INTISARI

KAJIAN INTERAKSI MOLEKUL CO DENGAN KLUSTER ATOM NIKEL MENGGUNAKAN METODE *DENSITY FUNCTIONAL THEORY* (DFT)

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Kajian interaksi gas CO pada kluster atom nikel dengan metode *Density Functional Theory* (DFT) telah dilakukan. Metode komputasi DFT dengan variasi fungsi densitas digunakan untuk menentukan model kluster nikel terstabil dari kristal Ni fcc (111). Pengamatan interaksi kluster nikel dengan satu molekul CO dan CO_2, interaksi penutupan permukaan (*coverage*) molekul CO pada kluster nikel, dan dilakukan juga pengamatan spektra vibrasi IR *stretching* ikatan C-O struktur kompleks nikel-karbonil.

Model kluster nikel terbaik yang ditentukan dengan optimasi geometri dengan metode DFT/B3LYP/LANL2DZ ECP adalah struktur kluster Ni_4. Kluster Ni_4 bersifat lebih selektif terhadap molekul CO daripada molekul CO_2 dengan urutan preferensi pengikatan ligan CO oleh kluster Ni_4 yaitu *hollow>bridge>on-top* sedangkan urutan preferensi pengikatan ligan CO_2 oleh kluster Ni_4 yaitu *hollow> on-top>bridge*. Kluster Ni_4 mengikat ligan CO dengan kuat ikatan ligan-kluster per jumlah ligan terbesar pada keadaan *low coverage*, dengan θ sebesar 0,33 dan nilai kuat ikatan per jumlah ligan CO sebesar -47,991 kkal/mol. Pengikatan ligan CO oleh kluster Ni_4 mengakibatkan *red shift* pada frekuensi serapan vibrasi IR *stretching* ikatan C≡O terhadap frekuensi serapan vibrasi IR molekul bebas.

Kata Kunci: Kluster Ni, Nikel-Karbonil Interaksi Penutupan Permukaan, DFT/B3LYP/LANL2DZ ECP

ABSTRACT

INTERACTION STUDY OF CO MOLECULES WITH NICKEL CLUSTERS USING DENSITY FUNCTIONAL THEORY (DFT) METHOD

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A theoretical study of the interaction of CO molecules on nickel atom cluster with the *density functional theory* (DFT) has been carried out. The DFT computational method with six variation of density functions were used to perform computational calculation on the determination of the most stable cluster model of nickel from Ni fcc crystals. Investigation of the interaction between nickel cluster and one CO and CO_2 molecule, and the surface enclosure by the CO ligands (*coverage interaction*), and the observation of IR vibration spectrum of CO bond stretching from the structure of nickel-carbonyl complexes also has been performed.

The best cluster model of nickel determined by geometry optimization using the DFT/B3LYP/LANL2DZ ECP method was the structure of Ni_4 cluster. Ni_4 cluster shown a selectivity toward CO than CO_2 molecules, with the preferred order of CO ligand binding position on Ni_4 cluster is *hollow>bridge>on-top*, meanwhile the preferred order of CO_2 ligand binding position on the same cluster is *hollow> bridge >on-top*. Ni_4 cluster bind the CO ligands with the strongest bond energy per ligand quantity at *low coverage* condition, with the θ value of 0.33 and the bond energy per ligand quantity of -47,991 kcal/mole. The binding of CO ligands by Ni_4 cluster has resulted in a *red shift* at the adsorbed frequency of IR *stretching* vibration of the C≡O bond compared to the adsorbed frequency of IR vibration from a free CO molecule.

Keywords: Ni Clusters, Nickel-Carbonyl, Surface Coverage Interaction, DFT/B3LYP/LANL2DZ ECP