Role of Water on CO oxidation over Boron-Nitrogen sheet supported Gold Clusters (Au_9) - A First Principles study

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Carbon monoxide (CO) is a highly toxic gas for human because of its high affinity with hemoglobin, and it causes many illnesses, suffocation, and sudden death. Therefore, the elimination of CO is attracted practical importance to control the environment. In many processes, the catalytic oxidation of CO to CO_2 over a heterogeneous catalyst surface is the suitable method in CO elimination. Due to the groundbreaking work of Haruta et al., [1] the use of gold nanoparticles as a catalyst to oxidize CO to CO_2 has become an interesting topic. Previously, many theoretical and experimental studies have explored the catalytic activity of Au clusters on pure metals and metal oxide surfaces. [2] Here we considered Au_9 clusters supported on a boron-nitrogen sheet (BN) and investigated its catalytic activity towards CO oxidation using first-principles calculations. Furthermore, we also explored the effect of water on the CO oxidation on Au clusters supported on the boron-nitrogen sheet. Our results indicate that Au_9 cluster is stably adsorbed on BN surface and the catalytic activity of Au_9 cluster is enhanced through electron transfer from BN to Au_9 cluster. We found that the stretching vibration of adsorbed CO on Au_9BN surface is blue-shifted with the increase of water content, which is in agreement with the previous experimental observation. [3] By exploring all possible CO oxidation pathways, we found that in presence with water on the Au_9BN surface, the reaction barrier of rate determining step of CO oxidation is only 0.40eV, which is significantly lower than the previously studies. Our calculated results suggest that Au_9 clusters supported on BN surface could be a promising catalyst for CO oxidation at low-temperature conditions.

References

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