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DFT Study Of CO_2 Adsorption On Ni_4M (M=Sc, and Y) Nano-Cluster

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ABSTRACT

In his project adsorption of carbon dioxide with different orientations on Ni_4M (M=Sc, and Y) clusters have been investigated. The adsorption energies for three different orientations of Ni4Sc-CO_2 are predicted to be 45.52, 32.03 and 11.04 Kcal/mol, while for Ni_4Y-CO_2 cluster, are in the order of 35.46, 10.03 and 14.83 Kcal/mol. Also, results show that the CO_2 molecule has the higher tendency to interact with Sc atoms of the cluster rather than Y atom. The maximum and minimum activation energy in Ni4Sc-CO_2 clusters are +22.19 and +4.27 (Kcal. mol^{-1}) respectively and the maximum and minimum activation energy in Ni4Y-CO_2 clusters are +20.12 and +5.16 (Kcal. mol^{-1}) respectively. Results of Thermodynamic investigation of CO_2 adsorption shows that, for all of the orientations of two metallic clusters, the adsorption process is exothermic.

Keywords: DFT, CO_2 Adsorption, Interaction Energy, Metallic Cluster, Reaction Mechanism

1-Introduction

Carbon dioxide (CO_2) is mainly the results of human activities such as deforestation and the burning of various fossil fuels for power generation and transport use and chemical processing. Atmospheric carbon dioxide also derives from multiple natural sources including volcanic outgassing, the combustion of organic matter, and the respiration processes of living aerobic organisms and have greenhouse effect that responsible for the global warming and changing the climate. Many researchers have been don a strong effort to transform CO_2 molecule into the more reactive species such as oxalic acid, and also artificial Photosynthesis, i.e. the renovation of carbon dioxide into carbohydrates by solar energy.
Adsorption of small molecules such as O_2, CO_2, NO, CO on pure copper [1], sodium [2], gold [3-6], platinum [7] palladium [8], and tin has been studied theoretically and experimentally by several researchers. However, it has been shown that the special selection of the alloy combination by the different composition of different metallic clusters gives a higher catalytic activity than pure metallic clusters. For example, in yttrium-doped gold clusters, the adsorption energy of CO molecules on gold clusters is reduced, but doping of the vanadium atom in the pure gold cluster increases CO adsorption [9]. Kumar Das et. al investigated the adsorption of CO and O_2 molecules on pure and bimetallic Sn_mGe_n ($m+n \leq 5$) clusters [10, 11]. They found that the addition of Sn atoms leads to the poisoning clusters, but the addition of Ge atoms promotes the adsorption of the CO molecule. In addition, donation and back donation of electron happened between the metallic cluster and CO molecule.
CO_2 capture ability investigations by a metallic, metal oxide and metal-rich minerals have been done by many research groups [12]. for example Nguyen et. al. investigate the CO_2 capture ability of doubly rhodium doped boron clusters Rh_2B_{18} and showed that this cluster can capture and cleaving of C-O bond of carbon dioxide. Although adsorption of CO_2 molecule on pure and bimetallic clusters have been the subject of a number of investigations, few of them have been focused on the first raw of transition metals. In my previews study, DFT Study of CO and NO Adsorption on Boron Nitride $(BN)_{n=3-5}$ is done[13]. This work aims at investigating the adsorption of CO_2 molecule on the bimetallic first raw transition metal Ni_4M (M= Sc, and Y) nanoclusters and broken mechanism of CO_2 based on chemical kinetics.

2- Computational Details