The potentials of boron-doped (nitrogen deficient) and nitrogen-doped (boron deficient) BNNT photocatalysts for decontamination of pollutants from water bodies

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Abstract

This work investigates the structural, elastic, electronic, and photoabsorption properties of boron- (N-deficient) and nitrogen- (B-deficient) doped single-walled boron nitride nanotube (SWBNNT) for photocatalytic applications for the first time. All calculations of the optimized systems were performed with DFT quantum simulation codes. The results of the structural analysis showed that SWBNNT is stable to both B and N dopants. It was also observed that the photodecomposition activity of the B-doped nanotube improved significantly under the condition of slight compressive stress, while it decreased for the N-doped nanotube. Therefore, N-doped SWBNNT showed poor performance under external pressure. Both B and N-doped systems could narrow the wide band gap of SWBNNT to the photocatalytic region below 3 eV, therefore this material can be used as photocatalysts in water splitting for hydrogen evolution, dye degradation, wastewater treatment, *etc.* Analysis of the optical properties revealed that B-doped SWBNNT absorbs more photons in the visible range than the N-doped SWBNNT and can therefore be considered as a more efficient photocatalyst. In addition, it was found that all doped nanotubes are anisotropic since the absorption in one direction of nanotube axes is worse than the other.