



Catalysis Today 126 (2007) 1-2



## **Preface**

Understanding catalysis is a major challenge that requires a multidisciplinary approach bringing together complementary perspectives. The operando methodology combines structure and activity measurements in a single experiment, using a reaction cell that meets the requirements for both, a catalytic reactor and an in situ cell. The actual state of a catalyst at work is shaped by the reaction conditions that may not be present after the catalytic act. Thus, operando methodology provides a grip on both structure and activity in a simultaneous fashion, which leaves us in an excellent position to assess the structure-activity relationships at a molecular level. When proposing the term "operando," I confirmed with a friend who is a university Professor, expert in Latin, about the appropriateness of such a term. Explaining him that the target was to look at a functional material under working conditions was a distant concept. So, I rephrased my question using a closer example. I asked him if it is correct to say "operando" if you are talking about people (rather than a catalyst) who is working. And he agreed. What is most exciting about operando is that it has indeed put many people to work in implementing the *operando* approach to amazing levels, bringing depth and breath that stand on very solid studies, using a single spectroscopy or combining several techniques, theoretical and experimental approaches and expanding/developing structural, time and spatial resolution. The contributions presented in Toledo prove a high level of maturity in the approaches to understand how catalysts operate, perform and behave.

The enterprise to understand catalysis and functional materials started in 2003, when *Operando*-I (http://www.icp. csic.es/operando/), organized in Lunteren (NL), was a great success. Many researchers shared they experience in performing advance *in situ* studies. Such a trend has consolidated in *Operando*-II (2006) (http://www.acaberlin.de/ operando/), Toledo (Spain); and it projects to an amazing future in the forthcoming *Operando*-III meeting (www.catalysis.de/operando), to be organized in Rostock (Germany) in 2009.

Operando-II brought exciting and stimulating presentations with a common objective: understanding catalysis. Multiple techniques can provide information on the states of a catalyst while it operates, bringing molecular knowledge on how reactants adsorb and interact with the surface. Such interaction transforms the reactants and modifies the catalyst structure. This symposium was a unique opportunity to integrate complementary perspectives on the states of the catalytic and other functional materials during operation. The impact of this symposium will be felt in the years to come. The plenary lecture by Prof. Thomas provided a perspective on the trajectory of *in situ* studies and opportunities for future developments. Prof. Weckhuysen's plenary shared with us the intimacies of the life of a catalyst. Prof. Daturi's plenary elaborated on the states of surface species during reaction. The final plenary lecture by Prof. Rupprechter underlined the molecular changes at the surface of catalysts during operation. The keynote lectures by Prof. Koptyug and Prof. Sels presented the power of NMR and fluorescence imaging techniques during catalytic operation. Prof. Gurlo, the opportunities for research in sensors. Prof. Bürgi and Prof. Gundwaldt shared with us their progress in liquid phase operando studies using ATR-IR/UV-vis and XAS, respectively. The oral and poster contributions covered every possible approach, and selected papers are presented in this Special Issue.

Such a successful event was essentially due to the participants, and we must also thank the support of our sponsors, which provided very important support to the organization of such an event. We thank the support by our Major Sponsor HORIBA Jobin-Yvon. Standard Sponsors, Varian Inc., PID Eng&Tech, Avantes/Instrumatic, Ocean Optics, Kaiser Optical Systems, Renishaw, Thermo Electron. We also appreciate the support by Bruker and CEPSA, Elsevier (Catal. Today), and the Royal Society of Chemistry (Phys. Chem. Chem. Phys.). The institutional support was particularly important from Spanish public organism CSIC, UNED University, the Spanish Ministry of Education of Science, Spanish Catalysis Society, and the UCLM University. The support from EU CONCORDE Action, the City of Toledo and Toledo Convention Bureau is highly appreciated. I would like to take advantage of these lines to thank the enormous effort

brought together by all the member of the Organizing Committee, Scientific Committee, aeCAT-Q, and Local Committee, who have worked amazingly well to make this symposium possible.

Looking forward to seeing you again at *Operando*-III. In the meantime, please, enjoy this Special Issue of Catalysis Today.

Miguel A. Bañares\*

CSIC – Instituto de Catalisis y

Petrolequimica Marie Curie, 2

E-28049-Madrid, Spain

\*Tel.: +34 91 585 4788/4879; fax: +34 91 585 4760 *E-mail address:* banares@icp.csic.es