## عنوان مقاله:

Theoretical Investigation of Hydrogen Adsorption on Ultra-Small Carbon Nanotubes


## محل انتشار:

سومین همایش پیل سوختی ایران (سال: 1388)

تعداد صفحات اصل مقاله: 5



## نویسندگان:

A. Zolfaghari - *Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran*

P. Pourhosseina - *Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran*

K. Nasiri Avanaki - *Shahid Rajaee Teacher Training University, Tehran, Iran*

H. Zolfaghari Jooyaa - *Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran*



## خلاصه مقاله:

The hydrogen adsorption on the surface of ultra small radius (3,0) was investigated. The structural and electronic changes due to physical and chemical adsorption were studied by density functional theory based calculations. The initial adsorptive orientation of hydrogen molecules with respect to the nanotube surface was obtained by the realistic molecular dynamics simulations. The resulted stable configuration was considered as the starting point for the rest electronic analysis. The total energies, atomic charges, and energy band gaps were calculated at three states, namely the pristine, physisorbed and hydrogenated (3,0) single walled carbon nanotube. The higher chemisorbed energy, in comparison with the general larger diameter carbon nanotubes, was attributed to the strong curvature effect of this ultra narrow nanotube. Both band structure and molecular orbital analysis clearly showed that chemisorption makes .the nanotube conducting along the tube axis



## کلمات کلیدی:

Ultra small nanotube; Hydrogen adsorption; MD simulations; DFT