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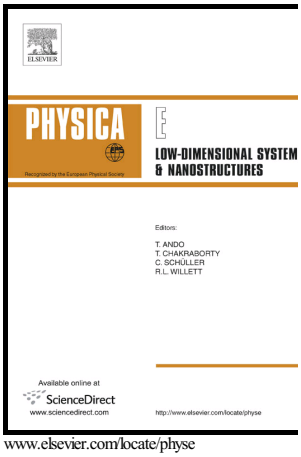

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Nitric Oxide Adsorption on Non-stoichiometric Boron Nitride Fullerene: Structural Stability, Physicochemistry and Drug Delivery Perspectives

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Abstract

The structural stability and physicochemical properties of the N-rich BN fullerene, $B_{24}N_{36}$, have been analyzed by means of the density functional theory at the level of the generalized gradient approximation. For this purpose, the Heyd-Scuseria-Ernzerhof (HSE) screened hybrid density functional and the 6-31G(d) basis set were used. The results indicate that the $B_{24}N_{36}$ fullerene is stable and behaves as a semiconductor compound. It has been found that while the polarity of the $B_{24}N_{36}$ fullerene is comparable with that of C_{60} fullerene, its chemical reactivity is notoriously higher. The spatial charge distribution of the BN fullerene allows nitric oxide adsorption, without compromising structural stability. Although the interaction between the NO molecule and BN fullerene is through van der Waals forces (dipole-dipole attraction), it has strong influence on the dipole moment,

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