An Innovative 3 steps Experimental Procedure to Better to Understand the Detection Mechanism of D-Limonene

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Over the past decades, *operando* approaches, surface studies, and theoretical simulations have shed light on the surface processes that drive the gas sensing responses of chemoresistive devices [1] for small molecules, such as NO_2, CO, H_2, O_3, and more deeply investigated the intermediate reactions of sample VOCs, such as ethanol, acetone and acetaldehyde. Nevertheless, these sensors can also detect more complex VOCs, such as D-Limonene. This gas is of interest in different applications, such as medical applications and precision agriculture and is exploited in the food and beverage industry, as a flavoring and preservative element, or in beauty and personal care products, in household products, and as the active principle in ecological pesticides.

In the experimental section, the optimal material for D-limonene sensing will be identified among seven nanostructured metal oxides (MOXs) based on WO_3, ZnO, and SnO_2, synthetized through different strategies for their functionalization, which were used to produce thick film sensors. On the best MOX candidate for D-Limonene detection a novel approach was applied to understand the sensing mechanism. The empirical procedure combines the investigation of surface chemical species formed during the analyte-sensor interaction through *operando* diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) with the characterization of MOX active sites via probe molecules and chemisorption analyses.

In the discussion of results some questions about the higher selectivity vs. D-Limonene compared to other materials, the rationale for the ideal operating temperature, and the role of active sites in the sensing mechanism will be addressed.

References

[1] Staerz, A.; Weimar, U.; Barsan, N., Current State of Knowledge on the Metal Oxide Based Gas Sensing Mechanism. *Sensors Actuators B Chem.*, *358*, 131531,(2022) doi:10.1016/j.snb.2022.131531.