Division 7 Physical Electrochemistry

2018 Report

Division 7 officers:

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

A.E. Russell, U. Southampton (Past Chair)

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

A. O'Mullane, Queensland University of Technology, L. Zhuang, Wuhan U. (Vice-Chairs, 2017-18)

The activities of Division 7 in 2018 are summarised below:

1. Organization and co-organization of symposia at annual ISE meetings

69th Annual Meeting of the ISE, Sep. 2-7, 2018, Bologna, Italy

Symposium 16: Micro- and Nano-scale Platforms to Study Electron Transport in (Bio) Molecular Systems: from Fundamentals to Molecular devices

Sponsored by:
Division 6, Molecular Electrochemistry
Division 7, Physical Electrochemistry
Division 2, Bioelectrochemistry

The symposium covered all aspects of electron transfer in molecular or biomolecular moieties that profit from an electrified interface and where the electrochemical control is or could find an essencial role. The symposium gathered works exploiting from fundamental approaches, including single-molecule or nanoscale platforms and computational modelling, all the way to micro-scale molecular junctions involving hybrid micro/nano-structured materials for device applications.

Symposium Organizers
Ismael Díez-Pérez (Coordinator), King's College London, UK, ismael.diez_perez@kcl.ac.uk
Sabrina Antonello, University of Padova, Italy
Angel Cuesta, University of Aberdeen, UK
Nadim Darwish, Curtin University, Australia
Giovanni Valenti, University of Bologna, Italy

Symposium 17: Physical Electrochemistry: Recent Developments in Spectroscopy, Microscopy and Theory for the Rational Design of Electrochemical Interfaces

Sponsored by:
Division 7, Physical Electrochemistry

This symposium covered recent developments in experimental and theoretical methods for the understanding and rational design of electrode surfaces, from model electrodes to novel nanostructured electrocatalysts and functional materials. This included (i) the fabrication of optimized interfacial architectures and functionalities for specific applications based on the ability to control and determine interfacial composition and the interactions between the system components at a molecular level and (ii) recent advances that combine electrochemical methods with in situ/operando spectroscopy, electrochemical scanning

probe microscopy, synchrotron-based techniques and theoretical calculations, and provide a detailed picture of the electrochemical interface at the atomic and molecular level. These lead to an understanding of the structure-reactivity and structure-selectivity relationships that dictate electrochemical reaction mechanisms and kinetics, and are crucial to the design and exploitation of improved materials. Applications involve to energy (conversion, production and storage), water (purification and remediation), (bio-)chemical sensing, environmental and process monitoring, surface protection, optical displays and electronics.

Symposium Organizers
Robert Hillman (Coordinator), University of Leicester, UK arh7@le.ac.uk
María Escudero-Escribano, University of Copenhagen, Denmark
Alessandro Minguzzi, University of Milan, Italy
Piercarlo Mustarelli, University of Pavia, Italy

Symposium 18: Theory: from understanding to optimization and prediction

Sponsored by:
Division 7, Physical Electrochemistry

This symposium coupled 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 A. Franco (Coordinator), Université de Picardie Jules Verne, France, alejandro.franco@u-picardie.fr
Marc Koper, Leiden University, The Nethrelands
Pawel Kulesza, University of Warsaw, Poland
Claudio Fontanesi, University of Modena and Reggio Emilia, Italy
Fabio La Mantia, University of Bremen, Germany
Petr Vanysek, Northern Illinois University, USA

Symposium 19: Single Entity Electrochemistry

Sponsored by:
Division 7, Physical Electrochemistry
Division 1, Analytical Electrochemistry
Division 2, Bioelectrochemistry

This symposium provided a vibrant forum to discuss this area of electrochemistry, bringing together experimentalists and theoreticians across several divisions to discuss a topic that is

at the forefront of fundamental electrochemistry and underpins many important technical applications.

