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Extended Abstract

Influence of Oxygen Vacancies in Gas Sensors Based on Tin Dioxide Nanostructure: A First Principles Study †

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† Presented at the 8th GOSPEL Workshop. Gas Sensors Based on Semiconducting Metal Oxides: Basic Understanding & Application Fields, Ferrara, Italy, 20–21 June 2019.

Published: 19 June 2019

The use of computer simulations for performance predictions has become almost essential. In the gas sensing field, the simulation of the physical-chemical properties of (Metal Oxide) MOX semicondutors can be used to predict the performance of sensors based on the material studied.

Tin dioxide is a typical n-type semiconducting material with a wide band gap of 3.6 eV [1]. It has attracted the attention of many researchers due to its broad spectrum of physical-chemical properties, indeed it has been used in several fields such as optoelectronic devices, electrocatalysis, ceramics and gas sensors. SnO_2 is the most studied semiconductor as sensing layer for chemoresistive gas sensors production [2]. Then, it represents the best candidate for the innovative work here proposed.

So far, literature presents lacks of studies on how number and arrangement of oxygen vacancies affects the sensing performance of chemoresistive gas sensors, which usually needs a high operating temperature. Therefore, in order to enhance the behavior of SnO_2 as active element in gas sensors devices, we propose a study concerning the impact of oxygen vacancies on its physical-chemical properties. Structural, electronic and electrical properties of the stochiometric SnO_2 and the reduced one were studied.

A series of first principles study was carried out using the Full Potential Linearized Augmented Plane Wave (FPLAPW) method [3] within the framework of Density Functional Theory (DFT) as implemented in the Wien2k code [4]. The principle of DFT simulations is to calculate the physical-chemical properties by solving the Khon and Sham equation.

The results showed a high electrical conductivity for samples with oxygen vacancies, which can give a decrease of the temperature that sensing material needs to be thermo-activated. The position of the impurity states is one of the important parameters, which involve the reactions on the material surface. Indeed, the arrangement of the impurities impact on the Energy that is necessary to ionize the impurity states.

Figure 1 illustrates the total density of state (DOS) of the stochiometric SnO_2 and the reduced ones with two different concentration (3.125% and 9.375%) of oxygen vacancies. It can be seen from this figure that in the case of reduced compounds, the impurity states are found to be present in the energy gap regions and, by increasing the concentration of the defects studied the positions of these states change and the excitation of electrons from this level will need less energy then.

The simulated results show an important impact of the oxygen vacancies on the electronic and electrical properties of SnO_2, which lead to experimental investigations to modify and tailor MOX semiconductors for gas sensing applications.

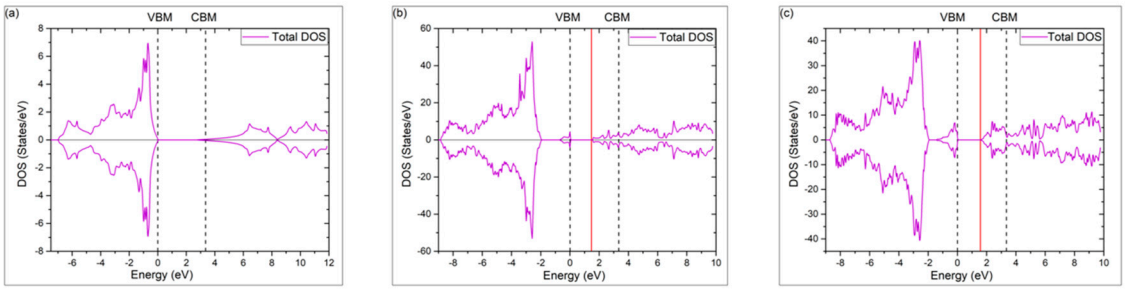

Figure 1. Total Density of States of (**a**) stochiometric SnO_2 (**b**) and (**c**) are Reduced SnO_2 ($Sn_{16}O_{31}$ and $Sn_{16}O_{29}$, respectively).

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