عنوان مقاله:

DFT Study Of CO2 Adsorption On Ni4M (M=Sc, and Y) Nano-Cluster

محل انتشار:

پنجمین کنفرانس ملی پژوهش های نوین در شیمی و مهندسی شیمی (سال: 1397)

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خلاصه مقاله:

In his project adsorption of carbon dioxide with different orientations on Ni4M (M=Sc, and Y) clusters have been investigated. The adsorption energies for three different orientations of Ni4Sc-CO2 are predicted to be 45.52, 32.03 and 11.04 Kcal/mol, while for Ni4Y-CO2 cluster, are in the order of 35.46, 10.03 and 14.83 Kcal/mol. Also, results show that the CO2 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-CO2 clusters are +22.19 and +4.27 (Kcal. mol-1) respectively and the maximum and minimum activation energy in Ni4Y-CO2 clusters are +20.12 and +5.16 (Kcal. mol-1) respectively. Results of Thermodynamic investigation of CO2 adsorption shows that, for all of the orientations of two metallic clusters, the adsorption process is exothermic

کلمات کلیدی:

DFT, CO2 Adsorption, Interaction Energy, Metallic Cluster, Reaction Mechanism