

COST
Domain Committee "CMST "

COST Action D-6
Start Date (*February 2006*)

***Molecular Structure-Performance
Relationships at the Surface of Functional
Materials***

**MONITORING
PROGRESS REPORT**

***Reporting Period: from February 2006
to December 2009***

This Report is presented to the relevant Domain Committee.
It contains three parts:

- I. Management Report prepared by the COST Office/Grant Holder***
- II. Scientific Report prepared by the Chair of the Management Committee of the Action***
- III. Previous versions of the Scientific Report; i.e., part II of past reporting periods***

The report is a "cumulative" report, i.e. it is updated annually and covers the entire period of the Action.

Confidentiality: the documents will be made available to the public via the COST Action web page except for chapter *II.D. Self evaluation*.

Based on the monitoring results, the COST Office will decide on the following year's budget allocation.

Executive summary (max.250 words): The groups at COST D36 address structure-activity relationships at the surface of functional materials under working conditions. This Action stands on a multidisciplinary approach based on combining and designing advanced in situ spectroscopic methods to characterize functional materials structure at work simultaneously to its performance measurement; talent on synthesis of nanoscaled materials (nanoparticles, nanocrystalline materials, core-shell structures, among others) and advanced theoretical modeling to describe structural and reactive features of functional materials and adsorbed molecules during operation. All working group have integrated synthesis, spectroscopy, performance measurement (catalysis, electrochemistry, biocompatibility) and theoretical modeling. This Action is characterized by knowledge permeation, which has an impact in fundamental and applied areas, such a biomimetic photocatalysis, hydrogen production, selective oxidation, sustainable chemistry, environmental catalysis or biocompatible vesicles for drug delivery inside the body. Advanced spectroscopic tools are developed, such as electrochemical Raman cells or scanning electro microscopy, or

I. Management Report prepared by the COST Office/Grant Holder



I.A. COST Action Fact Sheet

• COST Action D36 - Molecular Structure-Performance Relationships at the Surface of Functional Materials

• Domain CMST

• Action details:

CSO Approval: 14/06/2005 **End date:** 23/02/2011
Entry into force: 14/10/2005 **Extension:** none

• Objectives

The main objective of the Action is to increase the fundamental knowledge and understanding of the chemistry occurring at surfaces and interfaces and the factors that tune it. An interdisciplinary, combined effort is the approach. A fundamental approach is advocated, even for industrially oriented research projects. This requires precisely defined problems at all levels and an interdisciplinary approach i.e. synthesis and activation of the materials; measurement of the surface properties; understanding surface properties at the atomic, molecular or cluster level and theoretical understanding of these properties in relation to chemical composition and the structure of the surface. As a consequence, the secondary objective is to gain advanced knowledge for modelling/predicting of the structure/composition reactivity/surface properties relationships of the materials, by means of characterisation of the bulk and surface properties under real operation conditions and for preparing materials with tuneable properties.

• Parties: list of countries and date of acceptance

Country	Date
Austria	17/02/2006
Denmark	14/10/2005
Greece	14/10/2005
Latvia	15/12/2005
Portugal	22/05/2006
Sweden	14/10/2005

Country	Date
Belgium	14/10/2005
Finland	02/05/2006
Hungary	25/10/2005
Netherlands	13/10/2005
Romania	14/10/2005
Switzerland	14/10/2005

Country	Date
Bulgaria	21/11/2005
France	06/06/2006
Ireland	19/10/2005
Norway	14/10/2006
Slovenia	06/12/2005
Turkey	08/04/2009

Country	Date
Czech Republic	15/11/2005
Germany	13/10/2005
Italy	05/01/2006
Poland	14/10/2005
Spain	17/10/2005
United Kingdom	24/10/2005

Total: 24

• Intentions to accept: list of countries and date

• Other participants:

(Institution Name, Country, Town)

Chair:**Professor Miguel BANARES**

CSIC - Instituto de Catalisis Marie Curie, 2 E-28049 Madrid Spain
banares@icp.csic.es

DC Rapporteur:**Professor Vasile PARVULESCU**

Department of Chemical Technology & Catalysis Faculty of Chemistry University of Bucharest B-dul Regina Elisabeta 4-12 030016 Bucharest Romania
vasile.parvulescu@g.unibuc.ro

Science Officer:**Dr Erwan ARZEL**

COST Office
earzel@cost.esf.org
003225333817

Administrative Officer:**Svetlana VOINOVA**

COST Office
svoinova@cost.esf.org
+32 2 533 38 48

- **Action Web site:** <http://www.uma.es/costd36>
- **Grant Holder Representative** *none*
- **Working Groups** (list of WGs and names and affiliations of participants)

D36-001-05 Redox activity of host organometallic and structures at electrode interfaces

D36-003-06 Interfacial functionalization of (bi)-metallic nanoparticles to prepare highly active and selective catalysts: understanding synergy and/or promotion effect

D36-005-06 Structure-Reactivity Relationship of Pt and Pd Nanoarrays

D36-006-06 Understanding the chemical reactivity of alcohols over catalytic materials: from probe molecules to practical applications

D36-007-06 Molecular Catalysis and Photocatalysis at Soft Interfaces: Towards chemical fuel cells

D36-008-06 Biopolymers based surfactants- Stabilization and functionalization of particles and surfaces

I.B. Management Committee member list

Name	Country	E-mail

I.C. Overview activities and expenditure

2009 Budget

Total Action Budget:

Remaining Action Commitment:

Meetings

Meeting Type	Date	Place	Paid part	Cost	Total
Management Committee	24-févr-2006	Brussels (BE)	29	17930,14	
Management Committee	25-sept-2006	Brussels (BE)	4	1833,59	
Management Committee	02-oct-2006	Brussels (BE)	28	15255,57	
Working Group	19-nov-2006	Prague (CZ)	4	1978,31	
Working Group	24-nov-2006	Bruckmuhl (DE)	8	3473,28	
Working Group	30-nov-2006	Lausanne (CH)	4	2859,43	
Working Group	01-déc-2006	Warwick (uk)	8	4226,86	
Working Group	01-déc-2006	Palermo (IT)	7	5916,26	
Working Group	08-déc-2006	Barcelona (ES)	11	8385,23	
Working Group	17-mai-2007	Coimbra (PT)	10	8798,08	
In conjunction with Workshop/Conference	01-sept-2007	Espoo (FI)	41	32030,3	
Working Group	05-oct-2007	Stockholm (SE)	8	7065,89	
Working Group	16-nov-2007	Prague (CZ)	5	2719,79	
Working Group	26-nov-2007	Arcavacata di Rende (IT)	10	7401,25	
Working Group	16-déc-2007	Burgos (ES)	6	3326,08	
Working Group	04-avr-2008	Dijon (FR)	5	3125,15	
Working Group	10-mai-2008	Poznan (PL)	7	4376,94	
Working Group	15-mai-2008	Graz (AT)	6	7340,41	
In conjunction with Workshop/Conference	04-sept-2008	Dublin (IE)	27	18602,76	
Working Group	26-sept-2008	Villars (CH)	4	2655,7	
Working Group	24-oct-2008	Nice (FR)	14	12644,27	
Working Group	14-nov-2008	Delft (NL)	8	5336,46	
Working Group	28-nov-2008	Leiden (NL)	5	2361,52	
Working Group	11-déc-2008	Rome (IT)	10	7720,48	
Working Group	28-mars-2009	Espoo (FI)	6	3908,3	
Working Group	15-mai-2009	Palermo (IT)	13	11799,88	
Working Group	18-mai-2009	Maribor (SI)	12	9964,18	
Working Group	29-mai-2009	Paris (FR)	6	2752,39	
Joint Management Committee/Working Group	21-oct-2009	Malaga (ES)	76	63617,09	
					279405,59

