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Study of formaldehyde molecule adsorption on pristine, defect and functionalized carbon nanotubes by self-consistent charge density functional tight-binding method

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We aim to fabricate formaldehyde gas sensors for identifying formalin contamination of fresh raw food materials, especially seafood. Carbon nanotubes (CNTs) are one of materials widely used for fabrication of gas sensors because of their unique electronic properties. Unfortunately, pristine CNTs exhibit very low sensitivity for formaldehyde molecule adsorption. In this research, we have used self-consistent charge density functional tight-binding (SCC-DFTB) method to model the various CNTs including pristine, defect and N2 functionalization for finding the best structure for formaldehyde sensing. Pristine CNTs (9,0) containing 180 carbon atoms were built and their two ends were capped with hydrogen atoms to avoid the boundary effects. Then, the CNTs were made a vacancy defect and functionalized by N2 molecules. Interaction between a CNTs surface and formaldehyde molecule was investigated. Total energy of interaction was calculated. The primary results showed the total energy of pristine, defected and N2 functionalized CNTs was 0.13, 0.14 and 0.21 eV, respectively. The functionalization on CNT surfaces with N2 molecules improved a better interaction between formaldehyde molecules and CNTs.

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