

Division 7 Physical Electrochemistry 2019 Report

Division 7 officers:

A. Cuesta-Ciscar, U. Aberdeen (Chair)

A. A. Gewirth, U. Illinois (Past Chair)

S. Ye, Tohoku U. (Chair Elect)

P. Levecque, University of Cape Town, Katrin Domke, MPI for Polymer Research, Mainz (Vice-Chairs, 2019-20)

The activities of Division 7 in 2019 are summarised below:

Organization and co-organization of symposia at annual ISE meetings

1. 70th Annual Meeting of the ISE, Aug. 4-9, 2019, Durban, South Africa

Symposium 9: Electro-physical Chemistry and Application of Platinum Group Metals

Sponsored by:

Division 4, Electrochemical Materials Science

Division 5, Electrochemical Process Engineering and Technology

Division 7, Physical Electrochemistry

This symposium covered advances in the PGM physical chemistry, molecular compounds, metals and alloys that include at least one PGM and novel synthesis methods or materials.

Symposium Organizers:

Cobus Kriek (Coordinator), North-West University, South Africa, cobus.kriek@nwu.ac.za

Stanko Brankovic, University of Houston, USA

Angel Cuesta, University of Aberdeen, UK

Jessica Chamier, University of Cape Town, South Africa

Gary Patrick, Johannesburg, South Africa

Symposium 15: Computational Electrochemistry and Simulation: from Prediction of Properties to Optimization of Devices

Sponsored by:

Division 7, Physical Electrochemistry

This symposium aimed at coupling aspects of physical electrochemistry to elements of electrochemical engineering, in particular through the use of simulation techniques in strong connection with experimental characterization for validation.

The following topics were considered:

- Using simulation techniques such as ab initio calculations, molecular dynamics, dissipative particle dynamics, kinetic Monte Carlo, Continuum Fluid Dynamics, multiphysics and/or multiscale computational approaches for understanding and for the optimization and design of electrochemical cells
- Design of experimental validation techniques
- Methods for determination or estimation of parameters entering the computational models
- Comparison and correlation of behaviors and properties obtained at various scales and using different computational techniques

Applications include: charge transfer processes, electrochemical interfaces,

electrocatalysis, porous electrodes, photo-electrochemical cells, electrochemical cells for energy storage and conversion (batteries, supercapacitors, fuel cells, electrolyzers)

Symposium Organizers

Alejandro Franco (Coordinator), Université de Picardie Jules Verne, France

alejandro.franco@u-picardie.fr

Krishna Bisetty, Durban University of Technology, South Africa

Alex Quandt, University of the Witwatersrand, South Africa.

Symposium 16: Spectroscopy, Microscopy and Theory for the Rational Design of Electrochemical Interfaces

Sponsored by:

Division 7, Physical Electrochemistry

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- • Design of experimental validation techniques
- • Methods for determination or estimation of parameters entering the computational models
- • Comparison and correlation of behaviors and properties obtained at various scales and using different computational techniques

Applications include: charge transfer processes, electrochemical interfaces, electrocatalysis, porous electrodes, photo-electrochemical cells, electrochemical cells for energy storage and conversion (batteries, supercapacitors, fuel cells, electrolyzers)

