COMPUTATIONAL CHEMISTRY  
BI-WEEKLY SEMINAR SERIES  

TOPIC: Theoretical Studies on Biochemical Cycle of Nitrogen Catalyzed by Transition-Metal Complexes and Metalloenzymes  

SPEAKER: Hujun Xie, Zhejiang Gongshang University  

TIME: 2:00-2:45, May 7, 2015  

VENUE: Room 152, Geography Building, 3663 Zhongshan Road North, Shanghai (中山北路校区，地理楼152室)  

ABSTRACT OF THE TALK  

The nitrogen cycle in nature is one of the basic material cycles in the biosphere. It is related to the atmospheric nitrogen into the soil via microorganisms used by animals and plants, and finally returns to the atmosphere via microorganisms. The nitrogen cycle in terrestrial ecosystems includes the synthesis of organic nitrogen, ammonification, nitrification, denitrification and nitrogen fixation. In each aspect, one or more metalloenzymes are involved in catalytic reduction and oxidation reactions. Dr. Xie’s research focuses on the application of state-of-the-art theoretical techniques to elucidate the structure, bonding, reaction mechanisms and origins of various selectivities of organometallic reactions including the biological, inorganic and organometallic areas. In this talk, Dr. Xie will report the biochemical cycle of nitrogen catalyzed by transition-metal complexes and metalloenzymes, consisting of nitrogenase, nitrate reductase, nitrous oxide reductase etc.  

BIOGRAPHY  

Hujun Xie is Associate Professor of Department of Applied Chemistry at Zhejiang Gongshang University. He received his B.S. (2004) from Zhejiang University and Ph.D. (2009) from Xiamen University. He pursued the postdoctoral work in Zhejiang University and The Hong Kong University of Science and Technology from 2010 to 2014. His research involves the application of "state-of-the-art" theoretical techniques to elucidate the structure, bonding, reaction mechanisms and origins of various selectivities of organometallic reactions including the biological, inorganic and organometallic areas.