

DFT study of the mechanism of water activation and CO
oxidation on bimetallic Pt-M nanoparticle catalysts for
fuel cell applications

Yasuyuki Ishikawa, Alejandro Perez and Marius J. Vilkas
Department of Chemistry, University of Puerto Rico
P.O. Box 23346 San Juan, PR 00931-3346 USA

Heterogeneous catalysts are typically based on nanoscale metal particles. Recent experimental studies strongly indicate that size-selected metal clusters would exhibit much higher catalytic activity than bulk metals toward methanol/hydrocarbon oxidation. Thus, one key class of active catalysts for methanol oxidation may well be size-selected metal or bimetallic nanoclusters. By varying cluster surface composition, one can change electronic properties to adjust the chemistry of catalytic processes occurring on nanocluster surfaces. We address the problems of low catalytic activities and CO poisoning by first-principles-based theoretical examinations of the mechanism of water activation and CO oxidation on Pt-M bimetallic alloy and sequentially deposited nanoparticle catalysts. We show specifically how the M sites in the alloy and sequentially deposited catalysts influence catalytic performance. These features can be manipulated towards the design of new nanoscale catalysts.