عنوان مقاله:

Density Functional Study of the Effect of Diameter and Chirality on the Electronic Properties of Pure Single Walled Carbon Nanotubes

محل انتشار:

دومین کنگره بین المللی علوم و فناوری نانو (سال: 1387)

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خلاصه مقاله:

In the recent years, carbon nanotubes are receiving much attention due to their remarkable physical and electronic properties [1]. While there have been numerous investigations on the interactive properties of single-walled carbon nanotubes (SWNTs), there are very few reports describing the electronic properties of pure nanotubes. It is believed that a carbon nanotube may be considered as a single graphite sheet rolled up into a cylinder [2]. Although a graphite sheet itself is chemically inert, the rolling produces strains on the curved surface, which induces πσ– hybridization. Therefore, generally different interactive properties of SWNTs are explained by sp2-sp3 hybridization transformation [3,4]. It is expected that different properties of atomic oribitals such as energy, occupation, and their role in hybridization, as well as the total charge density, are affected by the curvature and chirality of SWNTs. This is our motivation for studying the electronic properties of the atomic orbitals of SWNTs

کلمات کلیدی: