

Supplementary Materials

ZnO structures with surface nanoscale interfaces formed by Au, Fe₂O₃, or Cu₂O modifier nanoparticles: characterization and gas sensing properties

Milena Tomić^{1,2}, Martha Claros³, Isabel Gràcia¹, Eduard Figueras¹, Carles Cané¹, and Stella Vallejos^{1,3*}

¹ Institute of Microelectronics of Barcelona (IMB-CNM, CSIC), Campus UAB, 08193 Cerdanyola del Vallès, Barcelona, Spain; milena.tomic@imb-cnm.csic.es (M.T.); isabel.gracia@imb-cnm.csic.es (I.G.); eduard.figueras@imb-cnm.csic.es (E.F.); carles.cane@imb-cnm.csic.es (C.C.)

² Autonomous University of Barcelona (UAB), Department of Electronic Engineering, Campus UAB, 08193 Cerdanyola del Vallès, Barcelona, Spain

³ CEITEC - Central European Institute of Technology, Brno University of Technology, 61200 Brno, Czech Republic; martha.claros@ceitec.vutbr.cz (M.C.)

* Correspondence: stella.vallejos@imb-cnm.csic.es (S.V.); Tel.: +34 935 947700

S1. Results – Material characterization

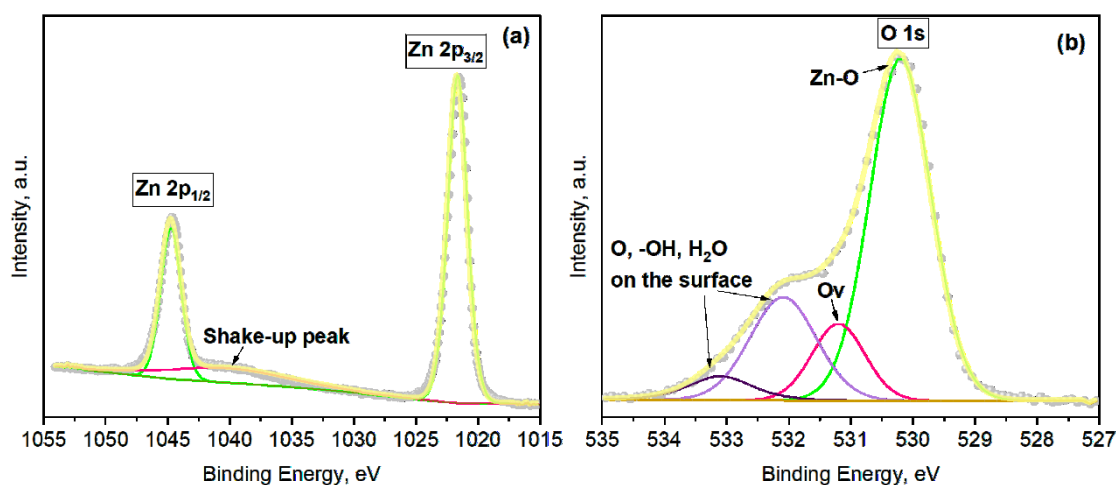


Figure S1. (a) Zn 2p, and (b) O 1s core levels XPS spectra for non-modified ZnO film. Grey dots represent the raw data, the solid yellow line corresponds to the envelope/fitting curve, and the other colored curves to the deconvoluted components.

The Zn 2p core-level spectrum recorded on non-modified ZnO film showed good agreement with the literature [1], proving the presence of Zn²⁺ state of zinc, with two main peaks at 1021.6 eV and 1044.7 eV that corresponds to the Zn 2p_{3/2} and Zn 2p_{1/2} peaks (**Figure S1a**), respectively, with the binding energy separation of 23.1 eV. Additional peak located at 1040.2 eV is related to the shake-up peak.

The O 1s XPS spectrum (**Figure S1b**) presents an asymmetric curve as reported earlier in the literature [2]. After the deconvolution, four different components are determined that indicate the presence of different oxygen species. The component centered at 530.2 eV is attributed to O²⁻ ions in the Zn-O bonding. The component at 531.2 eV is associated to O⁻ and O₂⁻ ions in the oxygen-deficient regions – oxygen vacancies. The components at 532.1 eV and 533.1 eV are connected to the presence of weak bonds from the physical or chemical adsorbed oxygen, hydroxides, and H₂O on the surface of ZnO film [3] [4] [5] [6].

