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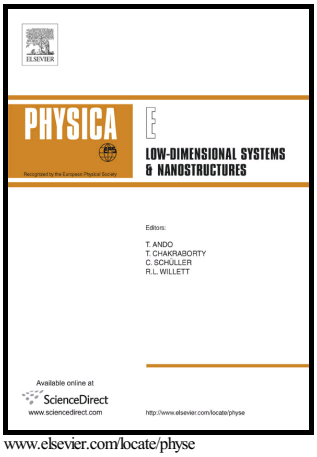

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Magnetic, electronic, optical, and photocatalytic properties of nonmetal- and halogen-doped anatase TiO_2 nanotubes

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Abstract

The structure stability, magnetic, electronic, optical, and photocatalytic properties of nonmetal (B, C, N, P, and S), and halogen (F, Cl, Br, and I)-doped anatase TiO_2 nanotubes (TNTs) have been investigated using spin polarized density functional theory. The N- and F-doped TNTs are the most stable among other doped TNTs. It is found that the magnetic moment of doped TNT is the difference between the number of the valance electrons of the dopant and host anion. All dopants decrease the band gap of TNT. The decrease in the band gap of nonmetal (C, N, P, and S)-doped TNTs, in particular N and P, is larger than that of halogen-doped TNTs due the created states of the nonmetal dopant in the band gap. There is a good agreement between the calculation results and the experimental observations. Even though C-, N-, and P-doped TNTs have the lowest band gap, they can not be used as a photocatalysis for water splitting. The B-, S-, and I-doped TiO_2 nanotubes are of great potential as candidates for water splitting in the visible light range.

Keywords: Nanotube, titania, titanium oxide, doping, electronic and optical properties, density functional theory