

ADSORPTION AND OXIDATION OF CO OVER Pt/Au CORE/SHELL STRUCTURED NANOPARTICLES: A FIRST PRINCIPLES STUDY

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The modification in reactivities of a metal catalyst by alloying with another metal has been widely explored in heterogeneous catalysis. The study of the mechanistic change during a reaction due to the alloying interaction is important to understand the behavior of the alloy catalyst. It has been shown recently that the gold-based PtAu alloy nanoparticles exhibit promising activity in the electrochemical oxidation of methanol and reduction of oxygen^a. The abundance and relative low cost of Au make the PtAu nanocatalysts ideal alternatives to the PtRu alloy catalysts.

Structures and energetics of PtAu clusters with different Pt/Au ratios have been studied using the density functional theory approach as implemented in VASP^b. The adsorption of CO on these nanoparticles have been studied and compared with that on the surface of a bulk PtAu alloy. C–O stretching frequencies for CO adsorption at different sites have been calculated. The results showed that both Pt and Au sites of the particles exhibit significant binding toward CO. Among all the sites explored, CO prefers Pt site that is adjacent to Au. These results are compared with CO adsorption on pure metal clusters as well as surfaces of bulk metals. Furthermore, the oxidation of CO over Pt/Au core/shell structured particles for 13- and 55-atom clusters have been studied and compared with that over the pure Au particles.

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^bG. Kresse and J. Hafner, *Phys. Rev. B*, **47**, 558 (1993); G. Kresse and J. Joubert, *ibid*, **59**, 1758 (1999)