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عنوان مقاله:

Quantum Mechanical Calculations On Absorption Of CH4 By Carbon Nanotube

محل انتشار:

اولین کنفرانس ملی علوم و فناوری نانو (سال: 1389)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

The results concerning an investigation employing the ab initio molecular orbital (MO) and Hartree-Fock (HF) methods to calculate structural optimization and the major stabilizing orbital interactions in nanotube and methane were evaluated by Natural Bond Oribital (NBO) methodology .Based on the optimized ground state geometries using HF/3-21G* method, the NBO analysis of donor-acceptor (bond- antibond) interactions revealed that the stabilization energies associated with the electronic delocalization.

کلمات کلیدی:

molecular orbital (MO), Hartree-Fock (HF), Natural Bond Oribital (NBO

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