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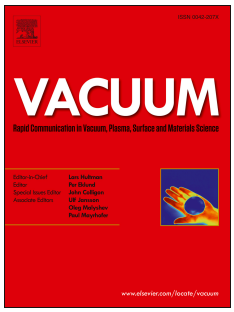

First-principle study of ammonia molecules adsorption on boron nitride nanotubes in presence and absence of static electric field and ion field

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First-principle study of ammonia molecules adsorption on boron nitride nanotubes in presence and absence of static electric field and ion field

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ABSTRACT

The adsorption of ammonia molecules (NH_3) on the surfaces of (4,4) boron nitride nanotubes (BNNTs), in presence and absence of applied static electric field (SEF, 0.03-z and 0.04-z) and ionic field (IF) of Be^{+2}, Mg^{+2}, Ca^{+2}, Sr^{+2} and Ba^{+2} has been investigated using density functional theory (DFT). The changes in geometric and electronic structures of all adsorption configurations were analyzed to characterize the sensitivity of BNNTs towards NH_3 molecules. Our calculations clearly showed that SEF and IF significantly impact the adsorption characteristics of NH_3 molecules on (4,4) BNNTs, indicating the chemisorption process. According to the results, the application of SEF and IF decreased the primary symmetry of BNNTs and consequently enhanced the chemical activity of BNNTs towards NH_3 molecules. Therefore, applying SEF and IF may be a suitable strategy for enhancing gas molecule adsorption capability of BNNTs, improving their sensor applicability.

Keywords: BNNTs; NH_3; Static electric field; Ion field; Chemisorption; DFT

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