

# Sensor and Actuators B: Chemical

## Improving methane gas sensing properties of multi-walled carbonnanotubes by vanadium oxide filling

George Chimowa,<sup>a</sup> Zamaswazi P.Tshabalala,<sup>a</sup> Amos A.Akande,<sup>a</sup> George Bepete,<sup>c</sup> Bonex Mwakikung,<sup>a</sup> Suprakas S.Ray,<sup>ab</sup> Evans M. Benecha<sup>d</sup>

<sup>a</sup> DST-CSIR National Centre for Nanostructured Materials, Council of Scientific and Industrial Research, Pretoria 0001, South Africa

<sup>b</sup> Department of Applied Chemistry, University of Johannesburg, Doornfontein 2028, Johannesburg, South Africa

<sup>c</sup> Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Wits 2050, Johannesburg, South Africa

<sup>d</sup> School of Interdisciplinary and Graduate Studies, University of South Africa, UNISA 0003, Pretoria, South Africa

### Abstract

Manipulation of electrical properties and hence gas sensing properties of multi-walled carbon nanotubes (MWNTs) by filling the inner wall with vanadium oxide is presented. Using a simple capillary technique, MWNTs are filled with vanadium metal which is later oxidized. It is observed that the methane gas detection response time at room temperature (293 K), is significantly improved from 138 s (in vanadium pentoxide) to 16 s (in filled MWNTs) while the recovery times changes from 234 s to 120 s respectively. The response sensitivity of the unfilled CNTs is improved from 0.5% to 1.5% due to the metal oxide filling. Using theoretical Density Functional Theory (DFT) electronic structure calculations, we show that the enhanced response is due to the increased density of states around the Fermi level of the composite material as a result of the encapsulated metal oxide. And we propose an adsorption mechanism at three different sites of the MWNTs surface based on the Langmuir model. This work also highlights the influence of ambient oxygen in carbon nanotube based sensors, an aspect that has not been clearly addressed in many previous theoretical and experimental studies.