

# Synergy between Metal Oxides, Metal-organic Frameworks, and Multivariate Statistics for Selective Room Temperature Gas Sensing

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## Summary:

The use of metal oxides for gas sensing applications is a common and commercialized strategy but, in most cases, these materials present two important drawbacks: a cross-sensitivity to common gas species and a high operation temperature (100-400 °C). It has been recently reported that, on its turn, metal-organic frameworks can sense gases at room temperature, offering the so-called "sieving effect" that allow them to work as filters for improved selectivity. This research explores metal-organic frameworks and their potential synergy with metal oxides and multivariate statistics to create next-generation gas sensors.

**Keywords:** Gas sensor, metal oxide nanowires, metal-organic frameworks, machine learning, greenhouse gas

## Headlines

Recently reported metal-organic frameworks offer the possibility of operating gas sensors at room temperature and, therefore, their integration in common use electronic devices.

The synergy of new sensing materials that exhibit the sieving effect, combined with multivariate statistic techniques, can enhance the selectivity of gas sensors.

## Background, Motivation and Objective

Metal oxides (MOx) have been investigated and commercialized as gas sensing materials for several decades because they offer high sensitivity, easiness of integration, robustness of the final device, and they are cost-efficient. However, they show cross-sensitivity to many gas species, especially to moisture, many times providing false readings. Furthermore, it is well-known that these materials need high temperatures (100-400 °C) to operate in optimal conditions [1], what makes it challenging to integrate MOx-based gas sensors in common electronic devices, such as smartphones, and, at the same time, this induces power consumptions that

hinder deploying these sensors in remote locations with reduced access to power grid.

Recently, metal-organic frameworks (MOFs) have been demonstrated to work as gas sensing materials as well, being sensitive to a large variety of gases while operating at room temperature, thus increasing their potential for practical applications, and presenting easiness of integration, robustness of the final device and cost-efficiency as good as MOx [2]. Moreover, they show the so-called sieving effect [3] through which MOFs, depending on the size of their pores, electron affinity and/or specific functional groups, can act as a filter for certain gases.

Our goal is to explore MOx, MOFs, and possible synergies between them to obtain novel gas sensors with enhanced features for practical applications such as room temperature operation with fast response times and/or increased selectivity.

## Methodology

By means of chemical vapor deposition, we synthesize assemblies of single-crystal MOx nanowires and, by using chemical routes, we synthesize MOFs, both directly and site-selectively integrated on interdigitate electrodes. In this

way, we obtain gas sensors that offer new sensing characteristics with few fabrication steps. These sensors operate at room temperature, opening the path to integration of gas sensors in common electronic devices. The obtained data are treated via multivariate statistic techniques to assess the discrimination power of the fabricated sensors.

## Results

We will present the gas sensing behavior observed for the fabricated MOx- and MOF-based sensors when exposed to CO<sub>2</sub> and CH<sub>4</sub> ranging from 300 to 1200 ppm and from 1 to 10 ppm, respectively, diluted in dry and humid synthetic air. As an example, Figure 1a shows one of the MOx single-crystal nanowire forests directly grown onto interdigitate electrodes, while Figure 1b demonstrates the discrimination power by means of principal component analysis of the response of one of the synthesized MOFs.

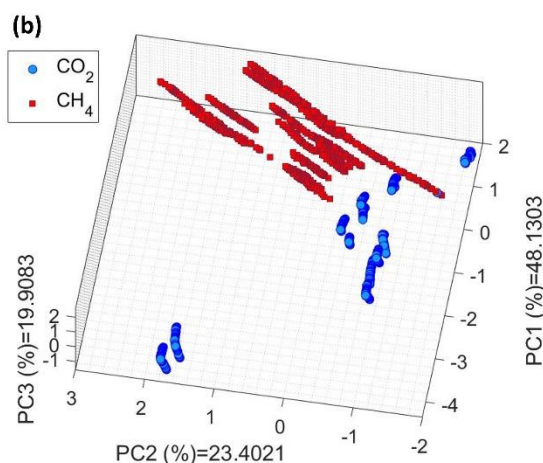
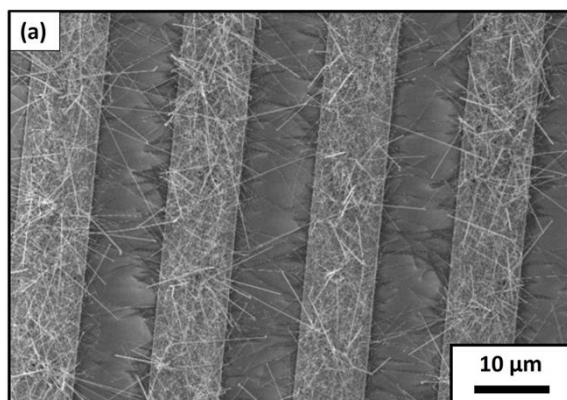


Fig. 1. (a) Metal oxide nanowires site-selectively grown on interdigitate electrodes by means of chemical vapor deposition and (b) results of principal component analysis from gas measurements of a metal-organic framework layer when exposed to carbon dioxide and methane ranging from 300 to 1200 ppm and from 1 to 10 ppm, respectively.

## References

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