

International Symposium
Frontiers in Surface and Materials Science: Theory and Practice

in honor of the 60th birthdays of Francesc Illas and Gianfranco Pacchioni

Auditori Antoni Caparrós, Parc Científic de Barcelona, c/ Baldiri Reixac 4
08028 Barcelona, Spain

November 14th, 2014

Website for Registration: <http://www.iqtc.ub.edu/frontiers/>
(please register before October 20, 2014)

PROGRAM

Chairs: **Dr. Anna-Maria Ferrari** (Università di Torino, Italy)

Prof. Josep Manel Ricart Pla (Universitat Rovira i Virgili, Tarragona, Spain)

14:00 Opening and welcome

Prof. Pere Lluís Cabot (Dean, Faculty of Chemistry, Universitat de Barcelona)

14:30 Prof. Javier Fernández-Sanz

Universidad de Sevilla, Spain

Chemical processes at metal-oxide surfaces

15:00 Prof. Paul Bagus

University of North Texas, USA

Understanding the Meaning of X-Ray Adsorption Edges In Heavy Metal Systems: A Challenge for Theory

15:30 Prof. Jean Paul Malrieu

Université Paul Sabatier de Toulouse, France

Spin (De)-Contamination of Broken-Symmetry Calculations of Magnetic Couplings: Deeper Analysis and New Suggestions

16:00 – 17:00 Poster session with refreshments

17:00 Prof. Elio Giamello

Università di Torino, Italy

Investigating defect centers in metal oxides: synergistic effects between Electron Magnetic Resonance and Computational Chemistry

17:30 Prof. Notker Rösch

Institute of High Performance Computing, A*STAR, Singapore

*Modeling Reactions on Transition Metals and Oxide Supports
– New Work Inspired by Collaboration with Old Friends*

18:00 Prof. Hans-Joachim Freund

Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Model Catalysts:

Almost 20 Years of Fruitful Exchange between Theory and Experiment

18:30 Closure of the Symposium

19:00 – 21:00 *Buffet dinner*

Accommodation

Barcelona offers numerous good opportunities for accommodation. Thus, everyone can make hotel reservation on his/her own, depending on the taste/needs. Please do that as early as possible. Some examples of suitable options for accommodation with single-room rates below or around 100 € per night are:

Residencia **Torre Girona** is at the working distance from the Meeting venue. Passeig dels Til·lers, 19, 08034 Barcelona, Tel.: (0034) 93 390 43 00, Fax: (0034) 93 205 69 10, http://www.resa.es/esl/residencias/torre_girona, torregirona@resa.es

Hotel** **Husa Bonanova Park**, Capità Arenas, 51, 08034 Barcelona, Tel.: (0034) 93 2040900 / (0034) 932045014 (fax), <http://www.hotelbonanovapark.com> , hotelbonanovapark@husa.es

Hotel** **Prisma**, Av. Josep Tarradellas, 119-121, 08029 Barcelona, Tel.: (0034) 934394207 / 934050427 (fax), <http://www.mediumhoteles.com>, prisma@mediumhoteles.com

Hotel** **Praktik**, Diputació, 32, Barcelona · tel. (+34) 93 467 31 15 fax. (+34) 93 467 31 10, <http://www.praktikhotels.com/>

Hotel*** **NH Rallye**, Travesera de les Corts, 150-152, 08028 Barcelona, Tel.: (0034) 93 3399050 / (0034) 93 4110790 (fax), <http://www.nh-hotels.com>, nhrallye@nh-hotels.es

Hotel*** **Apsis Sant Angelo**, Consell de Cent, 74, 08015 Barcelona, Tel.: (0034) 934 234 647, <http://www.hotel-santangelo.com>

Hotel*** **Century Park**, Valencia, 154, 08011 Barcelona, Tel.: (0034) 934 534 400, <http://www.hotelcenturypark.com>

Hotel**** **Senator Barcelona Spa**, Cardenal Reig, 11, Les Corts, 08028 Barcelona <http://www.barcelonasenatorhotel.com>

Aparthotel**** **Atenea Barcelona**, Joan Güell, 207-211, Les Corts, 08028 Barcelona, Tel.: (34) 934 906 640 <http://www.aparthotelatenea.com/en/?gclid=CKKM0p6yrbsCFSnpwgodRk4ATg>

Onix Fira***, Llansa, 30, 08015 Barcelona <http://www.barcelonaby.com/cgi/searchvenwide.cgi>