Theoretical study of CO oxidation on nanoalloy Ag$_7$Au$_6$ cluster

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Abstract: Density Functional Theory (DFT) calculations of the mechanism of carbon monoxide (CO) oxidation by oxygen (O$_2$) on Ag$_7$Au$_6$ cluster were carried out with the Gaussian 09 program package using the Perdew–Burke–Ernzerhof (PBE) functional with mixed basis set such as TZVP and LandL2DZ basis set. The TZVP basis set was used for carbon, nitrogen, and oxygen atoms, and the LanL2DZ basis set was used for gold and silver atoms. Calculation results showed that the adsorption energies of the most stable configuration of CO, O$_2$ and CO$_2$ on the Ag$_7$Au$_6$ catalyst in the range of -0.12 to -1.99 eV that are in good agreement with previous works. The CO oxidation via coadsorption mechanism is the dominant reaction pathway with small rate determining step of 0.26 eV. The mechanism start with CO and O$_2$ adsorbed on Ag$_7$Au$_6$ cluster to form OOCO complex with energy barrier of 0.10 eV then follow by COO$^-$O dissociation to form CO$_2$ molecule and O-Ag$_7$Au$_6$ intermediate. Next, second CO molecule adsorbed on Ag$_7$Au$_6$ cluster to react with O-Ag$_7$Au$_6$ intermediate to release CO$_2$ molecule with energy barrier of 0.26 eV. The result indicated that Ag$_7$Au$_6$ cluster was a suitable catalyst for CO oxidation.

Keywords: Oxidation; DFT; Coadsorption mechanism