

## Article

A theoretical survey on the chlorine dioxide (ClO<sub>2</sub>) and its decomposed species detection by the AlN nanotube in presence of environmental gases

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## Abstract

The adsorption of N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, hydrogen chloride (HCl), Cl<sub>2</sub>, hypochlorous acid (HClO), and ClO<sub>2</sub> gases was explored onto an AlN nanotube (AlNNT) through density functional theory computations. As N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, HCl, Cl<sub>2</sub>, 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 (ClO<sub>2</sub>) 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 ClO<sub>2</sub> adsorption and the electrical conductivity increases significantly. Therefore, the AlNNT can generate electrical signals when the ClO<sub>2</sub> molecules approach, being a hopeful sensor. It was found that this nanotube can selectively detect ClO<sub>2</sub> gas among the mentioned molecules. The recovery time for the AlNNT was computed to be 8.0 s for ClO<sub>2</sub> desorption, representing a short recovery time. Graphical abstract

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