

The relationships between atomic charges and magnetic response properties reflects conductivity of BN nanotubes

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Abstract

In this work, the potential relation between magnetic response properties (isotropic shielding (σ_{iso}) and total atomic magnetizabilities, $X(\Omega)$) with QTAIM atomic charges of boron and nitrogen atoms in (4,4), (5,3) and (7,0) single-walled boron nitride nanotubes (SWBNNTs) are investigated at DFT B3LYP/ 6-31G(d) level of theory using periodic boundary condition (PBC) approach. The results show that a liner correlation exists between atomic charges of B and N in (4,4) and (5,3) BNNTs and the isotropic shielding. The results show a solid correlation between chemical shielding and total-atomic magnetizabilities, $X(\Omega)$ in (4,4) BNNT with the lowest conductivity.