STSM

Beneficiary	Date	From	To	Cost	Total
Mr Jianjun Zhao	03-déc-2006	Berne (CH)	Coventry (uk)	1280	
Dr Monica Calatayud	20-déc-2006	Paris (FR)	Madrid (ES)	627	
Mr Akintayo Adisa	05-mars-2007	Manchester (uk)	Burgos (ES)	2440	
Ms Jana Bulickova	02-mai-2007	Prague (CZ)	Dresden (DE)	852	
Ms Ilaria Degano	07-mai-2007	PISA (IT)	Prague (CZ)	1200	
Ms Satu Korhonen	14-mai-2007	FI-02015 TKK (FI)	75252 Paris (FR)	1100	
Mr Jan Fiedler	16-mai-2007	Prague (CZ)	10125 Torino (IT)	1550	
Dr. Izabela Sobczak	01-mai-2007	Poznan (PL)	Delft (NL)	2470	
Dr Maciej Trejda	01-mai-2007	Poznan (PL)	Delft (NL)	2470	
Mr G�r�me Melaet	05-mai-2007	1050 Bruxelles (BE)	90146 Palermo (IT)	2450	
Dr Mich�le Salmain	24-sept-2007	Paris 75005 (FR)	Prague 8 (CZ)	1500	
Dr Viorel Chihaiia	01-oct-2007	Bucharest (RO)	Budapest (HU)	2000	
Ms Diana Costa	15-sept-2007	3004-535 Coimbra (PT)	Graz (AT)	2500	
Ms Satu Korhonen	01-oct-2007	FI-02015 TKK (FI)	Paris (FR)	2500	
Pr Bj�rn Lindman	03-janv-2008	Lund (SE)	Maribor (SI)	1400	
Mr Alberto Martinez	02-f�vr-2008	Burgos (ES)	Manchester (uk)	2500	
Mr Edgar Ventosa	03-f�vr-2008	Burgos (ES)	Coventry (uk)	2500	
Ms Nika Veronovski	01-mars-2008	2000 Maribor (SI)	00185 Roma (IT)	2500	
Mr Ivan Ivanov	14-avr-2008	1113 Sofia (CZ)	90146 Palermo (IT)	2100	
Dr Anna Elzbieta LEWANDOWSKA	18-mai-2008	MADRID (ES)	UTRECHT (NL)	1470	
Ms T�mea Benk�	24-mai-2008	Budapest (HU)	Palermo (IT)	1410	
Dr Filipe Antunes	17-mai-2008	Coimbra (PT)	Rome (IT)	2280	
Ms Tina Tkavc	01-avr-2008	Maribor (SI)	Lund (SI)	2500	
Dr Romana Sokolova	23-juin-2008	Prague (EE)	Pisa (IT)	1380	
Mr Germ�n Soldano	15-juin-2008	D89069 Ulm (DE)	Leiden (NL)	2500	
Dr Agnieszka RUPPERT	03-ao�t-2008	Utrecht (NL)	Paris (FR)	1560	
Ms Anna Wojtaszek	05-nov-2008	60-780 Pozna#324; (PL)	Paris (FR)	2500	
Ms Hanna Golinska	05-nov-2008	60-780 Poznan (PL)	E-28049 Madrid (ES)	2500	
Dr Anna Elzbieta LEWANDOWSKA	20-f�vr-2009	Madrid (ES)	Paris (FR)	1830	
Dr Giorgio Volpi	17-f�vr-2009	Turin (IT)	Prague (CZ)	2300	
Mr G�r�me Melaet	09-mars-2009	1050 Bruxelles (BE)	90146 Palermo (IT)	1250	
Mr Markus Vogelsang	01-mars-2009	Ulm (DE)	Manchester (UK)	2500	
Dr Ivan Ivanov	15-avr-2009	1113 Sofia (BG)	90146 Palermo (IT)	2300	
Ricardo L�PEZ MEDINA	14-avr-2009	Madrid (ES)	Poznan (PL)	1500	
Ms Daniela Plana	08-juin-2009	Manchester (UK)	Leiden (NL)	2450	

Ms Elizabeth Rojas Garcia	15-mai-2009	MADRID (ES)	PARIS (FR)	2500	
Dr Mohammad Mazharul Islam	20-juil-2009	Paris (FR)	Milano (IT)	2400	
Dr Elizabeth Santos, Dr	14-sept-2009	Ulm (DE)	Paris (FR)	1110	
Ms Ana Rita Almeida	14-sept-2009	Delft (NL)	Paris (FR)	2500	
Dr Gabriella Di Carlo	01-sept-2009	Palermo (IT)	Stockholm (SE)	3500	
Dr Noelia Beatriz Luque	15-oct-2009	Ulm (DE)	Paris (FR)	2500	
Mr Jordi Morros	09-déc-2009	Barcelona (ES)	Coimbra (PT)	1200	
					83.879

Workshops

Title	Date	Place		Cost	Total
WG 01 meeting: Redox activity of host-guest. organometallic and molecular structures at electrode interfaces	19-nov-2006	Prague (CZ)		545	
WG D38-06-06 meeting	24-nov-2006	Bruckmuhl (DE)		600	
WG D36-003-06 meeting	01-déc-2006	Palermo (IT)		700	
WG D36-008-06 meeting	08-déc-2006	Barcelona (ES)		700	
Action D36 WG 008 meeting	17-mai-2007	Coimbra (PT)		730	
Annual Workshop and MC meeting	01-sept-2007	Espoo (FI)		3.426	
D36 WG06 meeting	03-sept-2007	Espoo (FI)		329	
WG 003-06 meeting	05-oct-2007	Stockholm (SE)		573	
WG D36/007-06 meeting	16-nov-2007	Prague (CZ)		445	
WG D36/0008/06 Biopolymer based surfactants – stabilisation and functionalisation of particles and surfaces	26-nov-2007	Arcavacata di Rende (IT)		650	
WG D36/05/06 meeting	15-déc-2007	Burgos (ES)		600	
WG D36/007-06 meeting	04-avr-2008	Dijon (FR)		445	
WG D36/006/06 meeting	10-mai-2008	Poznan (PL)		650	
WG D36/008 meeting	15-mai-2008	Graz (AT)		520	
COST D36 Annual Workshop+MC meeting	04-sept-2008	Dublin (IE)		2.222	
COST WG D36/07 meeting	26-sept-2008	Villars (CH)		200	
WG D36/03 meeting	24-oct-2008	Nice (FR)		1.324	
WG D36/06-06 meeting	14-nov-2008	Delft (NL)		284	
WG D37/005-06 meeting	28-nov-2008	Leiden (NL)		360	
COST D36 WG7 meeting	28-mars-2009	Espoo (FI)		250	
Action D36 WG 03 meeting	15-mai-2009	Palermo (IT)		800	
WG D36/08 meeting	18-mai-2009	Maribor (SI)		1.400	
of	29-mai-2009	Paris (FR)		213	
Structure-performance relationships at the surface of functional	21-oct-2009	Malaga (ES)		10.000	

