THE STRUCTURE EFFECT OF AU AND PT CLUSTERS ON THE VIBRATIONAL SPECTRA OF ADSORBED METHANE MOLECULES

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The adsorption of CH_4 molecules on different Au and Pt clusters was investigated using density functional theory calculations. The results show that the vibrational spectra of CH_4 depend strongly on the adsorption site and orientation of CH_4 as well as the structure of Au and Pt isomers. Our results also indicate a possible increase of the peak temperature with cluster size and the broadening of the spectra that could be observed in the temperature-programmed desorption experiment.