Symposium Organizers
Pat Unwin (Coordinator), University of Warwick, UK, p.r.unwin@warwick.ac.uk
Paolo Actis, University of Leeds, UK
Damian Arrigan, Curtin University, Australia
Stefania Rapino, University of Bologna, Italy

Symposium 20: Interfacial Electrochemistry n Non-Aqueous Electrolytes

Sponsored by:
Division 7, Physical Electrochemistry
Division 3, Electrochemical Energy Conversion and Storage

In this symposium, recent advances in the experimental characterization, theoretical description and understanding of electrode / non-aqueous electrolyte interfaces were discussed. Specific topics included:

• Adsorption processes

• Double layer capacitance

• Electrodeposition

• Processes at model surfaces (*e.g.* single crystal electrodes)

• Charge transfer rates and mechanisms

• Structural characterization (by spectroscopy or scanning

probe techniques)

• Electrocatalysis in non-aqueous systems

• Stability of electrolytes

Symposium Organizers
Helmut Baltruschat (Coordinator), University of Bonn, Germany, baltruschat@uni-bonn.de
Nuria García-Aráez, University of Southampton, UK
Alessandro Lavacchi, ICCOM CNR Florence, Italy
Maria Assunta Navarra, University of Rome La Sapienza, Italy

70th Annual Meeting of the ISE, Durban, South Africa

- **Symposium 9** Electro-physical Chemistry and Application of Platinum Group Metals (Angel Cuesta)
- **Symposium 15** Computational Electrochemistry & Simulation: from prediction of properties to optimization of devices (Alejandro A. Franco)
- **Symposium 16** Spectroscopy, Microscopy and Theory for the Rational Design of Electrochemical Interfaces (Shaowei Chen, Manuela Rueda, Katarina Krischer)

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.

2. Organization and co-organization of ISE Topical Meetings

- Future meetings:

2019 Toledo, Spain "New electrochemical processes for the energy and the environment"

3. Sponsoring of International Conferences

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

"5th International Symposium on Surface Imaging /Spectroscopy at the Solid/Liquid Interface", 6-8 June 2018 in Krakow, Poland

"3rd International Conference on Proton- Coupled Electron Transfer", 10–14 June 2018, Blowing Rock, NC, USA

"Redox Films for Energy Conversion - bioelectrochemical and molecular systems", 10-11 September 2018, Marseille, France

"5th Ertl Symposium on Catalytic and Adsorption Reactions in chemical Processes", 25-28 November 2018 Gwangjun, South Korea

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).

4. Awards

The **Brian Conway Prize for Physical Electrochemistry** was awarded to Patrice Simon (CIRIMAT, CNRS-Université Paul Sabatier, Toulouse, France), in recognition of his ground- breaking work on materials for supercapacitors that has led to key advances in the field of porous carbons, pseudocapacitive materials and micro-supercapacitors.. Simon is particularly recognized for his research on the synthesis and electrochemical characterizations of these interfaces using advanced techniques (micro-electrodes, cavity micro-electrodes, Electrochemical Quartz Crystal Microbalance) in combination with structural in-situ and in-operando techniques.

Award Committee (two excellent nominations received)

A. A. Gewirth (chair)
A.E. Russell
M. Osawa
M.T.M. Koper
H. Abruña

In 2019 the Division is associated with the **Alexander Kuznetsov Prize for Theoretical Electrochemistry** and committee will be chaired by A. Cuesta.

5. Miscellaneous

- Due to personal reasons, Andy Gewirth will not be able to fulfill his duties as Past-Chair for some time. As a temporary solution it was proposed and accepted in the Division meeting to extend Andrea Russell's serving as Past-Chair for six months, until June 2019.
- During the Division meeting the following symposia were agreed to be proposed to be organized by Div. 7 for the 71st Annual Meeting:
    - The usual core symposium (organized by Paramaconi Rodríguez and

someone yet to be decided)
    - Electrocatalysis (Marcel Rich Helmut Baltruschat)
    - Atomistic insight into surface electrochemistry: links between electrochemistry and surface science, photovoltaics, etc (Katrin Domke, Julia Kunze). Could be a topical meeting
    - 2D materials (Robert Hilman, Marc Koper, Shen Ye and Nakkiran Arulmozhi). With materials divisions.
- Suggestions for topical meetings organized by (with support of) Div. 7 are strongly encouraged, as well as for symposia in the 72nd Annual Meeting. Please send suggestions to executive committee of division.