عنوان مقاله:
Study of Ethylene Adsorption on Pd

محل انتشار:
یازدهمین کنگره ملی مهندسی شیمی ایران (سال: 1385)

تعداد صفحات اصل مقاله: 12

نویسندگان:
Alireza Jalilazar - *Tarbiat Modarres University*

Hamid Mehdizadeh - *Tarbiat Modarres University*

Mehrdad Manteghian - *Tarbiat Modarres University*

Susan Khosroyar - *Islamic Azad University*

خلاصه مقاله:
In this paper, the effect of different parameters on the ethylene adsorption on Pd surfaces has been studied. The focus is on Pd (111) surface, because it is the most stable site, but Pd (100) and Pd (110) are included for completeness. Fully optimized geometries and adsorption energies obtained from nonlocal density functional calculations are presented for Pdn(C2H4) (n =1-6) clusters. The adsorption mode can be π or di- σ according to the cluster size. The di- σ adsorption mode is characterized by a strong distortion for both the ethylene and the metal cluster. The potential energy surfaces for the C-H activation show that the d10 configuration of palladium is suitable for the formation of the π molecular complexes, whereas the d9s1 configuration is suitable for the formation of the σ bonds of the vinylhydride products. This work demonstrates how the nature and bond strength of the surface species formed on the adsorption of ethylene on Pd may be altered by using modifiers.

کلمات کلیدی:
(Ethylene, Adsorption, Palladium (Pd