



# Electrocatalysis: Present and Future

An ELCAT meeting

Alicante, Spain  
14- 17 November 2011  
Hotel Husa Alicante Golf

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## Conference program

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Universitat d'Alacant  
Universidad de Alicante



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# ORGANIZING COMMITTEE

Elisabet Ahlberg

Juan M. Feliu

Enrique Herrero (secretary)

Timo Jacob

Petr Krtil

David Schiffrin

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## FOREWORD

This meeting is held within the framework of the FP7 Marie Curie Training Network ELCAT, devoted to Electrocatalysis. The subject deals with catalytic reactions in condensed media, mostly represented nowadays by the metal/solution interface. This type of studies started in relation to fuel cells and a lot of efforts have been dedicated to understand reactions such as oxygen reduction and the oxidation of low molecular weight organic molecules, specially formic acid, methanol and, more recently, ethanol, increasing the complexity of the reaction. Fundamental studies highlighted the importance of controlling the surface structure and composition in the reactivity of the electrode. This knowledge has been transferred to the reactivity of dispersed nanoparticles as practical electrocatalytic materials. On the other hand, the availability of data from well-defined experiments has been used as a guide to model these complex surface processes. The increasing expertise has also been used to study the reactivity of other small molecules, such as the reduction of carbon dioxide, to synthesize organic products that could be further used by the chemical industry, and nitrate reduction to nitrogen as a possible process to decontaminate waste waters. These two reactions, jointly with oxygen reduction and evolution, are the selected processes in ELCAT project.

The scope of Electrocatalysis, however, is not only related to fuel cells or small organic molecules but comprises a much broader field in which the interplay between molecules and surfaces has to be considered. The expertise gained with the studies of small molecules should be extended to more complex situations that eventually will enable to understand the reactivity of biologically relevant molecules attached to surfaces, hopefully in the nearest future.

The purpose of the ELCAT network is to transfer the present knowledge to the young generation of researchers and involves fundamental as well as practical approaches. Knowledge of the relevant experimental techniques and theoretical modeling of surface reactions in condensed media must finally merge in a better understanding of the electrocatalytic processes and enlarge the application of this knowledge to more complex systems.

I would like to thank to all the participants for their interest in the main subject of this meeting and I wish fruitful discussions and exchanges of ideas.

Juan M. Feliu

PS. Recently, Professor Dieter Kolb passed away. I would like to personally dedicate this meeting on surface reactivity to his memory and acknowledge his contributions to the field. JMF.

## SUNDAY, NOVEMBER 13<sup>TH</sup>

18:00-20:00 REGISTRATION AND WELCOME PARTY.

## MONDAY, NOVEMBER 14<sup>TH</sup>

08:30-09:00 OPENING

CHAIRPERSONS: M.T.M. KOPER, M. FIGUEIREDO

- 09:00-09:40 [I-01](#) Tailoring the Future of Electrocatalysis  
*N.M. Markovic*
- 09:40-10:00 [O-01](#) Electrocatalysis at bimetallic nanostructures  
*E. Santos*
- 10:00-10:20 [O-02](#) Substrate effect on Hydrogen electroinsertion into Pd/Pt(111): an in situ SXR D study  
*E. Sibert*
- 10:20-10:40 [O-03](#) Theoretical investigations on the adsorption and incorporation of hydrogen into the Pt(111) surfaces  
*P. Kaghazchi*
- 10:40-11:00 [O-04](#) Island formation on gold surfaces under electrochemical conditions  
*M. Mesgar*

11:00-11:30 COFFEE BREAK

- 11:30-12:00 [I-02](#) Electrocatalysis for Oxygen Reduction and Evolution  
*J. Rossmeisl*
- 12:00-12:20 [O-05](#) Ab Initio Study of the Electrochemical Pt(111)/H<sub>2</sub>SO<sub>4</sub> Interface  
*A. Comas-Vives*
- 12:20-12:40 [O-06](#) Water oxidation and catalyst recovery on binuclear molecular Mn(III-V) systems studied by first principles modeling  
*M. Busch*
- 12:40-13:00 [O-07](#) Theoretical study on the first step of oxygen reaction reduction  
*N.B. Luque*
- 13:00-13:20 [O-08](#) Parallel oxygen and chlorine evolution on iridium based oxides  
*E. Kuznetsova*

