

UNL Department of Chemistry & Co-sponsored by NCMN
PIM Divisional Seminar

February 15, 2016 @ 4:00 p.m.
Rm 548 Hamilton Hall

**Computational Nanocatalysis: From Single Atoms to Isolated
Bimetallic Clusters**

Dr. Jun Li

Department of Chemistry, Tsinghua University, Beijing 100084, China and the Environmental Molecular Sciences
Laboratory, Pacific Northwest National Laboratory, Richland WA 99352



Nanocatalysis is a key frontier in heterogeneous catalysis due to rapid development of synthesis and characterization of nanosized materials. Singly dispersed atoms anchored on the surface of metal oxides have been shown to have robust stability and significant catalytic activities [1]. Currently extensive experimental and theoretical studies have been carried out on single-atom catalysts (SAC) [2] as well as dynamically formed single-atom sites [3]. We also found that isolated bimetallic sites show high selectivity toward complete conversion of NO and CO to N₂ and CO₂ on cobalt oxides [4]. In this talk, I will provide an overview of the computational studies relevant to SACs using density functional theory (DFT). The special stability and catalytic activity of selected SACs involving Pt₁/FeO_x, Au₁/TiO_{2-x}, Au₁/CeO_{2-x}, and Rh₁Co₃/CoO_{1-x} bimetallics will be explained on the basis of electronic structures and metal-support covalent chemical bonding. The features of SACs and isolated bimetallic sites will be discussed based on extensive surface chemical bonding analysis.

References

- [1] B.-T. Qiao, A.-Q. Wang, X.-F. Yang, L. F. Allard, Z. Jiang, Y.-T. Cui, J.-Y. Liu, J. Li, T. Zhang, "Single-Atom Catalysis of CO Oxidation Using Pt₁/FeO_x", *Nature Chem.*, 2011, 3(8), 634–641.
- [2] X.-F. Yang, A.-Q. Wang, B.-T. Qiao, J. Li, J.-Y. Liu, T. Zhang, "Single-Atom Catalysts: A New Frontier in Heterogeneous Catalysis", *Acc. Chem. Res.*, 2013, 46(8), 1740-1748.
- [3] Y.-G. Wang, D.-H. Mei, V.-A. Glezakon, J. Li, R. Rousseau, "Dynamic Formation of Single-Atom Catalytic Active Sites on Ceria-Supported Gold Nanoparticles", *Nature Commun.*, 2015, 6, 6511.
- [4] S.-R. Zhang, L. Nguyen, J.-X. Liang, J.-J. Shan, J.-Y. Liu, A. I. Frenkel, A. Patlolla, W.-X. Huang, J. Li, F. Tao, "Catalysis on Singly Dispersed Bimetallic Sites", *Nature Commun.*, 2015, 6, 7938.