SCIENCE CHINA
Chemistry

• EDITORIAL •
• SPECIAL TOPIC • Heterogeneous catalysis theory

April 2015 Vol.58 No.4: 551–552
doi: 10.1007/s11426-015-5371-4

Preface

Science generally proceeds based on a mutual interaction between theory and experiment: theory can explain experimental phenomena and propose general rules for the design of new experiments while experiment can verify theoretical predictions and discover new phenomena to improve theories. Yet, the progress of heterogeneous catalysis mainly relied on experimental advances for a long time. In its early days, heterogeneous catalysis was an empirically applied field, in which the tests of reactivity and selectivity for synthetic catalysts were based largely on a trial-and-error approach. With the development of heterogeneous catalysis, a more rational approach to catalyst design was desirable. Various novel techniques of spectroscopic characterization were used to understand the catalytic processes at the microscopic or submicroscopic scales. In recent decades, the rapid increase of computer power and the development of robust and efficient numerical algorithms have made computer simulations an emerging technology to understand the underlying mechanisms of complex catalytic reactions. In particular, first-principle calculations in the framework of density functional theory have significantly improved our understanding of the catalytic reactions and of the spectroscopy of intermediates on the solid catalyst surface at the electronic and atomistic levels. More importantly, this makes rational catalyst design possible. In addition, the rapid development of theoretical treatment has recently made the computer simulation technology accessible to the field of more complex electro- and photo-catalysis involving the simulations of electrode potential and solid–liquid interfaces.

Theoretical catalysis is becoming an important component of the field of catalysis. In this special topic, various areas, ranging from heterogeneous catalysis to electro- and photo-catalysis along with those reactions that are catalyzed by metal, metal-oxide, or their combinations are covered. Herein, understandings of catalytic activity from the electronic structures of catalysts, especially the synergies between different components, are underlined and the general implications for catalyst design are discussed. Several articles explore the different aspects of electrocatalysis including electrochemical reactions in fuel cells and CO_2-electroreduction. The challenges to the theoretical treatments of the electrode potential and the description of free energy at solid–liquid interface are discussed. In addition, several articles investigated and compared photo-induced reaction pathways to heterogeneous catalysis with the same reactants and catalyst materials.

We are grateful to all the authors, Shengli Chen, Zhao-Xu Chen, Hongjun Fan, Qingfeng Ge, Xue-Qing Gong, P. Hu, Deyin Wu, Jinlong Yang and their co-workers, for their high-quality contribution to this special topic. We sincerely appreciate the splendid work for this special topic from Drs. Li Fu and Junjian Xu and their editorial and publication team. We hope that this special topic will provide a valuable reference for the current progress of theoretical studies in heterogeneous catalysis and inspire the advance of this research field in China.

P. Hu
East China University of Science and Technology
Zhipan Liu
Fudan University
2015-2-17

Professor Peijun Hu graduated from East China University of Science and Technology with a Bachelor's degree in 1982 and a Master's degree in 1985. Then he went to University of Cambridge, studying surface science and catalysis under the supervision of Sir David King, and received his Ph.D. in 1993. From 1993 to 1995, he did post-doctoral research under the supervision of Sir David King and Professor Mike Payne in Cambridge. In 1995, he joined Queen's University, Belfast, as a lecturer and was subsequently promoted to be Reader in 2001 and to be Chair Professor in 2004. In 2009, he was elected to be a member of Royal Irish Academy. His main research area is heterogeneous catalysis and he has published more than 160 papers, including 2 papers in *Nature*, 2 in *Nat. Commun.*, 16 in *J. Am. Chem. Soc.*, 5 in *Angew. Chem. Int. Ed.*, and 4 in *Phys. Rev. Lett.*

Professor Zhipan Liu received his Bachelor's and Master's degrees at Shanghai Jiao Tong University (1993–2000), and Ph.D. (2000–2003) at Queen's University, Belfast. He did post-doctoral research (2003–2005) at University of Cambridge. He has been a Full Professor in the Department of Chemistry, Fudan University, since 2005. He has been awarded a number of prestigious awards, including IUPAC Prize for Young Chemists (2004), National Science Fund for Distinguished Young Scholars (2009), and Changjiang Scholar of Ministry of Eductation. His major research interests include: (i) Theoretical Surface Science; (ii) First-principles Reaction Dynamics; (iii) Heterogeneous and Biological Catalysis; (iv) Electronic Structure calculations. He has published more than 100 scientific papers since 2001, including 19 papers in *J. Am. Chem. Soc*., 5 papers in *Phys. Rev. Lett.*, and 1 in *Angew. Chem.* The published papers have been cited over 3800 times.