materials					
					27.966

General Support Grants

Title	Date			Cost	Total
					0

Schools

Type	Date	Place	title	Cost	Total
SCHOOL_STUDENTS	24-nov-2008	Leiden (NL)	D36 TRAINING SCHOOL on ELECTROCATALYSIS at NANOSCALE techniques and applications	9000	
SCHOOL_LLECTURERS	05-oct-2009	Ulm (DE)	Hetero- and Electrocatalysis at the Nanoscale: Theory and Modeling	9653,84	
SCHOOL_ORGANISER	05-oct-2009	Ulm (DE)	Hetero- and Electrocatalysis at the Nanoscale: Theory and Modeling	1100	
SCHOOL_STUDENTS	05-oct-2009	Ulm (DE)	Hetero- and Electrocatalysis at the Nanoscale: Theory and Modeling	7800	
					27553,84

Honoraria

Title	Date	Expert		Cost	Total
					0

Grant

Grant Holder	Date			Cost	Total
					0

Dissemination

Title	Date			Cost	Total
					0

418804,77

II. Scientific Report

II.A. Innovative networking

Six Working Groups affording complementary areas constitute the Action; representative information is provided about all WG's.

II.A.1. Innovative knowledge/scientific breakthrough resulting from COST networking

WG-D36/001/06. A joint experiments brought results by performing high sensitivity low-frequency impedance measurements, which could discriminate subtle effects of intramolecular interactions [Pospíšil et al., *Carbon*, **48** (2010) 153]; this solves a problem of supramolecular protection of reactive forms of fullerene. It is expected that those derivatives may find application on pharmacology and other fields.

WG-D36/003/06. A **Brussels/Palermo** collaboration on total oxidation of CH₄ over very active and selective Pd/TiO₂-SiO₂ catalysts demonstrated, for the first time that that two forms of sulphate species exist. The sulphate species responsible for deactivation can be removed (reactivation) by methane at 350°C. A **Sweden/Palermo** collaboration develops novel nanocrystalline CeO₂; the nanocrystalline cubic ceria was obtained at room temperature with a specific surface area of 180 to 250 m²/g and maintains its features up to 400 °C.

WG-D36/005/06. Significant progress has been achieved on theoretical electrocatalysis at metal nanostructures (H₂ evolution reaction) that provides valuable insights into the dynamics of hydrogen evolution and oxidation at nanostructured surfaces. Key objectives have been completed, like the synthesis of Pd and Au-Pd core-shell nanostructures with various shell thicknesses or the electrostatic assembly of 2D and 3D arrays of the nanostructures at electrode surfaces [Li et al., *J. Phys. Chem. C* **112**(2008)9686; Bradbury et al. *CHIMIA*, **62** (2008) 841]. **Warwick** has developed its carbon nanotube growth protocols for single-walled carbon nanotube (SWNT) networks with a wide range of surface densities [Dumitrescu, et al., *Adv. Mater.* **21**(2009)3105]. The **Burgos/Helsinki** teams developed an innovative Raman cell for spectroelectrochemistry; this technique allows obtaining in-situ spectroscopic information about the reaction products generated during the electrocatalytic reactions.

WG-D36/006/06. Combines advanced in situ spectroscopic investigation with advanced DFT calculations on novel materials and catalytic processes for glycerol valorisation. **CaO catalyzed Glycerol Conversion (Utrecht/Paris)** requires both strong basic sites and Lewis acid sites are necessary for the etherification of glycerol. The more basic the character of the oxide, the more exothermic is the adsorption and the higher the dissociation extent; modeling results match experimental data. **Novel functionalized mesoporous materials (Poznan/Madrid/Delft) and metals doped silica-based (Paris/Poznan)** afford oxidation (**Delft**) and ammoxidation of glycerol (to acrylonitrile, **Madrid**) in aqueous media. Modeling presented uncovers glycerol mechanism and confirm that V, Nb, Ta were incorporated in the zeolite framework; and gold grafted silica materials. Furthermore, the **photo-catalytic oxidation of cyclohexane with TiO₂ anatase** - The photocatalytic oxidation of cyclohexane to cyclohexanone (**Delft**), calculated by periodic DFT (**Paris**).

WG-D36/007/06 develops the idea of reactivity at the liquid–liquid interfaces, addressing the oxygen reduction reaction for fuel cell applications and more recently to hydrogen generation. This will lead to a novel class of “chemical fuel cells” based on a soft interfaces; the work stands on complementarity: institutions with expertise in synthesis of molecular catalysts, theoretical electrochemistry, photoelectrochemistry at liquid–liquid interfaces, molecular dynamics and quantum–mechanical calculations.

WG-D36/008/06 develops novel ideas of studying DNA-lipid interactions based on phase diagrams; on a new family of non haemolytic cationic lysine based surfactants and to develop new reaction water media to prepare hydrophobic inulin surfactants. Thus, they have developed a novel technique based on Layer-by-Layer deposition to produce hollow nanocapsules. Also a new cubic liquid crystalline phase of DNA-lipid assembly has been

established, with relevance for nuclear organisation.

II.A.2. Spin off of new EC RTD Framework Programme projects

- i. Surface Electrochemical Reactivity in Electrocatalysis: A Combined Theoretical and Experimental Approach" (ELCAT): multisite Initial Training Network within the EU Seventh Framework Programme involving **ULEI/ULM**.
- ii. Integrated processing of lignocellulosic materials to chemicals (**LIGNOCELLUCHEM**), proposal, not granted
- iii. Proposal Reference oc-2009-1-4159; "Rational catalyst design through precise mechanistic and kinetic understanding"; Call identifier: FP7-2009-BIOREFINERY; ENV.2009.3.3.2.2 Sustainable Biorefineries
- iv. Proposal FP7 Call title FP7-NMP-2010-SMALL-4 NMP.2010.1.2-2: Substitution of materials or components utilizing "green nanotechnology"
- v. COST Domain Chemistry and Molecular Sciences and Technologies; Proposal Reference oc-2009-1-4487; "Holistic Approach Towards Controlling Heterogeneous Catalysed Reactions

II.A.3. Spin off of new National/Regional Programme projects

- i. Foundation for Polish Science Team Programme and European Regional Development Fund. 2009 – 2013. "*Atomic and molecular level devising of functional nanostructures for magnetic and catalytic applications*"
- ii. Four national projects were approved and granted. One international project for the cooperation France-Czechia was awarded. Another international project between Italy and Czechia is now under evaluation.
- iii. Study of the formation of Pd nanoparticles at L/L interfaces using a new mobile slit spectroelectrochemical cell: project funded by Junta de Castilla y Leon (Spain) **Burgos/Helsinki/Manchester**.
- iv. Development of Optically Transparent Electrodes based on Single Walled Carbon Nanotubes: project funded by the Junta Castilla y Leon (Spain) **Burgos/Helsinki**.
- v. Novel carbon nanomaterial networks as ultrasensitive/efficient platforms for analysis and electrocatalysis. Research Council for Natural Sciences & Engineering of the Academy of Finland involving **Helsinki**.
- vi. MEC-FCT; Date: 2008-2009; IP: Dr. M. R. Infante (Spain)-M. G. Miguel (Portugal); 2007PO0050 "*Tensioactivos biocompatibles en la complexación de biopolímeros*";
- vii. MEC-FCT (submitted); Date: 2010-2011; IP: Dr. M. R. Infante (Spain)-M. G. Miguel (Portugal) *Nuevos tensioactivos biocompatibles derivados de aminoácido en la liberación controlada de ADN*"

II.B. Inter-disciplinary networking

All the work done by this Action stands on complementarity of theoretical modelling and experimental work (synthesis, advanced in situ measurements during operating conditions), and thus, all the publications result from COST framework collaboration. The level of interdisciplinarity is excellent to provide scientific impact, as the examples described above demonstrate. An additional advantage of COST framework is its flexibility that allows interactions between laboratories in different WG's within the Action, but also between laboratories in **different COST Actions**, in particular, we have close interactions with **COST Action D35 and D41**. This year, a STSM has been done from D36 to a D41 laboratory, and the counterpart mission will probably take place in the next few months. For example, the application of in-situ methods involves a close cooperation within the project participants and with one **D35 project**. Partner laboratories achieved numerous results in the field of interfacial organometallic redox chemistry and in mechanistic studies of new organic compounds. An inter-disciplinary level of research proved to be a pre-requisite for identification of decomposition pathways of certain pollutants. A study of pesticides serves as one of the examples. Another example has stands on the STSM scientific mission from **D36 to D41** ("*Mechanisms of hydrogen diffusion on the anatase TiO₂(101) surface: Investigation from the first principles*"). The level of interdisciplinarity afforded in this action is rendering novel results and breakthrough developments described above that have an

impact on sustainable process and energy use, as well as on biocompatibility. These developments will result in significant socio-economic impact.

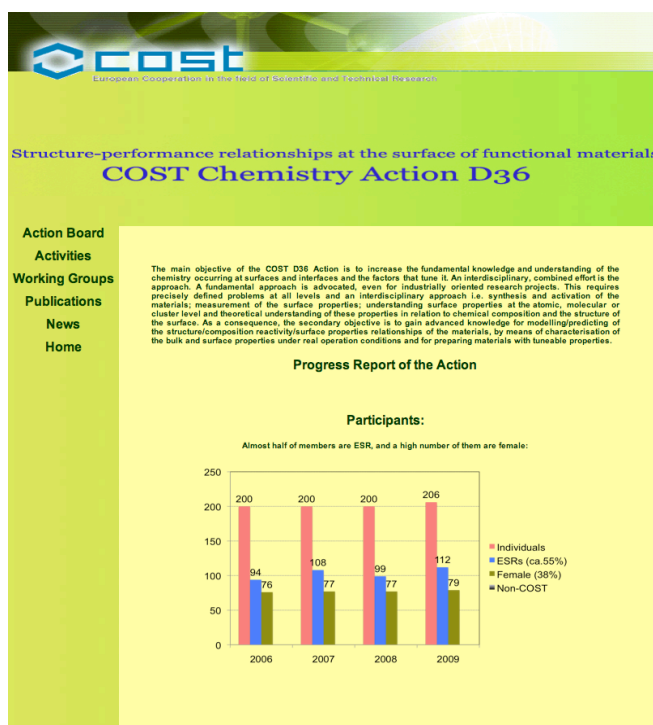
II.C. New networking

Three new laboratories from Turkey have joined three WG's during 2009 after Turkey became MC member: (1) Bilkent University (prof. Kantcheva); (2) University, Ankara (Dr. A.Cihaner); (3) Prof Mustafa Ersoz, Selcuk University (Konya). A Czech group (Institute of Organic Chemistry and Biochemistry, prof. I. Stibor) joined the action as well. At present, the total number of participants in the Action is 192 individuals of whom 41 % is female and 51% ESR; this is also reflected in MC composition (35% females). The participation of ESR is very high, ESR do almost all STSM and 30 ESR attended the **second Training School**. New networking has resulted in a number of new projects, as described in **Section II.A**. The Involvement of researchers from outside of COST Countries is evident also on works made on gas transport in a microporous solid using an innovative slice selection procedure and applied to the diffusion of benzene in zeolites was carried out by the French group lead by Prof. Jacques Fraissard. This research involved researchers from outside the COST countries, particularly involved people from Ternopil, Ukraine. Moreover they used ^{129}Xe spectroscopy of adsorbed xenon for exploring microporous carbon materials.

OUTREACH Activities stand on conferences, publications (95 papers, listed in Annex), workshops and Training Schools. Our **Second Training School on Heterogeneous Catalysis and Electrocatalysis at the Nanoscale** (Reisensburg Castle, near Ulm, 4-8.October.2009), devoted to *theory and computer modelling of interfacial reactions with strong emphasis on the relationships between heterogeneous catalysis and electrocatalysis*. As part of the key deliverables of **WG D36/005/06**, the Ulm group led the organisation of a Training School devoted to methods and models relevant to electrocatalysis and heterogeneous catalysis. A panel of **twenty** experts delivered lectures on: Electron transfer theories: from Marcus theory to theories of electrocatalysis; Simulation methods: Monte Carlo and Molecular dynamics, both classical and quantum versions; Quantum chemical methods; Relation between electrocatalysis and heterogeneous catalysis. Over **30 participants (100% ESR)** from the whole of the Action D36 took part on the 4-day event and the feedbacks received were overwhelmingly positive. The Action Chair **presented COST Action D36 during COST-Day** celebrated in Madrid on November 2009 to publicize COST Actions to a broader range of people involved in fundamental and applied research.

The **WEBPAGE** has been enabled at www.uma.es/costd36 in which information to WG's, deliverables and activities are available.

Rising of research funds comes from the relevant national funding agencies of each laboratory; in addition, the Engineering and Physical Science Research Council (UK), CONACYT (Mexico); The Swiss National Science Foundation (CH), the International Society of Electrochemistry, the Lorentz Center Leiden (NL), National Physical Laboratory (UK), Birmingham Science City: Innovative Uses for Advanced Materials in the Modern World (West Midlands Centre for Advanced Materials Project 2; AM2 and Hydrogen-Energy (both Advantage West Midlands supported projects, with AM2 also part-funded by the European Regional Development Fund).



II.D. Self evaluation

The most relevant achievement has been the consolidated entanglement of different expertisness in the working groups. Several WG's use regularly theoretical chemistry to describe structure under working conditions, and predict performance and spectra. Such modelization has been contrasted with actual in situ determination of both spectra and performance values. This is providing a tool not only to describe reality, but for data interpretation and understanding the causes that determine the actual structure and performance of catalysts, electrocatalysts, biocompatible systems and phenomena during environmental processes and cultural heritage degradation. In this line, it is particularly attractive that such cross-fertilization is no only happening within working groups, but also among working groups.

