Article

A theoretical survey on the chlorine dioxide (ClO2) and its decomposed species detection by the AlN nanotube in presence of environmental gases

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Abstract

The adsorption of N2, O2, H2O, hydrogen chloride (HCl), Cl2, hypochlorous acid (HClO), and ClO2 gases was explored onto an AlN nanotube (AlNNT) through density functional theory computations. As N2, O2, H2O, HCl, Cl2, and HClO approach the AlNNT, their adsorption releases 7.1, 12.6, 22.3, 26.5, 30.2, and 41.2 kJ/mol of energy, respectively, indicating a physisorption. In addition, the electronic properties of the nanotube do not change significantly. As chlorine dioxide (ClO2) approaches the AlNNT, its adsorption releases 97.4 kJ/mol of energy. Electronic analysis showed that the AlNNT HOMO–LUMO gap reduces from 4.10 to 2.80 eV (~ − 31.7%) by ClO2 adsorption and the electrical conductivity increases significantly. Therefore, the AlNNT can generate electrical signals when the ClO2 molecules approach, being a hopeful sensor. It was found that this nanotube can selectively detect ClO2 gas among the mentioned molecules. The recovery time for the AlNNT was computed to be 8.0 s for ClO2 desorption, representing a short recovery time.Graphical abstract