NRC主催／物理工学コース／談話会

平成27年12月15日（火）9:45 ～ 10:30

総合研究棟W棟 2階 W202 会議室

Abhishek Kumar Singh 助教授

Materials Research Centre, Indian Institute of Science, Bangalore

Bimetallic Catalyst: A solution to Pt-Poisoning-Free CO Oxidation

Late-transition-metal-doped Pt clusters are prevalent in CO oxidation catalysts, as they exhibit better catalytic activity than pure Pt, while reducing the effective cost and poisoning. However, completely eliminating the critical problem of Pt poisoning still poses a big challenge. Here we report for the first time that, among the bimetallic clusters ((Pt3M where M = Co, Ni, and Cu)/MgO(100)), the CO adsorption site inverts for Pt3Co/MgO(100) from Pt to Co, due to the complete uptake of Pt d-states by lattice oxygen. While this resolves the problem of Pt poisoning, good reaction kinetics are predicted through low barriers for Lanmuir-Hinshelwood and Mars van Krevelen (MvK) mechanisms of CO oxidation for Pt3Co/MgO(100) and Li-doped MgO(100), respectively. Li doping in MgO(100) compensates for the charge imbalance caused by a spontaneous oxygen vacancy formation. Pt3Co/Li-doped MgO(100) stands out as an exceptional CO oxidation catalyst, giving an MvK reaction barrier as low as 0.11 eV. We thereby propose a novel design strategy of d-band center inversion for CO oxidation catalysts with no Pt poisoning and excellent reaction kinetics. R. Ahmad and A. K. Singh, ACS Catalysis 5, 1826 (2015).

どなたでもお気軽にご参加ください

世話人：大野かおる（内4254）