Joint CQSE and CASTS Seminar

Weekly Seminar
Jun. 1, 2012 (Friday)

TIME Jun. 1, 14:30 ~ 15:30
TITLE Theoretical Study of Ammonia Oxidation on RuO2(110) Surfaces: Mechanism and Microkinetics
SPEAKER Prof. Jyh-Chiang Jiang
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Previous ammonia oxidation studies reported ca. 100% NO selectivity and the absence of N_2O on RuO_2(110) in ultrahigh vacuum (UHV) at 530 K, $p(NH_3) = 10^{-7}$ mbar, and $O_2/NH_3 = 20$ (Wang, Y.; Jacobi, K.; Schone, W.-D.; Ertl, G. *J. Phys. Chem. B* **2005**, *109*, 7883). Differently, the steady-state and transient experiments over polycrystalline RuO_2 at ambient pressure reveal that N_2 is the predominant product. The NO selectivity was as low as 6% at $O_2/NH_3 = 2$ and reached a maximum of 65% at the highest temperature (773 K) and effective oxygen-to-ammonia ratio of 140, whereas the maximum N_2O selectivity was 25% at 100% NH_3 conversion. (Perez-Ramırez, J. et al. *J. Phys. Chem. C* **2010**, *114*, 1660). Such contradiction of product distribution stimulates us to carefully examine ammonia oxidation on RuO_2(110) combined with DFT calculations and microkinetic modeling.

In my presentation, I'll demonstrate the theoretical simulations of temperature programmed desorption (TPD) spectra of ammonia on RuO_2(110) surface, which is well agreeable to experimental observation by Wang et al (*J. Phys. Chem. B* **2005**, *109*, 7883). Then, I'll show the product distribution, based on our mirokinetic analysis combined with DFT calculation, at different temperature, pressure, and NH_3/O_2 ratios.

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