Volume 16 | Number 27 | 21 July 2014 | Pages 13543–14310

PCCP

Physical Chemistry Chemical Physics

www.rsc.org/pccp

Themed issue: Electrocatalysis - Fundamental Insights for Sustainable Energy

ISSN 1463-9076

ROYAL SOCIETY OF CHEMISTRY

EDITORIAL

Marc T. M. Koper and Yasuhiro Iwasawa

Electrocatalysis

PCCP

EDITORIAL

Electrocatalysis

Marc T. M. Koper[a] and Yasuhiro Iwasawa†[b]

Cite this: *Phys. Chem. Chem. Phys.*, 2014, **16**, 13567

DOI: 10.1039/c4cp90068e

www.rsc.org/pccp

Electrocatalysis is the field of chemistry that deals with the catalysis of redox reactions and that links electrochemistry to catalysis. Electrocatalysis is a key discipline for the development of energy storage, fuel cells, solar fuels, electrosynthesis and all other electrochemical processes and devices in which the control of interfacial charge transfer reactions plays an important role. With the projected future "electrification" of our society through solar and wind energy, the conversion of electricity to chemical bonds and *vice versa* will be an essential field of physical chemistry in the decades to come. Basic fundamental understanding of these processes, both in model studies and at a more device-related level, requires detailed quantitative physical chemistry approaches. The present themed issue of PCCP balances fundamental and more applied studies in the field of electrocatalysis.

In the last 10–15 years, our fundamental understanding of electrochemistry and electrocatalysis has benefited tremendously from the application of first-principles computational chemistry techniques using density functional theory (DFT). In this issue, this development is illustrated by contributions from the groups of Janik (DOIs: 10.1039/C4CP00266K and 10.1039/C4CP00760C), Rossmeisl and Krtil (DOI: 10.1039/C4CP00571F), Dodelet and Vidal (DOI: 10.1039/C3CP55331K), Groß (DOI: 10.1039/C4CP00237G), Liu (DOI: 10.1039/C4CP00037D), and Atanassov and Kiefer (DOI: 10.1039/C4CP01634C). In many instances, such DFT calculations directly target the explanation or prediction of experimental results. This is an important development underscoring the physical chemistry approach and supporting the discovery of new materials for electrochemical energy storage and conversion.

Mechanistic studies combining well-defined surfaces with electrochemical and *in situ* spectroscopic measurements remain at the basis of our empirical understanding of electrocatalytic reactivity. In this issue, we find such studies on diverse reactions for electrochemical energy storage and electrosynthesis, such as formic acid oxidation (Feliu *et al.*, DOI: 10.1039/C4CP00304G), oxygen reduction for fuel cells and lithium–air batteries (Sung *et al.*, DOI: 10.1039/C4CP00187G; Stephens and Chorkendorff *et al.*, DOI: 10.1039/C4CP00319E; Wan *et al.*, DOI: 10.1039/C4CP00757C; Mayrhofer *et al.*, DOI: 10.1039/C4CP00585F; Bandarenka *et al.*, DOI: 10.1039/C4CP00260A; Vidal *et al.*, DOI: 10.1039/C3CP55331K; Ramaker and Roth *et al.*, DOI: 10.1039/C4CP00192C; Uosaki *et al.*, DOI: 10.1039/C4CP00394B; Alonso-Vante *et al.*, DOI: 10.1039/C3CP54564D; Wu *et al.*, DOI: 10.1039/C4CP00225C; Chen *et al.*, DOI: 10.1039/C4CP00257A; Hoshi *et al.*, DOI: 10.1039/C4CP00243A; Kanan *et al.*, DOI: 10.1039/C4CP01337A; Kiefer *et al.*, DOI: 10.1039/C4CP01634C), methanol and ethanol oxidation (Sun *et al.*, DOI: 10.1039/C3CP55059A; Behm *et al.*, DOI: 10.1039/C4CP01229A), carbon dioxide reduction (Fontecave *et al.*, DOI: 10.1039/C4CP00451E; Jaramillo *et al.*, DOI: 10.1039/C4CP00692E), water oxidation (Rossmeisl *et al.*, DOI: 10.1039/C4CP00571F; Lee *et al.*, DOI: 10.1039/C4CP00385C), and chlorine evolution (Schuhmann and Strasser *et al.*, DOI: 10.1039/C4CP00896K). These papers cover the use of various different electrocatalyst materials, from model single-crystal surfaces (Attard *et al.*, DOI: 10.1039/C4CP00564C; Hoshi *et al.*, DOI: 10.1039/C4CP00243A), oxide catalysts (Savinova *et al.*, DOI: 10.1039/C4CP00341A; Rossmeisl and Krtil *et al.*, DOI: 10.1039/C4CP00571F; Lee *et al.*, DOI: 10.1039/C4CP00385C), to molecular catalysts (Dodelet and Vidal *et al.*, DOI: 10.1039/C3CP55331K; Fontecave *et al.*, DOI: 10.1039/C4CP00451E). A perspective paper by Rodriguez and Koper (DOI: 10.1039/C4CP00394B) provides an overview of the use of gold electrodes (both single crystalline and nanoparticulate) as an electrocatalyst material.

We as Guest Editors are very happy with the broad view on electrocatalysis that the present themed issue provides and hope that this collection of articles will inspire more authors to submit their best electrocatalysis work to PCCP. Finally, we would like to thank all contributors for their support of this special issue by submitting such excellent papers.

[a] *Leiden Institute of Chemistry, Leiden University, PO Box 9502, 2300 RA Leiden, The Netherlands. E-mail: m.koper@chem.leidenuniv.nl*

[b] *Innovation Research Center for Fuel Cells, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan. E-mail: iwasawa@pc.uec.ac.jp*

† Emeritus at the University of Tokyo, Tokyo, Japan.