13:20-15:00 LUNCH

CHAIRPERSONS: E. AHLBERG

- 15:00-16:00 [I-03](#) A comparison between artificial and natural water oxidation.  
*Per Siegbahn*
- 16:00-17:00 [I-04](#) Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level  
*J. Ulstrup*
- 17:00-17:30 [I-11](#) Modelling the catalytic voltammetry of reversible enzymes. Application to hydrogenases.  
*V. Climent*

## TUESDAY, NOVEMBER 15<sup>TH</sup>

CHAIRPERSONS: S. HORSWELL, M. DUCA

- 09:00-09:40** [I-05](#) In situ, Real Time Monitoring of Electrocatalytic Reactions  
*K. Uosaki*
- 09:40-10:00** [O-09](#) The Mechanism of Formic Acid Electrooxidation on Metal Electrodes  
*A. Cuesta*
- 10:00-10:20** [O-10](#) Glycerol electro-oxidation over glassy-carbon-supported Au particles: The influence of the support coverage on the electrode catalytic activity  
*J.F. Gomes*
- 10:20-10:40** [O-11](#) DEIS study of ethanol and acetaldehyde oxidation on Pt in acid solutions  
*A. Lasia*
- 10:40-11:00** [O-12](#) Pd-modified Ni Foam Electrodes and their Use as Anodes for the Oxidation of Methanol, Ethanol, Ethylene Glycol and Glycerol in Basic Media  
*M. Musiani*

### 11:00-11:30 COFFEE BREAK

- 11:30-12:00** [I-06](#) In situ XAS studies of core-shell PEM fuel cell catalysts: the opportunities and challenges  
*A.E. Russell*
- 12:00-12:20** [O-13](#) DEMS Study on the Oxidation of Ethanol at Poly and Single Crystal Platinum Surfaces  
*E. Mostafa*
- 12:20-12:40** [O-14](#) Scanning electrochemical cell microscopy: A novel approach towards new fundamental insights into nanoscale electrocatalysis  
*S.C.S. Lai*
- 12:40-13:00** [O-15](#) Reactions of fuel cell interest at mesoporous materials  
*G. García*
- 13:00-13:20** [O-16](#) Synthesis and Electrochemical Properties of Au-Rh Nanomaterials  
*W. Siriwatcharapiboon*

### 13:20-15:00 LUNCH

CHAIRPERSONS: P. KRTLIL, M. MESGAR

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*E. Savinova*
- 15:30-15:50** [O-17](#) Towards Nano-engineered Pt-skin high surface area catalysts  
*D.F. van der Vliet*
- 15:50-16:10** [O-18](#) Cathodic corrosion as a facile and effective method to prepare clean metal and metal alloy nanoparticles  
*P. Rodríguez*
- 16:10-16:30** [O-19](#) Understanding the importance of surface cleanliness in shape controlled Pt nanoparticles  
*F.J. Vidal-Iglesias*
- 16:30-16:50** [O-20](#) Electrocatalytic reduction of CO<sub>2</sub> by Au/Cu alloys  
*E. Volker*
- 16:50-17:10** [O-21](#) Electroreduction of carbon dioxide on copper-based electrodes: Activity of copper single crystals and copper-gold alloys  
*T. Doneux*
- 17:10-17:30** [O-22](#) Experimental and theoretical studies on the intermediates in the electrochemical reduction of carbon dioxide  
*L. Soare*

