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Non-covalent green functionalization of Boron Nitride Nanotubes with Tunable aryl alkyl Ionic Liquids: A Quantum Chemical Approach

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Abstract

The quantum mechanical treatments of the non-covalent interactions of the (8,0) zigzag single-walled boron nitride nanotube (BNNT) with the five types tunable aryl alkyl ionic liquids (TAAILs) as well as corresponding cations were carried out at the M06-2X/6-31+G(d):PM6 level of theory to better understand the trends in interaction between BNNT and ILs. Two different complexes (\mathbf{A}_{\parallel} and \mathbf{B}_{\perp}) were found in non-covalent interaction between BNNT surface and [X-PhMIM][BF₄] (X = NH₂, CH₃, H, CHO and NO₂) TAAILs. Comparison of interaction energies indicates that the \mathbf{B}_{\perp} complexes are more stable than \mathbf{A}_{\parallel} ones. A detailed analysis of the geometric and electronic properties, charge transfer, electron density properties, global reactivity descriptors, work function, dipole moment and electron density of the states for pure BNNT and different configurations of the modified BNNT were carried out. It is predicted that the π - π stacking of BNNT with the TAAILs is accompanied by a decrease in the energy gap. ChelpG analysis reveals that the interaction of ILs with BNNT induces the charge transfer from anion to cation. Inspection of the results shows that the charge in the \mathbf{A}_{\parallel} complexes is transferred from IL to BNNT for electron donating substituents and from BNNT to IL for H and electron accepting ones. The results also show that the charge in the \mathbf{B}_{\perp} complexes is transferred from IL to BNNT with the exception of IL containing the NO₂ substituent. To understand the behavior of non-

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