Low-operating temperature chemiresistive gas sensors: DFT calculations and electrical charaterization

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Despite advantages highlighted by Metal OXides (MOX) based gas sensors, these devices still show drawbacks in their performances, so further investigations are necessary. Researchers tried to address these problems in several ways, which includes new synthesis methods for innovative MOX-based materials, such as solid solutions (WO_3-SnO_2, SnO_2-TiO_2), addition of catalysts (Pd, Au, Pt etc.) and doping by using external atoms or oxygen vacancies[1]. Concerning this last issue, literature presents a lack of studies on how arrangement and number of oxygen vacancies affect the sensing performance and only a few preliminary works highlighted interesting results[2]. Another way to overcome MOX sensor drawbacks is to investigate other kinds of materials, such as metal-organic framework or 2D materials, which recently highlighted interesting results. Among the various 2D materials, phosphorene is one of the best candidates for such technological application, since it shows a chemiresistive activity at room temperature. The purpose of this work was focused on the study of materials addressed to gas sensing application operating at low temperatures, both tuning electrical properties of a well-known metal oxides, i.e. tin oxide (SnO_2), through a control of oxygen vacancies, and investigating a promising 2D material, i.e. black phosphorus.

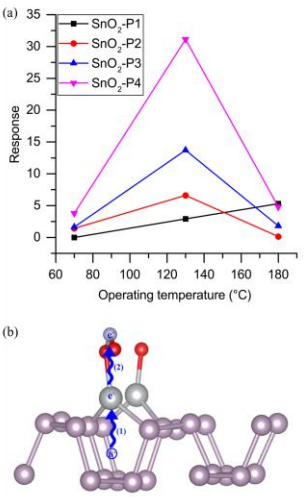

Fig. 1: (a) SnO_2 sensors response at different operating temperatures to 0.5 ppm NO_2. (b) Mechanism involved in the interaction between NO_2 gas molecule and nickel-decorated phosphorene (the Fermi-level control mechanism[4]).

The effect of oxygen vacancies on the structural, electronic, and electrical properties of bulk SnO_2 at two different concentrations was studied, then the formation of surface oxygen vacancies was investigated to study the adsorption of oxygen molecules from the surrounding atmosphere on the stoichiometric and reduced SnO_2 surface. Reduced SnO_{2-x} was synthesized and devices based on the produced material were fabricated and tested (Fig. 1a). The results showed a high response of the sensors towards low concentrations of nitrogen dioxide NO_2 (500 ppb) at 130°C instead of 450°C, the operating temperature of the available SnO_2-based gas sensors. For phosphorene, DFT calculations were carried out to explain how nickel influences its electronic properties since the decoration with nickel showed better stability of the sensor and high response towards NO_2 at room temperature[3]. The sensing mechanism was studied and explained using charge transfer analysis[4](Fig. 1b).

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