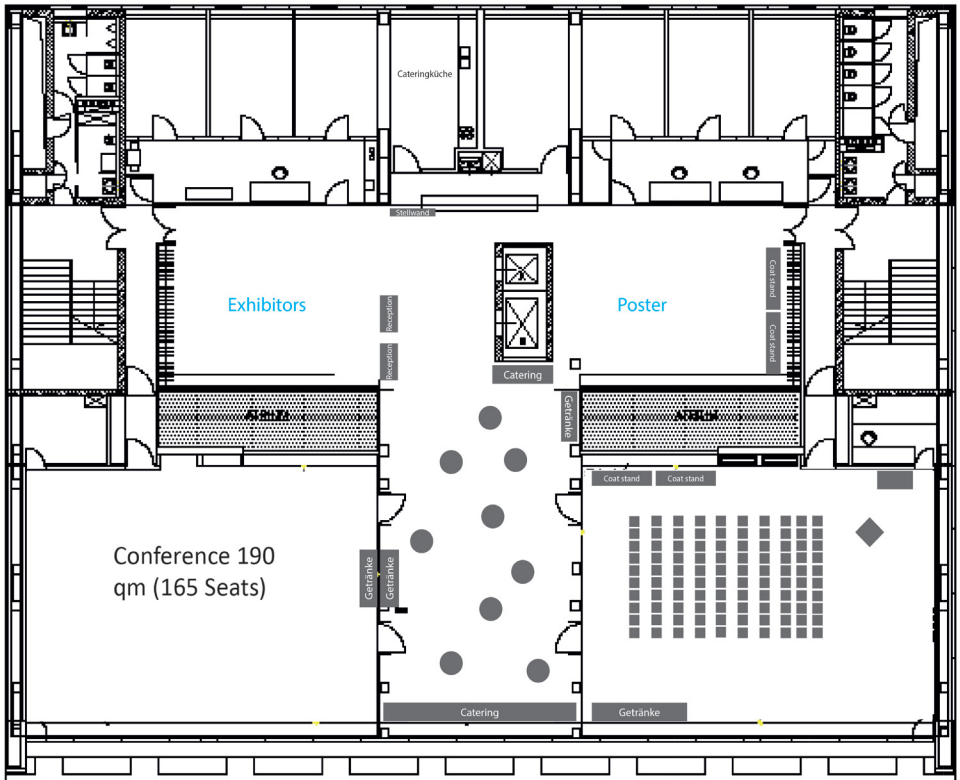
Y

Yamakawa, Shunsuke, (*Tue s02*)08:45
Yamakov, Vesselin, *s03-006*
Yamane, Daisuke, *s01-008*
Yan, Peng, (*Mon s01*)16:50
Yoon, Soobin, *s06-004*
Yu, Jia, (*Wed s05*)16:30

Z

Zagar, Cristian, (*Mon s05*)08:45
Zaveri, Aryan, *s03-007*
Zenyuk, Iryna, (*Thu s06*)09:50
Zhang, Chao, (*Mon s01*)13:40
Zhang, Ningxin, *s06-009*
Zhang, Qingxin, *s06-011*

Zhang, Yufan, (*Thu s06*)10:10
Zhao, Chen, (*Wed s04*)14:00
Zhao-Karger, Zhirong, (*Wed s04*)15:00
Zhu, Xinwei, *s02-028*, *s02-028*
Zubov, Alexandr, *s04-003*



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UNIVERSITY**

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6th Floor (6.OG, top level)

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Templergraben
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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 Kulikovskiy
	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			Invited: Tanja Vidakovic-Koch
	11:30-11:50	Poster Session 1 symposia 1 & 2	Poster Session 2 symposia 3, 4, 5 & 6	Poster Session 2 symposia 3, 4, 5 & 6	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	Rebeka 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	
	15:00-15:20	Alexandra Celinda Dávila-López	Katharina Helmbrecht	Niklas Herrmann	
	15:20-15:40	Coffee break	Coffee break	Coffee break	City tour : 16:00
	15:40-16:10	Invited: Kai Exner	Invited: Federico Calle-Vallejo	Birger Horstmann	
	16:10-16:30	Annalisa Paolone	Kari Laasonen	Jens Noack	
	16:30-16:50	Andreas Heuer	Zdenek Futera	Astrid Maass	
17:00-17:30	Opening Ceremony	Michael Busch	Manuel Kolb	Vladislav Mints	
	17:30-17:50	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			
	18:50-19:10				
	19:10-19:30				
	19:30-19:50				
18:45-21:00	Welcome Reception			bus depart : 19:00 / return : 22:45	
				Banquet : 19:30	

S2 - Theory and computation of interfacial and nanoscale phenomena
S3 - Advances in first principles electrochemical methods
S4 - Modeling functional materials: microstructure to complex electrodes
S5 - Accelerated materials development: rapid path from idea to integration
S6 - Modeling dynamic phenomena in electrochemical systems
S6 - Modeling based diagnostics of electrochemical materials and cells