北京大学量子材料科学中心

International Center for Quantum Materials, PKU

中心系列讲座 ICQM Weekly Seminar Series

Chemical Reactions on Nano-Particle and Metal/Oxide Interface

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Time: 4:00pm,Apr. 17, 2012 (Tuesday)

时间: 2012年4月17日（周二）下午4:00

Venue: Conference Room A (607), No. 5 Science Building

地点: 理科五号楼607会议室

Abstract

Chemical reactions catalyzed by metal nanoparticles dispersed typically on oxide supports are fundamental and yet important process in energy conversion and production of the chemicals. Among others, size of the metal nanoparticles and interface between metal and oxide are crucial, and will be addressed by density functional theory calculations in this talk. I will discuss the size effect on the electronic properties, morphology and stability of the metal nanoparticles as well as the influence on the chemical reactions. A generic metal-cation ensemble at the metal and oxide interfaces as the active site for the chemical reactions will be illustrated. I will highlight how the insights from theoretical simulation could be used to rationalize the design of the materials with better chemical activity.

Reference:

1.Q. Fu, W. X. Li, X. H. Bao et al, Science (2010) 328, 1141
2.X. G. Ku, W. X. Li et al, ChemSusChem (2012), doi: 10.1002/cssc.201100525
3.D. P. Sun, W. X. Li et al, J. Phys. Chem. C (2012), doi: 10.1021/jp300924k

About the Speaker

Prof. Wei-Xue Li studied physics at Wuhan University and received his PhD **from** Institute of Mechanics, CAS in 1998. From 1999 to 2004, he worked as a postdoctoral in Fritz-Haber Institute MPG (Berlin) and Aarhus University (Denmark). In July 2004, he was awarded “CAS Hundred Talent” and joined State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics (CAS). Since then, he heads the Theoretical Catalysis Group at Dalian and MPG-CAS Partner Group associated with Fritz-Haber Institute. His research interests focus on computational simulation of catalytic reactions on heterogeneous surfaces, in particular nanoparticles and metal/oxide interfaces.