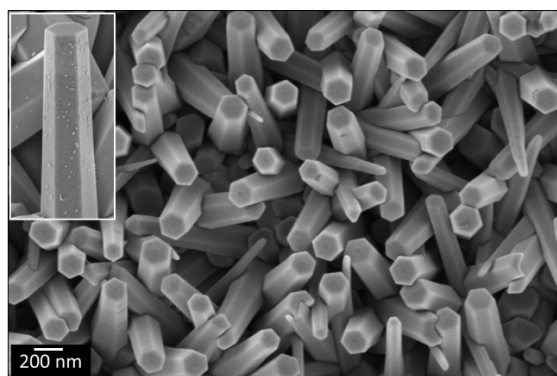


Figure S2. SEM images of the Ag@ZnO structured film (the inset shows a magnified image of a single Ag-modified ZnO rod).

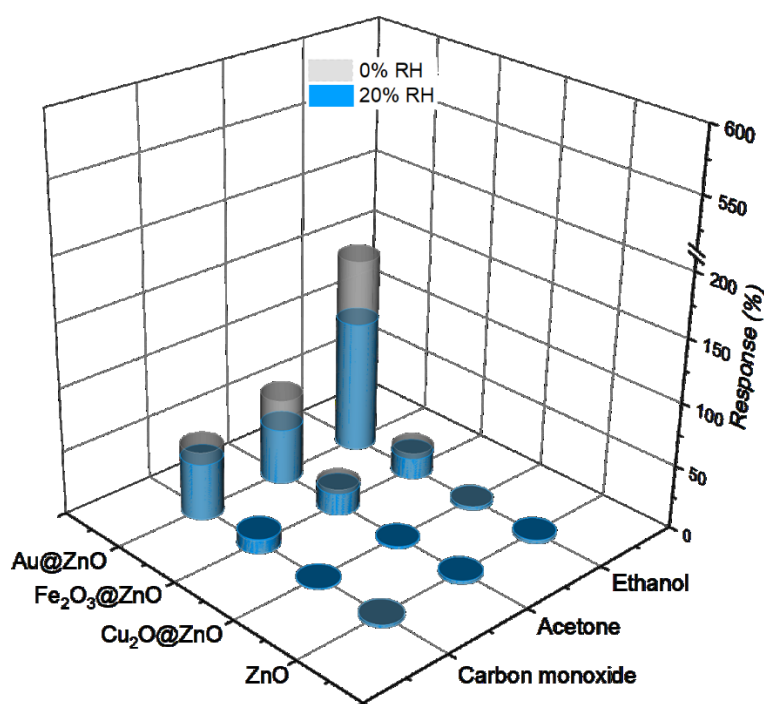


Figure S3. Responses towards 80 ppm of ethanol, acetone, carbon monoxide for the ZnO, Au@ZnO, Fe₂O₃@ZnO, and Cu₂O@ZnO sensors at 0% and 20% RH.

References:

- [1] S. Vallejos *et al.*, "ZnO rods with exposed {100} facets grown via a self-catalyzed vapor-solid mechanism and their photocatalytic and gas sensing properties," *ACS Appl. Mater. Interfaces*, vol. 8, no. 48, pp. 33335–33342, 2016, doi: 10.1021/acsami.6b12992.
- [2] J. H. Zheng, Q. Jiang, and J. S. Lian, "Synthesis and optical properties of flower-like ZnO nanorods by thermal evaporation method," *Appl. Surf. Sci.*, vol. 257, no. 11, pp. 5083–5087, 2011, doi: 10.1016/j.apsusc.2011.01.025.
- [3] S. Jain, J. Shah, N. Negi, C. Sharma, and R. K. Kotnala, "Significance of interface barrier at electrode of hematite hydroelectric cell for generating ecopower by water splitting," *Int. J. Energy Res.*, vol. 43, pp. 4743–4755, 2019, doi: 10.1002/er.4613.
- [4] H. Wang, S. Baek, J. Song, J. Lee, and S. Lim, "Microstructural and optical characteristics of solution-grown Ga-doped ZnO nanorod arrays," *Nanotechnology*, vol. 19, no. 7, p. 075607, Jan. 2008, doi: 10.1088/0957-4484/19/7/075607.
- [5] E. De La Rosa *et al.*, "Controlling the growth and luminescence properties of well-faceted ZnO nanorods," *J. Phys. Chem. C*, vol. 111, no. 24, pp. 8489–8495, Jun. 2007, doi: 10.1021/jp071846t.
- [6] L. J. Meng, C. P. Moreira de Sá, and M. P. dos Santos, "Study of the structural properties of ZnO thin films by x-ray photoelectron spectroscopy," *Appl. Surf. Sci.*, vol. 78, no. 1, pp. 57–61, May 1994, doi: 10.1016/0169-4332(94)90031-0.