Int. J. Mol. Sci. **2001**, *2*, 165-166

International Journal of
Molecular Sciences
ISSN 1422-0067

www.mdpi.org/ijms/

Foreword

Papers from Euroconference on Molecular Mechanism of Heterogeneous Catalysis Held in San Feliu de Guixols (Spain) in June 2001

Francesc Illas [1] and Josep Manel Ricart [2]

[1] Departament de Quimica Fisica, Universitat de Barcelona, & Centre de Recerca en Quimica Teorica, Parc Cientific de Barcelona C/ Marti i Franques 1, 08028 Barcelona, Spain. Phone : 34-93-402 1229, fax 34-93-402 1231, e-mail: f.illas@qf.ub.es. http://www.qf.ub.es/c1/area4a1.html (Personal Page: http://www.qf.ub.es/c1/xino.html)
[2.] Department of Chemical Physics and Inorganics, Faculty of Chemistry, University Rovira i Virgili, P. Imperial Tàrraco, 1, 43005 Barcelona Spain. e-mail: ricart@quimica.urv.es, Tel. +34 977 559568, Fax. +34 977 559563 http://www.quimica.urv.es/~ricart/

Received: 9 November 2001 / Accepted: 9 November 2001 / Published: 9 November 2001

Heterogeneous catalysis is of immense technological and economic importance on a global scale because it provides the backbone of the world's chemical and oil industries. This is the reason for intense research in both academic and industrial laboratories. Because of the innate complexity of practical catalytic systems it has been suggested that progress should be achievable by investigating key aspects of catalysis by experimental studies on idealized model systems. In fact, surface science was initially meant to investigate the mechanisms of heterogeneous catalysis by performing careful experiments under well controlled conditions. However, even under these extremely controlled conditions and in spite of the development of new and sophisticated experimental techniques that enable resolution at the atomic scale it is still very difficult, almost impossible, to obtain precise information about the molecular mechanisms that underlie catalytic processes without the help of unbiased, ab initio, theoretical support. Spectacular advances in computers and supercomputers together with developments in electronic structure theory have broken the limitation that had constrained practical applications of ab initio theory to systems of academic interest. Nowadays, accurate first-principles calculations on realistic systems of industrial and technological interest are becoming possible. Notwithstanding, there is still a gap between the systems of potential industrial interest and those which can be studied by sophisticated experimental or theoretical techniques.

The main objective of thie Euroconference on Molecular Mechanism of Heterogeneous Catalysis held in San Feliu de Guixols (Spain) in June 2001 has been contributed to close this gap by bringing together leading scientists working in heterogeneous catalysis from both theory and experiment whose common goal is a fundamental understanding of molecular mechanisms in catalysis. Consequently, the

programs has covered a wide range of topics all related to catalysis, from the models of surface science, to catalysis by different materials (oxides, sulphides, metals, bimetallic catalysts, zeolites, etc.), covering various catalytic processes (homogeneous catalysis, electrocatalysis, supported catalysis and their models, promotion effects in catalysis, etc.) as well as theory of catalysis, addressing, among other aspects, kinetics problems and activation barriers.

The present special issue is representative of the whole program although it contains only a reduced number of contributions.

Acknowledgements: The guest editors wish to express their gratitude to the Spanish Ministerio de Ciencia y Tecnologia for supporting publication costs of this special issue and to the Universitat de Barcelona, Generalitat de Catalunya, Elsevier, the European Science Foundation and the European commission for having made this Euroconference possible.