

CBC SEMINAR ANNOUNCEMENT



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Solid-Liquid Interface Photo-Electrochemical Catalysis From First Principles

In this talk, I will give a short review on theoretical progress on catalysis and present our recent results in understanding solid-liquid interface catalysis [1-4]. Methodologically, we developed a periodic continuum solvation model based on the modified-Poisson-Boltzmann equation within the periodic DFT slab framework, which is designed for studying complex catalytic reactions at the solid-liquid reactions under the influence of electrochemical potentials, surface charges and solution [3,4]. Using the approach, we investigated water oxidation on RuO₂ surface and oxygen reduction on Pt surface, and calculated Tafel kinetics quantitatively. We show that the elementary electrocatalytic reactions on surface can be classified into two general classes according to their redox properties, whose activity exhibits distinct potential dependence. Our approach has also been utilized to investigate some other catalytic reactions on nanoparticles in aqueous surroundings [1,2].

References

- 1) Li, Y.-F.; Liu, Z.-P.* "Particle Size, Shape and Activity for Photocatalysis on Titania Anatase Nanoparticles in Aqueous Surroundings", J. Am. Chem. Soc. 2011, 133,15743
- 2) Shang, C.; Liu, Z.-P.* "Origin and Activity of Gold Nanoparticle as Aerobic Oxidation Catalyst in Aqueous Solution" J. Am. Chem. Soc. 2011, 133,9938
- 3) Fang, Y.-H.; Liu, Z.-P.* "Mechanism and Tafel Lines of Electro-oxidation of Water to Oxygen on RuO₂(110)", J. Am. Chem. Soc. 2010, 132, 18214
- 4) Li, Y.-F.; Liu, Z.-P.*; Liu, L.;Gao, W. "Mechanism and Activity of Photocatalytic Oxygen Evolution on Titania Anatase in Aqueous Surroundings", J. Am. Chem. Soc. 2010, 132, 13008

Date:	27th July 2012 (Friday)
Time:	11:00am – 12:30pm
Venue:	NTU SPMS CBC Building Level 2, Conference Room
Host:	Assoc Professor Chen Hongyu