The base for this success is based on the multidisciplinary approached envisaged for every WG, which has resulted in the fact that all WG's tackle specific applications standing on the four pillars of the Action: well-defined model systems, advanced in situ characterization during working conditions, performance measurement and theoretical modelling to describe structure and reactivity. Thus, every WG is a multidisciplinary team tackling a given problem. The applications of the different WG's are different; yet, they share some common characteristics. The Training School celebrated in Ulm (October, 2009), on catalysis at nanoscale has been a major success, not only for the visibility of COST Action D36 to non-COST members, but also to trigger interaction among students of different working groups. This and the previous Training School in 2008 are promoting STSM's between laboratories belonging to different WG's. This is resulting in a progressive trend to interact among laboratories of different WG's, which is a major success for such cross-fertilization is a promise of exciting progress in the near future. The STSM's are indeed the most powerful tool of COST Actions, which in combination with the Workshops is fundamental for an efficient flow and exchange of information and knowledge. The COST Action constitutes an excellent frame for such interactions.

The lack of direct support for COST Action members in some countries results in a serious limitation for an efficient development of their activities, which research has to be run on the group's budget.

ANNEXES

- I. Previous scientific reports**
- II. PUBLICATIONS 2009**
- III. PLENARY/INVITED/KEYNOTE LECTURES 2009**
- IV. WG's annual summary (6)**
- V. STSM reports (14)**
- VI. PROCEEDINGS BENAHAVIS Annual COST D36 Workshop**
- VII. 2nd TRAINING SCHOOL – REGENSBURG CASTLE, near ULM**
- VIII. Presentation at “COST Day” in Madrid, 27.Nov.2009**

ANNEX I. Previous scientific reports

A. Results achieved during the period Feb. 2006 to Jan. 2008

The Action started in Feb. 2006, the main objective is to increase the fundamental knowledge and understanding of the chemistry occurring at surfaces and interfaces and the factors that tune it. An interdisciplinary, combined effort is the approach, i.e. synthesis and activation of the materials; measurement of the surface properties; understanding surface properties at the atomic, molecular or cluster level and theoretical understanding of these properties in relation to chemical composition and the structure of the surface. This allows for gaining advanced knowledge for modeling/predicting of the structure/composition reactivity/surface properties relationships of the materials, by means of characterization of the bulk and surface properties under real operation conditions and for preparing materials with tenable properties. The first MC meeting extended an invitation for WG proposals, which were evaluated according to COST procedures. The first MC agreed that a Steering Committee would be sufficient for many decisions, making the management of D36 faster and easier at a better cost. The second MC meeting, on 2.Oct.2006 selected six WG's, based on the external reports and internal discussions, after hearing the report from the Steering Committee that met on 25.Sep.2006. These WG started their action immediately, so that kick-off meetings were celebrated before the end of the year 2006.

This Action possesses a broad scope, yet sharing common interdisciplinary approach focused on understanding functional materials. All the WG's aim at elucidating, understand and optimize nanostructured functional materials, through the careful design of nanostructures, investigations of reactivity and rationalization through detailed theoretical modeling and advanced *in situ* and *operando* studies. The scope of applications is very broad, catalysis, sensing, coating and microelectronics, environmental applications and in the formulation of biocompatible colloids. Therefore the Action was designed to have a significant number of Working Groups reaching a critical mass to tackle several target systems.

2007 has been the first year when the WG's have actually developed their actions, which started during December 2006, after the specific WG's were approved. 2007 has been a particularly active year, despite the transition time between June-August in which activities could not be funded. All the groups have geared up very efficiently and a total of 12 STSM have been done, along with 7 WG meetings, a MC meeting and a workshop. The WG's presented the results of their first months of research at a workshop in Finland on September 1st and 2nd, 2007, which was coordinated with the MC meeting and one WG meeting. This workshop was also open to non-COST members and there was an interaction with COST Action D41, whose chairman, Prof. Pacchioni gave a plenary lecture to show the activities at D41 and common interests with D36; all groups in D36 are using theoretical modelling to study their systems, which is a key activity in D41 go understand oxides. In turn, Dr. Bañares, presented an equivalent talk, presenting D36 and results from D36, relevant to D41 participants.

Within COST Action D36, every working group has initiated collaborative research under the scope of this Action: to combine of *in situ* studies, theoretical calculations, advanced synthesis and characterization to understand the structure-performance relationships at a molecular level, and thus tune their properties. Every Action aims at different processes and materials, which are determined by the reactivity at the surface of solids or at liquid/liquid interfaces. Some groups study catalysis, electrocatalysis, and electrochemical reactivity for degradation or valorization of molecules at the surface. Other groups analyze interface reactivity: liquid/liquid interfaces for catalytic processes, or solid/liquid interface reactivity for several functional materials. Every WG tackles the effect of the nanostructure on the structural and reactive property on applications. All the groups share similar experimental approaches, electrochemical, catalytic or electrocatalytic, at solid/gas, solid/liquid or liquid/liquid interfaces. All the WG's apply theoretical modelling to describe the structure and reactivity at the surface or interface of the reactive materials, but also to predict reactivity under different conditions. The WG's use theoretical calculations to describe the state of the materials during operation conditions and to assign spectroscopic bands of the materials. A common experimental approach the different WG's is the use of *in situ* and *operando* spectroscopic characterization of the materials during operation conditions. The developments of each WG are disclosed at the Annexes, they exhibit exciting progress since all groups are moving towards a similar combined experimental approach where well defined nanostructured materials are prepared, characterized *in situ* during operation and modelized to tackle very different application arenas. It is

expected that the activities of the different WG's will initiate some degree of entanglement during 2008.

January-December, 2008

The year started with a change in a WG, Prof. B. Grzybowska's group left WG-D36-006-03 due to retirement, and it was replaced by the team of Prof. Korećki, both located at the Institute of Catalysis and Surface Science of the Polish Academy of Science in Krakow.

During the second full year of the Action, all WG's have consolidated and have extended their activities aiming at a progressive entanglement of expertisness, combining experimental approach where well defined nanostructured materials are prepared, characterized *in situ* during operation and modelized in order to develop a molecular knowledge of the structure-activity relationships. This is being applied to corrosion and cultural heritage degradation (WG D36-001-06), electrochemistry and catalysis on nanoscaled systems (WG D36-001-06, WG D36-005-06, WG D36-006-01), catalysis and sustainable processes (WG D36-003-06, WG D36-005-06, WG-D36-006-06, WG-D36-007-06) and surfactants and biocompatible materials (WG-D36-008-06).

Among the major developments, it is interesting to highlight:

The extension of the joint research in **WG-D36-001-06** about host-guest complexes and their electrochemical reactivity to other type of possible complexes of fullerene and cyclodextrins. This WG investigated new compounds with cyclodextrin moiety covalently attached to the fullerene structure. The water-soluble complex of fullerene and gamma-cyclodextrin was characterized by the electrochemical impedance spectroscopy. This work was aimed at the optimization of *conditions for the electrocatalytic nitrogen conversion to ammonia at mild conditions*. This WG described a *new type of cationic catalysis*, which is based on ion pair interactions of nitro-aromatic radical anions generated at the electrode surface with alkali metal cations. The ion pair formation effectively diminishes the electrostatic repulsion of radicals from the interface. The effect is a strongly enhanced further reduction to reactive dianions of nitro-compounds.

