عنوان مقاله:

(CO Oxidation on Pt(001) , Pd(001) and Rh(001) surfaces the Density Functional Theory Study(DFT

محل انتشار:

همایش منطقه ای شیمی (سال: 1389)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Oxidation of Carbon Monoxide on Pt (001) , Pd (001) and Rh (001) surfaces is studied using Ab initio calculations with Density Functional Theory (DFT).The aim of this study is the catalytic oxidation of CO to CO2 on an oxygen procoverd Pt (001), Pd (001) and Rh (001) surfaces. The interaction between CO and O on metals surfaces are an important issue in CO oxidation and also is promotion and poisoning effects of catalysis. We disscused on M-O and M-CO bonding. The results are breaking of an O-metal bond to the formation of a CO2 molecule [1].Density Functional Theory (DFT calculations show that the carbon monoxide is performed on the top site of Pt (001) , Pd (001) and Rh (001) . The Langmuir-Hinahelwood mechanism have been proposed for catalytic reactions [2]. Also ,we investigate the transition state (TS). All calculations were made using Gaussian 03. Optimized geometric were determind at Density Functional Theory (DFT) with B3lyp .We used 6-31G (d) basis set for CO and O ,located are top site on metals surfaces ,and Lanl2DZ basis set for Pt , Pd and Rh .At final ,we calculated the transition state (TS) using scan program in the structure offered.

کلمات کلیدی:

.(COoxidation, Lanl2DZ basis set, Langmuir-Hinshelwood mechanism, DFT theory, Transition State(TS

لینک ثابت مقاله در پایگاه سیویلیکا: