International Journal of New Chemistry, 2015, 2(6), 213-222
Published online January 2015 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X

Open Access

A DFT study of the nuclear magnetic properties of fullerenes

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Received 30March 2015; Accepted 20 April 2015; Published 20 April 2015

Abstract

The stable configurations, electronic structure and magnetic properties of $B_{16}N_{16}$, B_8C_{24}, Al and P inserted $(BC_3)_8$ was studied by performing density functional theory (DFT) calculations of the NMR parameters. The results indicate that B_8C_{24} has semiconductivity property and be effectively modified by inserting groups due to the introduction of certain impurity states within the band gap of the pristine nanostructure, thereby reducing the band gaps. The band gap B_8C_{24} cage is reduced from 2.18 eV to 1.96 (for Al-inserted) and 1.76 eV (for P-inserted), respectively. The calculation of chemical shielding (CS) tensors shown that the B_8C_{24} inserted with Al and P atoms possess a C_{3v} local symmetry with special chemical shifts patterns. Theoretical analyses by molecular orbital under C_{3v} symmetry explain the impurity energy levels and chemical sheilding tensors.The present results are expected to open a way to change the electronic and magnetic properties of studied nanocages, which is helpful to design or develop novel nanodevices based on these structures.

Keywords: $B_{16}N_{16}$, B_8C_{24}, AlB_7C_{24}, $B_7C_{24}P$, Fullerene, Density Functional Theory