In **WG-D36-003-06**, the joint research on nanoscaled bi-metallic Au-Ag/ Fe₃O₄ materials shows that the morphology of the cluster assembly can be tuned by changing composition and deposition condition. *Such research is fundamental for the understanding of the catalytic behavior of gold catalysts supported on iron oxides, widely investigated by the other WG participants in several reactions such, the oxidation reaction of CO, water-gas shift reaction, and also oxidation of VOC.*

In **WG-D36-005-06**, the joint research activities have afforded significant progress towards: The joint work has examined in detail the synthesis of Au-Pd core-shell nanostructures employing seeding-growth methods. The synthesis consists of reducing PdCl₄²⁻ at the surface of 20 nm Au cores in the presence of ascorbic acid. This method allows adjusting the average shell thickness between 1.6 and 9.0 nm. They have also explored conducting polymers as supports for Pt catalysts. Thus, modifying highly oriented pyrolytic graphite (HOPG) with a thin poly(3,4-ethylenedioxythiophene) (PEDOT) layer provided a route for catalytic surfaces with higher density of smaller nanoparticles than in likewise produced HOPG-supported arrays. Ultra-small (ca 1 nm) particles have been deposited within zeolite membranes via different methods. Similarly, protected Au NPs have been deposited by chemical reaction at the water/toluene interface

Simultaneously, joint work has resulted in the development of a novel strategy to prepare composite catalytic materials based on the layer-by-layer electrochemical generation of a hybrid material consisting of polyaniline (PANI) and Pt NPs, it is possible to tune the electrocatalytic performance for the oxidation of methanol. The layer-by-layer approach preparation of the nanocomposite and modification of the Pt nanoparticles with a layer of PANI resulted in substantially higher catalytic efficiency for methanol oxidation.

The groups formulated a general theory of hydrogen electrocatalysis based on extensive calculations with density functional theory (DFT). They first applied this theory successfully to the hydrogen evolution reaction on a series of pure metals (Pt, Au, Cd) and then they turned to systems of special interest to this COST group. The energy of activation for the hydrogen reaction was lower on Pd layers on Au(111) than on pure.

The reactivity of monoatomic nanowires was found to significantly enhance with respect to bulk metals. Thus, on platinum wires the energy of dissociation of water is greatly reduced. Likewise, the energy of adsorption for hydrogen on gold wires is much lower, leading to hydrogen adsorption at potentials above the equilibrium potential for hydrogen evolution.

In **WG-D36-006-06**, the achievements range from the development of kinetic models and fundamental understanding of catalysts active in the conversion of glycerol and alcohols by selective (amm)oxidation or etherification to value added products, there is an important degree of interaction among groups and methodologies. In particular focus is on combining information from advanced *operando* spectroscopy tools, and DFT calculations. In 2008, activities within the framework of this COST action have focused on an enhancement of the interaction of the various groups involved in the form of STSM agreements. In particular, intensive interactions between the groups of Banares/Ziolek, Thielens/Ziolek, and of Calatayud/Weckhuysen were established. Furthermore two working group meetings were held, the first in Poznan, Poland, and the second in Delft, The Netherlands. In the following an extended summary of the various achieved results on the basis of the two working group meetings is provided, including those reported of various STSM's. Finally, an overview is given of the various papers that have been published as a result of the cooperation of the various parties in our working group.

A large variety of catalysts has been synthesized, with promising characteristics for alcohol conversions. In particular the acid-base properties and nature of the surface sites have been well characterized. The catalysts can be divided in three categories, i.e. CaO and related materials, supported metal oxides (Fe-Mo, Cr, (alkali promoted) V-Sb, and Nb), and catalysts based on Au. Extensive DFT modelling has been conducted to reveal the structure of a variety of these systems, as well as the interaction with alcohols and the modes of reduction. CaO was found a promising catalyst for the target reaction of the conversion of glycerol, yielding etherification. Combinations of V and Sb were found very active in the ammoxidation of glycerol, in particular in the combination with the use of microwaves. Fe-Mo catalysts have to be further evaluated for the conversion of glycerol, as well as the Cr, and Au-catalysts. Tool development has focused on the analysis of liquid phase processes, and includes the evaluation of Raman spectroscopy and ATR in combination with microreactors, which appears an ideal combination for transient experiments. Many activities are planned for 2009, in particular focusing on extending the work in the combination of *operando* analyses, reactivity evaluation, and DFT modelling of the conversion of glycerol in particular, and alcohols in general.

In **WG-D36-007-06**, during 2008, the main achievements have been:

- the synthesis of hydrogen peroxide in biphasic systems using decamethylferrocene as an oxygen ligand. The reaction is controlled by the proton pump reaction from aqueous to the organic phase.
- the demonstration that free base porphyrins such as H₂TPP can activate oxygen to catalyse its reduction.
- The design, synthesis and characterisation of highly efficient amphiphilic porphyrins for oxygen reduction
- The development of new computational techniques to study the structure of liquid-liquid interface by molecular dynamics.

In **WG-D36-008-06**, the emphasis has been on several applications of surfactants. Essentially, adsorption of bio-surfactants (protein and sugar-derived surfactants) on surfaces and DNA encapsulation. Collaboration dealt with interactions between Gemini surfactants and homo-polymers, to find rational explanation on the interactions between such association colloids and macromolecules.

The relations between size and thermodynamic stability of vesicles made of common lipids and arginine-based surfactants was performed. Experiments were performed by DLS, electrophoretic mobility and TEM. The results are reflected in 4 contributions to literature (vide Annex on publications).

The stabilization of titania nano-particles mediated by adsorption of surfactants was addressed by an investigation dealt with DLS and electrophoretic mobility.

Annex I, on Scientific Achievements by every Working Group provides more information about the developments and projects in progress in the different working groups.

B. Dissemination of results

During hardly more than one year, the groups have been most active, and there has been an important degree of dissemination, in several fields. The total number of **papers** done under COST D36 is already 76, which on average, means almost two papers per laboratory. Two of them are reviews. In addition, there have been three **book chapters** and members in two laboratories in WG D36/008/06 have filed two **patents**.

The WG members have been very active and they have already reported their activities on 44 occasions at conferences and workshops. I'd like to highlight that among these, there have been several keynote and plenary lectures. One of them, within the exchange between COST D41 and COST D36, which is commented below.

- **Invited Plenary Lecture** H. Girault, at **14th annual meeting of the Chinese Electrochemical Society**, Xiamen, China on 7-9, Nov., 2007
- **Invited presentation**, M. A. Bañares "Molecular structure-activity relationships on supported oxide catalysts, relevance of additives and reaction conditions. A case study from COST D36 Action", **COST Action D41 "Inorganic Oxides: Surfaces and Interfaces"** 2007 Annual Meeting of the COST D41 Action, Berlin, 21-23, Oct. 2007
- **KEYNOTE LECTURE** "Operando Raman Methodology: the combination of kinetic and structural information in a single experiment to understand catalytic operation"; 6-8.Dec.2006, in **APCAT-4 (Asia Pacific Conference on Catalysis)**, Singapore. Miguel A. Bañares.
- **PLENARY LECTURE** - "Niobium as a promoter for oxidation catalysts", **6th International Symposium on Group Five Elements**, May 7-10, 2008, Poznań, Poland -
- **KEYNOTE** - "Structure-Performance Relationships in Supported Vanadia Catalysts under Working Conditions based on Complementary Operando Raman-GC and *in situ* XANES spectroscopies", **SNBL Workshop on simultaneous Raman-X-ray diffraction/absorption studies for the *in situ* investigation of solid-state transformations, and reactions at non ambient conditions. 18-19 June 2008, ESRF, Grenoble, Francia**
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Web site

WG D36-007-06 GIRAULT has already established a wiki site (WIKI.EPFL.CH) to allow all WG members share results, presentation, articles. A general access site is in preparation now, it provides links to COST D36 events and information about the WG's involved in this action.

Publication of a special issue in "CATALYSIS TODAY" on the first COST D36 workshop



On December 2008, a special issue in Catalysis Today, edited by Dr. Sanna Airaksinen - host and organizer of the symposium- has been published. It is devoted to the First COST D36 workshop, celebrated in Helsinki on September 2007 (As described in Annex IV). Catalysis Today is a top-notch international journal. The special issue reports 13 papers reflecting the contributions presented there. This special issue is an important vehicle to disseminate the activities run at this Action and raises its visibility. It should be underlined that several non-COST participants attended this workshop, and this trend is expected to rise during the next workshop, to be held near Malaga, Spain, in 2009. An outline of the issue is presented here:

Catalysis Today

Volume 139, Issue 3 pp. 153-242 (30 December 2008)

First Workshop of COST Action D36 "Molecular Structure - Performance Relationships at the Surface of Functional Materials", Edited by Sanna Airaksinen

1. "Preface", , Sanna Airaksinen

2. "Selective H–D exchange catalysed by aqueous phase and immobilised Pd nanoparticles", Pages 154-160, James A. Sullivan, Keith A. Flanagan, Holger Hain
3. Hydrotalcite docked Rh-TPPTS complexes as efficient catalysts for the arylation of 2-cyclohexen-1-one in neat water, Pages 161-167 F. Neațu, M. Besnea, V.G. Komvokis, J.-P. Genêt, V. Michelet, K.S. Triantafyllidis, V.I. Pârvulescu
4. NO reduction by CO over gold based on ceria, doped by rare earth metals, Pages 168-173, Lyuba Ilieva, Giuseppe Pantaleo, Ivan Ivanov, Radka Nedyalkova, Anna Maria Venezia, Donka Andreeva
5. Support effect on the catalytic performance of Au/Co₃O₄–CeO₂ catalysts for CO and CH₄ oxidation, Pages 174-179, L.F. Liotta, G. Di Carlo, A. Longo, G. Pantaleo, A.M. Venezia
6. Formation and structure of Au/TiO₂ and Au/CeO₂ nanostructures in mesoporous SBA-15, Pages 180-187, A. Beck, A. Horváth, Gy. Stefler, R. Katona, O. Geszti, Gy. Tolnai, L.F. Liotta, L. Guzzi
7. Gold, vanadium and niobium containing MCM-41 materials—Catalytic properties in methanol oxidation, Pages 188-195, Izabela Sobczak, Natalia Kieronczyk, Maciej Trejda, Maria Ziolek
8. Nb-containing mesoporous materials of MCF type—Acidic and oxidative properties, Pages 196-201, Maciej Trejda, Jolanta Kujawa, Maria Ziolek, Julita Mrowiec-Białoń
9. Sb–V–O-based catalysts for the ammoxidation of propane with a fluidized bed reactor, Pages 202-208, M. Olga Guerrero-Pérez, José L. Rivas-Cortés, J.A. Delgado-Oyagüe, J.L.G. Fierro, Miguel A. Bañares
10. Combining theoretical description with experimental in situ studies on the effect of alkali additives on the structure and reactivity of vanadium oxide supported catalysts, Pages 209-213, Anna E. Lewandowska, Mònica Calatayud, Enrique Lozano-Diz, Christian Minot, Miguel A. Bañares
11. A DFT study of methanol dissociation on isolated vanadate groups, Pages 214-220, L. Gracia, P. González-Navarrete, M. Calatayud, J. Andrés
12. Nature of vanadium species in V substituted zeolites: A combined experimental and theoretical study, Pages 221-226, F. Tielens, M. Trejda, M. Ziolek, S. Dzwigaj
13. CO₂ adsorption on (0 0 1) surfaces of metal monoxides with rock-salt structure, Pages 227-233, Ramzi Hammami, Adnene Dhouib, Sébastien Fernandez, Christian Minot
14. Modeling of gas transport in a microporous solid using a slice selection procedure: Application to the diffusion of benzene in ZSM5, Pages 234-240, Michel Petryk, Sebastien Leclerc, Daniel Canet, Jacques Fraissard

Lorentz center **Electrocatalysis@Nanoscale:**
Techniques and Applications
Workshop November 24 – 28 2008, Leiden, The Netherlands

Scientific Organizers:

- M.T.M. Koper, Leiden
- A.I. Yanson, Leiden
- D.J. Fermin, Bristol
- P.R. Unwin, Warwick

Invited Speakers:

- Helmut Baltruschat, Bonn
- Bernard Boukamp, Twente
- Robert Dryfe, Manchester
- Joost Freunek, Leiden
- Serge Lemay, Delft
- Julie Macpherson, Warwick
- Claf Magnussen, Kiel
- Bruno Pichler, Berlin
- Antonio Bode, Alicante
- Elizabeth Santos, Cordoba
- David Schiffrin, Liverpool
- Wolfgang Schmickler, Ulm

Local Organizers:

Prof. Dr. Marc Koper, Dr. Alex Yanson

International Organizers:

Dr. David Fermin (Bristol), Prof. Dr. Patrick Unwin (Warwick) (WG D36-005-06)

Logos: NPQ, FOM, COST, Lorentz center

www.lorentzcenter.nl

Second COST D36 Workshop, in September 2008, Dublin

The second COST D36 workshop took place in Dublin on September 2008. Several non-COST speaker participated actively, as invited speakers.

Training School (in collaboration with Lorentz Workshop) on "Electrocatalysis@nanoscale: techniques and applications"

Lorentz Center, Leiden University, The Netherlands, 24-28 November 2008

Local Organizers:

Prof. Dr. Marc Koper, Dr. Alex Yanson

International Organizers:

Dr. David Fermin (Bristol), Prof. Dr. Patrick Unwin (Warwick) (WG D36-005-06)

The purpose of this Training School was to bring together junior scientists from all WG's in COSTD36 Action and non-COST students to learn about the principles and possible applications of the various experimental techniques applicable to the study of the electrocatalytic systems. The Training School was held in the framework of a "Lorentz Workshop" at the Lorentz Center of Leiden University. The format of the meeting was set up so as to actively

involve participants in solving their own research questions. Student participants were asked to formulate a pertinent research question from their own research before the start of the Training School. After the specialist training lectures in the morning and early afternoon sessions, in the afternoon discussions, students presented their research questions in small groups of 6 students and two experts.

