عنوان مقاله:

Carbon Nanotubes Functionalized by Li, Na and K atoms: A Density-Functional Study

محل انتشار:

همایش ملی نانو فناوری و شیمی سبز (سال: 1391)

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خلاصه مقاله:

Carbon nanotubes functionalized by metals have great potential for applications in hydrogen storage, chemical sensors, and nanodevices. In this article, we report the study of the adsorption of three alkaline metal atoms on carbon nanotubes using density functional theory calculations. A detailed comparison of the binding energies, equilibrium positions, Mulliken charges has been performed for three metal doped carbon nanotubes. Binding energies of metal doped carbon nanotubes indicate that these structures are stable and show site dependence. We found that K has the most binding energy with Carbon nanotubes. The results indicate that the charge transfer occurs .from metal to Carbon nanotubes and K has the most atomic charge

کلمات کلیدی:

Functionalization; Doping; Density Functional Theory; Carbon Nanotube; K, Na, Li