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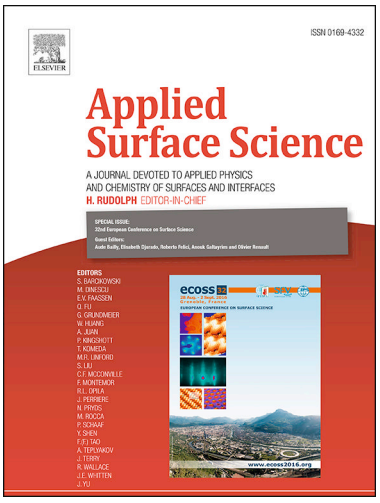

Full Length Article

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Sensing Properties of Pristine Boron Nitride Nanostructures towards Alkaloids: A First Principles Dispersion corrected Study

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Abstract

To understand the underlying physics behind the interaction of biomolecules with the nanomaterials to use them practically as bio-nanomaterials is very crucial. A first principles calculation under the frame work of density functional theory is executed to investigate the electronic structures and binding properties of alkaloids (Caffeine and Nicotine) over single walled boron nitride nanotube (BNNT) and boron nitride nanoribbon (BNNR) to determine their suitability towards filtration or sensing of these molecules. We have also used GGA-PBE scheme with the inclusion of Van der Waals interaction based on DFT-D2. . Increase in the accuracy by incorporating the dispersion correction in the calculation is observed for the long range Van der Waals interaction. Binding energy range of BNNT and BNNR with both alkaloids have been found to be - 0.35 to - 0.76 eV and -0.45 to -0.91 eV respectively which together with the binding distance shows physisorption binding of these molecules to the both nanostructures. The transfer of charge between the BN nanostructures and the adsorbed molecule has also been analysed by using Lowdin charge analysis. The sensitivity of both nanostructures BNNT and BNNR towards both alkaloids is observed through electronic structure calculations, density of states and quantum conductance. The binding of both alkaloids with BNNR is stronger. The analysis of the calculated properties suggests absence of covalent interaction between the considered species (BNNT/BNNR) and alkaloids. The study may be useful in designing the boron nitride nanostructure based sensing device for alkaloids.

Keywords: Boron Nitride Nanostructure, Alkaloids, Electronic Properties, Binding energy, Quantum Conductance, Sensors.

1. Introduction