Electrocatalysis is a highly interdisciplinary discipline of science of great importance for our future energy economy (batteries, fuel cells, hydrogen production...). A good background in electrocatalysis, which would enable one to tackle all the important research problems in this area, requires knowledge of chemistry, physics, catalysis, materials science, electronics, nanotechnology, biochemistry, etc. This aspect is also reflected in the many different experimental techniques that are available to study electrocatalytic and electrochemical processes, which range from modifications of the classical spectroscopic techniques (Infrared, Raman, UV-VIS) to scanning probe microscopies (AFM, STM) to techniques based on electrical response (voltammetry, impedance spectroscopy, scanning electrochemical microscopy). Such a School was most successful, bringing COST and non-COST participants among professors and students. Many interactions are crystallizing among participants from different groups, inside and outside D36.

Scientific and Technological Cooperation

- *Cooperation and contacts with scientific institution, other research programmed and potential users.*
 - o An interaction has been established with Prof. G. Pacchioni, Chairman of **COST D41** due to complementary approaches in the area of oxide materials. It was agreed to promote mutual interactions by arranging a joint workshop after the second year, when a body of research is significant in both Actions. As a first Approach, Prof. Pacchioni, presented the Action D41 and representative results to D36 members at the First D36 Workshop, in Espoo, Finland, September 2007. In turn, Dr. Bañares presented the Action D36 and representative results to D41 members at the 2007 D41 Workshop, in Berlin, Germany, October 2007. *Preliminary contacts have already been established between specific laboratories in D36 and D41.*
 - o COST Action D36-006-06. The group of Paris has joined the Group of Madrid in a multidisciplinary project funded by CSIC in Spain on magnetic and catalytic properties of nanoscaled mixed oxide materials (Materials with new interface magnetism: origin, and application screening (MAGIN) 200680F0123, 199 000 €. (January 2007-December 2008). A workshop shall be organized on March.2008 among all groups involved (physics, chemists, materials science, magnetism, DFT modellization).
- *Transfer of results*
 - o The WG initiated their activities ca. three months ago, so there has not been transfer yet. It should be highlighted that two WG's possess industrial partners involved.
 - o Laboratories in WG-008-06 INFANTE have filed two patents.
- *Contacts in the ERA (EUREKA, ESF, European coordinative research frameworks ...)*
 - o The results obtained within the WG's should constitute a seed for project proposals under FP7 in the near future. Several consortia are now in progress of building up.
 - o The First COST Workshop in Espoo, Finland, resulted in a proposal for a new Action, coordinated by one of the non-COST invited speakers, Prof. G. Rupprechter ref. OC-2007-1457 "SPECTROSCOPY OF FUNCTIONING CATALYSTS" (under DC CMST)

ANNEX II. PUBLICATIONS 2009

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2. M. Hromadová, L. Pospíšil, R. Sokolová, N. Fanelli; „New electrochemical oscillator based on the cation-catalyzed reduction of nitroaromatic radical anions.“; **Electrochim. Acta**, **54** (2009), 4991
3. L. Adriaenssens, L. Severa, T. Šálová, I. Císařová, R. Pohl, D. Šaman, S. V. Rocha, N. S. Finney, L. Pospíšil, P. Slavíček, F. Teplý; „Helquats: A Facile, Modular, Scalable Route to Novel Helical Dications“; **Chemistry Eur. J.**, **15** (2009) 1072.
4. L. Pospíšil, M. Hromadová, M. Gál, M. Valášek, N. Fanelli, V. Kolivoška; „Irregular Polarographic Currents Obey Feigenbaum Universality Route from Order to Chaos“; **Coll. Czechoslovak Chem. Commun**, DOI: 10.1135/cccc2009120
5. G. Volpi, C. Garino, L. Salassa, J. Fiedler, K. I. Hardcastle, R. Gobetto, C. Nervi; „Cationic Heteroleptic Cyclometalated Iridium Complexes with 1-Pyridylimidazo [1,5- α]Pyridine Ligands: Exploitation of an Efficient Intersystem Crossing“; **Chem. Eur. J**, **15** (2009), 6415.
6. S. Roy, B. Sarkar, C. Duboc, J. Fiedler, O. Sarper, F. Lissner, S. M. Mobin, G. K. Lahiri, W. Kaim; „Heterohexanuclear (Cu₃Fe₃) Complexes of Substituted Hexaazatrinaphthylene (HATN) Ligands: Twofold BF₄⁻ Association in the Solid and Stepwise Oxidation (3 e) or Reduction (2 e) to Spectroelectrochemically Characterized Species“; **Chem. Eur. J** **15** (2009), 6932
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8. L. Ilieva, G. Pantaleo, I. Ivanov, R. Nedyalkova, A.M. Venezia, D. Andreeva, „NO reduction by CO over gold based on ceria, doped by rear earth metals“, **Catal. Today**, **139** (2008) 168-173.
9. L. Ilieva-Gencheva, G. Pantaleo, N. Mintcheva, I. Ivanov, A. M. Venezia, D. Andreeva, „Nanostructured Gold Catalysts Supported on CeO₂ and CeO₂-Al₂O₃ for NO_x reduction by CO: Effect of Catalysts pretreatment and Feed Composition“, **J. Nanoscience & Nanotechnology**, **8** (2008) 867.
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12. Kancheva, O. Samarskaya, L. Ilieva, G. Pantaleo, A.M. Venezia, D. Andreeva, „In situ FT-IR investigation of the reduction of NO with CO over Au/CeO₂-Al₂O₃ catalysts in the presence and absence of H₂“, **Appl. Catal. B: Environ.**, **88** (2009) 113-126.
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 25. A. Rutkowska, D. Walker, S. Gorfman, P. A. Thomas and J. V. Macpherson, **J. Phys. Chem. C** 113 (2009) 17087.
 26. I. Dumitrescu, P. R. Unwin and J. V. Macpherson, **Chem. Commun.** 45 (2009) 6866.
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ANNEX III. PLENARY/INVITED/KEYNOTE LECTURES 2009

Plenary/Invited/Keynote Lectures

1. J. Fraissard, The search for lost illusions **Plenary lecture**, International congress "XEMAT 2009" **Ruka**, Finland, 7-10/06/2009
2. J. Fraissard, **Keynote lecture VIII International Conference, "Mechanisms of Catalytic Reactions"**, **Novosibirsk**; "Modeling of gas transport in a microporous solid using a slice selection procedure: Application to the diffusion of benzene in ZSM5", 29 June- 2 July 2009 .
3. Prof. Hubert H. Girault **Plenary lecture 42nd Heyrovsky discussion**, Trest, Czech Republic June 2009. "Hydrogen Production at Soft Interfaces"
4. Prof. Hubert H. Girault; **keynote lecture at the 8th Turkish Electrochemistry Meeting** "Bio-inspired electrochemistry: H₂ production and O₂ reduction".
5. Prof. Girault gave a **plenary lecture to the Chinese Electrochemical special meeting in Beijing** (August 2009) entitled " Bio-inspired electrochemistry at soft interfaces".

In attached files at our webpage www.uma.es/costd36 :

- ANNEX IV. *WG's annual summary (6)***
- ANNEX V. *STSM reports (14)***
- ANNEX VI. *PROCEEDINGS BENAHAVIS Annual COST D36 Workshop***
- ANNEX VII. *2nd TRAINING SCHOOL – REGENSBURG CASTLE, near ULM***
- ANNEX VIII. *Presentation at “COST Day” in Madrid, 27.Nov.2009***