

## عنوان مقاله:

The Atomic Charge and Magnetic Shielding Relationship in (5,0) zigzag Carbon Nanotube with and without Potassium doping

## محل انتشار:

دومین همایش ملی پژوهش های کاربردی در علوم شیمی، زیست شناسی و زمین شناسی (سال: 1393)

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## خلاصه مقاله:

In this study, the relationship between isotropic shielding and atomic charge (with Mulliken, NBO, QTAIM) in (5,0) zigzag single walled carbon nanotube (SWCNT) with potassium doping and without potassium doping using Density Functional Theory (DFT) based on Periodic Boundary Condition (PBC) approach are investigated. When in (5,0) zigzag SWCNT, the relationship between the  $^{13}\text{C}$  isotropic shielding and the atomic charge by Mulliken, Natural Bond Orbital (NBO) and Quantum Theory of Atoms In Molecules (QTAIM) at the PBEPBE/6-31G(d) level of calculations being studied, It is clear that there are linear relationship between  $^{13}\text{C}$  chemical shielding and atomic charge in carbon nanotube without potassium doping and there are nonlinear relationship between  $^{13}\text{C}$  chemical shielding and atomic charge in carbon nanotube with potassium doping.

## کلمات کلیدی:

Magnetic shielding, Atomic charge, Mulliken, QTAIM, NBO, PBC

## لینک ثابت مقاله در پایگاه سیویلیکا:

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