Hydrogen Atom Transfer in Coinage Metal Cluster Complexes: A Density Functional Theory Study

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Copper-based catalysts are used in chemical industries to convert carbon monoxide and water to carbon dioxide, hydrogen and methanol. Methanol and ethanol are two of the most common reaction intermediates and precursors in the synthesis, decomposition, and oxidation reactions involving hydrocarbons, such as the Fischer-Tropsch process. To understand the catalytic mechanism, the adsorption behaviours of methanol on copper, silver, and gold clusters have been investigated by infrared-photodissociation spectroscopy and theoretical calculations.

In this study, we examine the adsorption of ethanol onto small copper clusters, Cun, using density functional theory. Initially, a CH_3CH_2OH-Cu_n complex is formed and subsequently, there may be hydrogen atom transfer to form a $CH_3CH_2OCu_nH$ complex. We examine the energetics of this process for n=1-4 and, for comparison, we also examine the corresponding processes for (i) adsorption of methanol and water, and (ii) adsorption onto small silver and gold clusters. Additionally, the energetics of hydrogen atom transfer for charged clusters and small copper clusters alloyed with silver and gold, $Cu_xAg_yAu_z$, ($x + y + z <= 3$) were also examined. Equilibrium geometries and vibrational frequencies were obtained, as well as thermochemical values for the transfer of a hydrogen atom from oxygen to the metal atom.