## WEDNESDAY, NOVEMBER 16TH

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P. Zelenay
- 09:40-10:00**    [O-23](#)    Electrocatalytic reduction on nitrogen containing compounds in platinum modified single crystals  
M. Figueredo.
- 10:00-10:20**    [O-24](#)    Mechanism of Nitrate Ions and NO Electroreduction on Pt(100)  
A. Danilov
- 10:20-10:40**    [O-25](#)    Casting the dice: nitrite reduction at Pt(100) and cubic nanoparticles  
M. Duca
- 10:40-11:00**    [O-26](#)    Nitrate electro reduction on Pt nanoparticles/Cu phthalocyanin sported on carbon  
J. Souza-García

**11:00-11:30**    COFFEE BREAK

- 11:30-12:00**    [I-09](#)    Oxygen reduction reaction activity, selectivity and surface properties of nanostructured metallic centred catalysts  
N. Alonso-Vante
- 12:00-12:20**    [O-27](#)    Metal Nanoparticles Confined in LbL Polyelectrolyte Multilayers for Electrocatalysis  
E.J. Calvo
- 12:20-12:40**    [O-28](#)    Wet Chemistry Synthesis of Nitrogen-Doped Carbon as Non-Precious Electrocatalysts for Oxygen Reduction  
Y. Zhang
- 12:40-13:00**    [O-29](#)    Oxygen reduction on Pt-Cu nanoparticles embedded in Nafion® or polystyrene  
A. Boschín
- 13:00-13:20**    [O-30](#)    Screening of metal electrocatalysts for organic halides activation: an SECM approach  
C.M. Sánchez-Sánchez

**13:20-15:30**    LUNCH

**15:30-17:00**    POSTER SESSION

**20:30-24:00**    GALA DINER

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L. Kibler
- 09:40-10:00**    [O-31](#)    Electrocatalytic Properties of Strained Pd Shells grown on Au Nanostructures  
D.J. Fermin
- 10:00-10:20**    [O-32](#)    Highly dispersed Pt<sub>3</sub>Co/C nanoparticles: correlation between the fine nanostructure and the ORR activity  
L. Dubau
- 10:20-10:40**    [O-33](#)    Preparation of highly distributed Pt electrocatalysts supported on hydrophobic graphitized carbons without increasing electrochemical carbon corrosion  
H. Kim
- 10:40-11:00**    [O-34](#)    Electron Transfer across a Nanowire/Electrolyte Solution Interface: Catalysis or Inhibition?  
R. Nazmutdinov

**11:00-11:30**    COFFEE BREAK

- 11:30-11:50**    [O-35](#)    Enhanced Catalytic activity of Fe and Co phthalocyanines for the reduction of O<sub>2</sub> when linked to Au(111) via conjugated SAMs of aromatic thiols  
J. Zagal
- 11:50-12:10**    [O-36](#)    Competitive adsorption processes on Pt(100) face in sulfate solutions  
A. Rudnev,
- 12:10-12:30**    [O-37](#)    Molecular electrocatalysis at liquid-liquid interfaces: a biologically inspired system for oxygen reduction  
P. Peljo.
- 12:30-12:50**    [O-38](#)    Electrochemical synthesis of hydrogen peroxide  
E. Vesterberg
- 12:50-13:10**    [O-39](#)    Combined SECM + XPS Study of (Ru<sub>1-x</sub>:Ti<sub>x</sub>)O<sub>2</sub> (x=0, 0.5, 1) Coatings of Industrial Relevant Electrodes  
L.A. Näslund

**13:10-13:30**    CLOSING

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- [I-04](#) Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level  
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- [I-08](#) Electrocatalysis of Oxygen Reduction on Non-Precious Metal Fuel Cell Catalysts  
*P. Zelenay, G. Wu, H. T. Chung and C. M. Johnston*
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*N. Alonso-Vante*
- [I-10](#) New information about elementary steps in electrocatalysis  
*L.A. Kibler, E. Heider, F.W. Hartl and T. Jacob*
- [I-11](#) Modelling the catalytic voltammetry of reversible enzymes. Application to hydrogenases.  
*F. Grey, S. Hexter, V. Climent and F. Armstrong*



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