Symposium Organizers

Shaowei Chen (Coordinator), University of California at Santa Cruz, USA,

shaowei@ucsc.edu

Dave Billing, University of the Witwatersrand, South Africa

Charl J. Jafta, Oak Ridge National Laboratory, USA

Katharina Krischer, Technische Universität München, Germany

Bin Ren, Xiamen University, China

Manuela Rueda, Universidad de Sevilla, Spain

2. 71st Annual Meeting of the ISE, Belgrade, Serbia

- **Symposium 5** Coupling electrochemical and optical methods to study chemo- and bioobjects: light as sensor and actuator (Kylie Vincent, Stijn Mertens)
- **Symposium 13** Electrochemistry in the digital age: model-supported process analysis and design (Michael Eikerling)
- **Symposium 16** Two-dimensional materials: An electrochemical perspective (Robert Hillman, Shen Ye)
- **Symposium 18** Nanoelectrochemistry and electrocatalysis – from fundamentals to applications (Helmut Baltruschat)
- **Symposium 19** Electrochemical surface and interface (Paramaconi Rodriguez, Enrique Herrero, Katrin Domke, Julia Kunze-Liebhäuser, Natasa Vasiljević, Daria Vladikova)
- **Symposium 20** Cutting Edge Electrochemical Measurement Techniques (Liwei Chen, Bin Ren, Olaf Magnussen)

Please look out for the call for abstracts for the Annual meeting and plan on submitting yours in good time to support the Division's symposia.

Organization and co-organization of ISE Topical Meetings

- Past meetings:

25th ISE Topical Meeting, *New electrochemical processes for the energy and the environment*, May 2019, Toledo, Spain

- Future Meetings:

28th ISE Topical Meeting, *Challenges in Molecular Electrochemistry and Surface Reactivity*, March-April 2021, Santiago, Chile

ISE Topical Meeting, *Experimental and Modelling tools for Electrochemical Energy Devices*, Stockholm (Sweden), 2022

ISE Topical Meeting, *Theory, modeling and simulation in Electrochemistry*, Germany 2022

Sponsoring of International Conferences

The Division has sponsored or agreed to sponsor the following Meetings:

15th International Conference on Electrified Interfaces (ICEI), November 3rd-8th 2019, Valdivia, Chile

50th Electrochemistry Gordon Research Conference, January 5-10th 2020, Ventura, California, USA

9th meeting on Electrochemistry in Nanoscience, May 25th-27th 2020, Paris, France

If you are seeking support for a school, symposium, or conference from the Division, please submit your request as early as possible using the forms provided on the ISE website. Please make it very clear if you are seeking financial support (typically only €300 to €400 is provided per event in total from the ISE).

Awards

The **Alexander Kuznetsov Prize for Theoretical Electrochemistry 2019** was awarded to Jan Rossmeisl (University of Copenhagen, Denmark), in recognition of his outstanding contribution to the field, in particular the development of a computational hydrogen electrode and, more recently, the development of a method to explicitly include the effect of the electrolyte in atomic scale simulations. Prof Rossmeisl computational work has allowed to make predictions regarding the electrocatalytic activity of novel materials for a large variety of reactions relevant for electrochemical energy conversion and storage that were later confirmed experimentally. His work can be considered as seminal and inspirational and has had impact beyond academia.

Award Committee

A. Cuesta (chair)

A.E. Russell

S. Yen

J. Chen

M. Eikerling

In 2020 the Division is associated with the **Brian Conway Prize for Physical Electrochemistry** and committee will be chaired by A. Cuesta.

Miscellaneous

- Andy Gewirth returned to his duties as Past-Chair on 26th February 2019. Between 1st January and 25th February Andrea Russell's serving as Past-Chair was extended to cover for his absence as agreed during the Division Meeting in Bologna.
- During the Division meeting the following symposia were agreed to be proposed to be organized by Div. 7 for the 72nd Annual Meeting:
 - The usual core symposium (Coordinator Keiji Murakoshi)
 - Photodriven electrochemistry/Ultrafast electrochemistry (Coordinator David Fermin / Yujin Tong)
 - Electrochemical Switches, Pumps, and Machines (Coordinator Frank Marken). With Division 6
 - Physical Electrochemical Aspects of Organic Electrosynthesis (Coordinator Mark Koper). With division 6
 - Battery, interfaces, spectroscopy. Division 7 as co-chair
- Suggestions for topical meetings organized by (with support of) Div. 7 are strongly encouraged, as well as for symposia in the 73rd Annual Meeting. Please send suggestions to executive committee of division.