عنوان مقاله:

Electronic and transport properties of Beryllium-intercalated zig-zag carbon nanotube

محل انتشار:

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خلاصه مقاله:

In this paper, the electronic and transport properties of carbon nanotubes intercalated with beryllium atomhave been investigated using density functional theory combined with non-equilibrium Green's functionformalisms by SIESTA software for use in carbon nanotube based electronic devices. The band structure,density of states and transport spectra of carbon nanotubes intercalated with beryllium atom were calculated toconfirm the higher metallic properties of this structure. the study of the device mode platform showed theenhancement of current and effective conductance as a result of the structural change due to the intercalationof Be atom in the pure structure. Finally, the under study model is proposed for the design of ultra-fast devicesbased on carbon nanotubes

کلمات کلیدی:

Carbon Nanotube, Density Functional Theory, Transport, Ultrafast Electronic Devices, SIESTA Software :

لینک ثابت مقاله در پایگاه سیویلیکا: