A theory-guided design of catalysts for fuel cell application

Yasuyuki Ishikawa
Department of Chemistry, University of Puerto Rico
P.O. Box 23346 San Juan, PR 00931-3346 USA

Heterogeneous catalysts are typically based on nano-sized metal clusters. The dynamics of the nanocluster surface reactions depend on the properties of the cluster surface as well as those of the adsorbed reactants, intermediates and products. Systematic exploration of catalytic systems must be based on an understanding of the fundamental processes taking place on the nanocluster surfaces. Supported and unsupported metal clusters have received attention because they are finite systems that differ a great deal physically and chemically from bulk metals. Metal clusters exhibit pronounced variations in electronic and chemical properties as the number of metal atoms in the cluster is varied. Recent studies strongly indicate that size-selected metal clusters would exhibit much higher catalytic activity than bulk metals toward methanol oxidation. Thus, one key class of active catalysts for methanol oxidation may well be size-selected metal or bimetallic clusters. By varying cluster size, one can change electronic properties to adjust the chemistry of catalytic processes occurring on cluster surfaces. We address the problems of low catalytic activities and CO poisoning by first-principles based, theoretical examinations of the mechanism of dehydrogenation of methanol on pure Pt and mixed Pt-M metal particle catalysts.