Catalysis Today 165 (2011) 1

Contents lists available at ScienceDirect

Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

Preface

This special issue of Catalysis Today was developed on the basis of the successful symposium on "Theory, Modeling and Simulation in Energy Production and Utilization" that we organized at the 239th ACS national meeting, held in March 21–25, 2010, in San Francisco. A significant number of presentations are related to catalysis, particularly, heterogeneous catalysis, due, in large part, to our background and expertise. We approached Dr. J. (Jerry) Spivey, the Associate Editor, at the meeting and expressed our interests in organizing a special issue for Catalysis Today. Dr. Spivey was very supportive and instructed us to submit a proposal. We selected "Theoretical Catalysis" as the theme and our proposal was promptly approved.

This special issue published 21 articles dealing with a range of topics in heterogeneous catalysis, including metal-catalyzed surface reactions, oxide and oxide-supported metal catalysts, as well as zeolite. Several papers deal with different aspects of electrocatalysis, reflecting its importance in developing more efficient catalysts for fuel cell application. Synergy between different components in bimetallic, even trimetallic, systems has been demonstrated in a number of cases. In addition to first-principles mechanistic studies, several papers reported results of integrating the information on elementary steps into kinetic models through kinetic Monte Carlo or mean-field based microkinetics. We hope the work in this special issue provides insights into specific catalysts or catalytic process in particular and demonstrates the importance and potential of theory and simulation in catalysis in general.

We would like to thank the authors who responded to our invitation and contributed to the special issue. We are also grateful to the outstanding reviewers who evaluated the manuscripts rigorously and made sure the accepted papers compatible with the high quality of Catalysis Today. Several papers had to go through iterations of revision and reviewing. The guidance and help that Dr. Spivey provided throughout the process are greatly appreciated. Finally, we would express our appreciation to Mary Harty and her team at Elsevier for their professional services.

Managing Guest Editor
Qingfeng Ge*
Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, IL 62901, USA

Guest Editor
Jian-guo Wang
Institute of Industrial Catalysis, College of Chemical Engineering and Materials Science, Zhejiang University of Technology, Hangzhou 310032, China

Guest Editor
Jun Li
Department of Chemistry, Tsinghua University, Beijing 100084, China

* Corresponding author. Tel.: +1 618 453 6406; fax: +1 618 453 6476.
E-mail addresses: qge@chem.siu.edu (Q. Ge), jgw@zjut.edu.cn (J.-g. Wang), junli@tsinghua.edu.cn (J. Li)

Available online 9 April 2011

doi:10.1016/j.cattod.2011.03.001