عنوان مقاله:

A DFT study of the nuclear magnetic properties of fullerenes

محل انتشار:

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خلاصه مقاله:

The stable configurations, electronic structure and magnetic properties of B16N16, B8C24, Al and P inserted (BC3)8 was studied by performing density functional theory (DFT) calculations of the NMR parameters. The results indicate that B8C24 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 B8C24 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 B8C24 inserted with Al and P atoms possess a C3v local symmetry with special chemical shifts patterns. Theoretical analyses by molecular orbital under C3v 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

کلمات کلیدی:

B16N16, B8C24, AlB7C24, B7C24P, Fullerene, Density Functional Theory

لینک ثابت مقاله در پایگاه سیویلیکا: