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Preface

Heterogeneous catalysis has a role of ever increasing importance for the manipulation and control of chemical reactions. With knowledge of the basic reasons and fundamental chemical mechanisms of catalytic processes it is more easily possible to modify and tune the properties of catalytic materials to achieve the desired reaction properties. Theoretical understanding of catalysis can help to provide us with this knowledge and hence theoretical research is an important aspect of the study of catalysis. A primary purpose of the 6th International Conference on Theoretical Aspects of Heterogeneous Catalysis, CAT-96, held June, 2–7, 1996 in Tarragona, Spain, was to exchange information about recent theoretical advances in the understanding of surface properties and processes relevant to catalysis. The subjects considered at CAT-96 covered a broad range of topics in the following areas:

Metal and/or metal oxides in catalytic systems
Theoretical concepts and computational methods
Reactions on surfaces and clusters
Acid–base catalysis
Thin films and supported clusters
Surface reaction dynamics

A second purpose of CAT-96 was to encourage, develop and strengthen interaction between theory and experiment. To help achieve this purpose, there were several presentations at CAT-96 which described experimental research and which helped to establish connections be-

tween measurements of catalytic properties and the theoretical interpretation of those properties. Still another important objective of CAT-96 was to stimulate the interaction of scientists in academic institutions and industrial research laboratories. To help focus the participants of CAT-96 on the potential for academic–industrial interaction, the opening lecture at the conference was given by Dr. Jacinto Monge who is a Research Area Director at the REPSOL Research and Development Laboratories in Madrid, Spain.

The CAT-96 meeting follows five previous bi-annual meetings in the series on the theory of heterogeneous catalysis. The first meeting was held at Lyon, France, 1986, with succeeding meetings at Zakopane, Poland, in 1988, at Berkeley, California, in 1990, in Krakov, Poland, in 1992 and Berlin, Germany, in 1994. The meeting in 1998 will be in Cambridge, England. This special issue of *Journal of Molecular Catalysis* collects the papers presented at CAT-96 and will provide an archival record of the work discussed at the meeting which will be valuable for the participants as well as for others who were unable to attend.

On behalf of the organizing committee, we wish to express our gratitude for the generous support provided to CAT-96 by several institutions and private companies. These included: ‘Ministerio de Educación y Ciencia, DGICYT’, ‘Generalitat de Catalunya’, ‘Universitat de Barcelona’, ‘Universitat Rovira i Virgili’, ‘Fundació Catalana per a la Recerca’, ‘Societat Catalana de Química’, ‘Col.legi de Químics de Catalunya’, REPSOL, Hoechst, Afora, Dow,

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