Despite advantages highlighted by Metal OXides (MOX) based gas sensors, these devices still present drawbacks in their performances (e.g. selectivity, stability and high operating temperature), so further investigations are necessary. Researchers tried to address these problems in several ways, which includes new synthesis methods for innovative materials based on MOX, such as solid solutions, addition of catalysts and doping of MOX by using external atoms or oxygen vacancies. Concerning this last issue, literature presents a lack of studies on how the arrangement and number of oxygen vacancies affect the sensing performance and only a few preliminary works highlighted interesting results. Another way to overcome MOX sensor drawbacks is to investigate novel class of materials, such as metal organic framework or 2D materials. Among these, phosphorene is one of the best candidates for such technological application~~,~~ since it shows ~~a~~ chemoresistive activity at room temperature.

The goal of this work is to decrease the operating temperature of SnO_2 based gas sensors by exploiting the oxygen vacancies. First, a theoretical investigation was done in the framework of Density Functional Theory (DFT) to investigate, on the atomic scale, how oxygen vacancies influence the physical and chemical properties of the material. 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 in order to study the adsorption of oxygen molecules from the surrounding atmosphere on the stoichiometric and reduced SnO_2 surface. Then, reduced SnO_{2-x} was synthesized and devices based on the produced material were fabricated and tested. The results showed a high response of the sensors towards low concentrations of nitrogen dioxide NO_2 (500 ppb) at 130°C instead of the typical operating temperature of 450°C for SnO_2-based gas sensors. This decrease in the operating temperature results in a decrease of the power consumption of the device, opening up to its possible employment on portable devices like mobile phones. The results were interpreted characterizing the material by mean of X-ray Powder Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscope (SEM) and Ultraviolet–visible spectroscopy (UV-visible) analysis. In the end, the experimental results were compared to the DFT outputs obtained.

As mentioned before, phosphorene is one of the promising 2D materials for gas sensing applications, but it still presents some drawbacks, mainly due to the material degradation over the time when exposed to ambient conditions. Many investigations were done on decorating phosphorene with metal atoms in order to enhance its performance for different technological applications. Nickel is one of metals proposed for such purpose, but few studies were done on nickel decorated phosphorene for gas sensing applications, especially for gas sensing application. In the innovative work here proposed, DFT calculations were carried out to explain how nickel influences the electronic properties of phosphorene since the decoration with nickel showed better stability of the sensor and high response towards NO_2 at room temperature. The theoretical results explained this behavior by studying the adsorption of oxygen molecules on pristine and nickel loaded phosphorene. The DFT calculations showed that oxygen molecules dissociate on the layer of pristine phosphorene and react with phosphorus atoms (oxidation of the material), while in the presence of the nickel atoms the later play the role of acceptors and interact with the oxygen molecules. Finally, the sensing mechanism towards NO_2 was investigated theoretically by studying the charge transfer occurring at the surface of the material during the adsorption process.