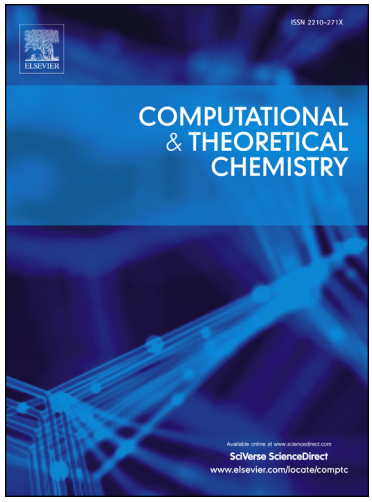

Electric field effects on the adsorption of formaldehyde molecule on the ZnO nanotube surface; A theoretical investigation

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Electric field effects on the adsorption of formaldehyde molecule on the ZnO nanotube surface; A theoretical investigation

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Abstract

In this work, we performed a theoretical investigation of adsorption of formaldehyde molecule (HCHO) on the exterior surface of single-walled (8, 0) zinc oxide nanotube (ZnONT). We considered the effect of external electric fields (EF) on the adsorption properties. Details of the geometric structures, adsorption energies, band gap and charge transfer have been considered. The obtained results show that the electric field can easily modulate the band gap and the adsorption energy of formaldehyde on ZnONT, furthermore as the electric field increases in parallel direction to the ZnO tube axis, these modulation increased noticeably. Comparison of (10,0), (5,5) and (8,0) ZnONT/HCHO demonstrates that the adsorption energy and band gap are sensitive to the tube diameter and chirality. However, with and without the electric field effect (8,0) ZnO nanotube is a better candidate for formaldehyde adsorption rather than those of (10,0) and (5,5) ZnONT. The present results can be providing useful guidance to develop novel nanotube-based sensors for the detection of formaldehyde molecules.

Keywords: ZnO nanotube; Formaldehyde; DFT study; Adsorption; Electric field effect.