COMPOSITION EFFECT OF BIMETALLIC PT/AU NANOPARTICLES ON THE ADSORBED CO VIBRATION FREQUENCY

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The CO virbational frequency shifts upon its adsorption on bimetallic Pt/Au clusters were studied using density functional theory (DFT) calculations. The CO molecule was adsorbed at different sites of a bimetalic Pt/Au cluster to determine the favorable adsorption site. Various Pt compositions of Pt/Au clusters were used to study the CO adsorption process. The DFT calculations have shown that the CO vibrational frequency was shifted from 2134 cm^{-1} of an isolated molecule to the range of 2000-2100 cm^{-1} after the adsorption to a Pt/Au cluster. In general, the redshift is larger when a CO molecule is adsorbed to a Pt atom in the cluster. Furthermore, the DFT results are supported by the new FTIR experimental measurement (C. J. Zhong, et al, private communication). Detailed comparison between the DFT results and the experimental date will be presented and discussed.