

## **PL-2.5** Engineering Heterostructured Nanomaterials for Nanoelectronic and Biomedical Applications

## Oleg Lupan<sup>1,2</sup>

<sup>1</sup> Technical University of Moldova, 168 Stefan cel Mare Av., MD-2004 Chisinau, Moldova
<sup>2</sup> Kiel University, Kaiserstraße 2, D-24143 Kiel, Germany
oleg.lupan@mib.utm.md, ollu@tf.uni-kiel.de

Engineering heterostructured nanomaterials for nanoelectronics, as well as for biomedical applications have attracted huge attention in the past decade. It is because heterostructured nanomaterials are constructed by two or more single-component nanoparticles with certain structure, order of nanolayers and synergistically enhanced functional properties.

Heterostructures made of nanoparticles and nanostructured thin films or metal-organic frameworks are integrating advantages of porosity, nanosize, structure, optical and electrical performances. Recently, diverse nano-heterostructured materials are engineered and grown through various approaches and strategies and have proved promising potential for applications in battery safety sensors (BAS), gas, vapor and UV sensors, as well as biosensensors for biomedical applications [1-7].

Novel two-in-one battery safety sensors have been developed based on the CuO/Cu<sub>2</sub>O and TiO<sub>2</sub>/CuO/Cu<sub>2</sub>O heterostructures, as an example of real application [1-4]. These sensors enable early detection of solvents or the vapors of their degassing products, which are produced by Li-Ion batteries at the onset of runaway [1-5]. Coating ZnO nanocolumns using Al<sub>2</sub>O<sub>3</sub> and thermally annealing offers the resulting Al<sub>2</sub>O<sub>3</sub>/ZnO heterostructure that enhances the gas sensing properties towards the detection of the components in the electrolytes of the lithium-ion batteries. Columnar films of Al<sub>2</sub>O<sub>3</sub>/ZnO with a thickness of 10 nm for the top-coating layer exhibit the highest sensitivity and selectivity towards the vapors of C<sub>3</sub>H<sub>4</sub>O<sub>10</sub>. Experimental and computed results indicate that relative humidity will not affect the sensing properties of the such heterostructures towards the volatile organic compounds (VOCs) and degassing products used in the electrolytes of lithium-ion batteries [1-6].

As well as, new 2-in-1 sensor for NH<sub>3</sub> and H<sub>2</sub> detection is discussed, which ensure stable, precise and very selective characteristics for the tracking of these vapors at low concentrations. The fabricated TiO<sub>2</sub> layers, which were annealed at 610 °C formed two crystal phases, anatase and rutile, and after coverage with a thin PV4D4 polymer nanolayer via initiated chemical vapor deposition (iCVD), show response to ammonia at room temperature and exclusive hydrogen detection at elevated operating temperatures. These results open new possibilities for applications, e.g. like biomedical diagnosis, biosensors, and the development of non-invasive technology [7]. Compared to unprotected CuO/Cu<sub>2</sub>O/ZnO:Fe the coated CuO/Cu<sub>2</sub>O/ZnO:Fe exhibit a much better sensing performance at higher relative humidity and tunability of the gas selectivity [3].

The higher responses to specific volatile organic compounds, VOCs, are controlled and tailored for the samples synergistically enhanced with dopants and nanoparticles simultaneously. In addition, the recovery times are reduced for the developed nanocolumnar layers for a range of operating temperatures. The response of the synergistically enhanced sensors to gas molecules containing certain functional groups is in excellent agreement with density functional theory calculations performed in our work too [8].

This new fabrication strategy can underpin the next generation of advanced materials for photocatalytic, VOC, and gas sensing applications and prevent levels that are hazardous to human health and can cause environmental damage. As well as, it can be used for detecting gases used as traces for specific molecules, that act as biomarkers in exhaled breath or outgassing VOCs of various biological systems.

Acknowledgments. This research was funded by the SulfurSilicon Batteries (SuSiBaBy) Project (LPW-E/3.1.1/1801), which was funded by the EUSH and EFRE in SH.

## References

- Lupan O., Ababii N., Mishra A.K., Bodduluri M.T., Magariu N., Vahl A., Krüger H., Wagner B., Faupel F., Adelung R., de Leeuw N.H., Hansen S.: Heterostructure-based devices with enhanced humidity stability for H<sub>2</sub> gas sensing applications in breath tests and portable batteries. Sensors Actuators A Phys 329, 112804 (2021). <u>https://doi.org/10.1016/j.sna.2021.112804</u>
- Schröder S., Ababii N., Brînză M., Magariu N., Zimoch L., Bodduluri M.T., Strunskus T., Adelung R., Faupel F., Lupan O.: Tuning the Selectivity of Metal Oxide Gas Sensors with Vapor Phase Deposited Ultrathin Polymer Thin Films. Polymers (Basel) 15, 524 (2023). <u>https://doi.org/10.3390/polym15030524</u>
- 3. Schröder S., Ababii N., Lupan O., Drewes J., Magariu N., Krüger H., Strunskus T., Adelung R., Hansen S., Faupel F.: Sensing performance of CuO/Cu<sub>2</sub>O/ZnO:Fe heterostructure coated with thermally stable ultrathin hydrophobic PV3D3 polymer layer for battery application. Mater Today Chem 23, 100642 (2022). https://doi.org/10.1016/j.mtchem.2021.100642
- Lupan O., Santos-Carballal D., Ababii N., Magariu N., et al.: TiO<sub>2</sub>/Cu<sub>2</sub>O/CuO Multi-Nanolayers as Sensors for H<sub>2</sub> and Volatile Organic Compounds: An Experimental and Theoretical Investigation. ACS Appl Mater Interfaces 13, 32363–32380 (2021). <u>https://doi.org/10.1021/acsami.1c04379</u>
- Lupan O., Magariu N., Santos-Carballal D., Ababii N., Offermann J., Pooker P., Hansen S., Siebert L., de Leeuw N.H., Adelung R.: Development of 2-in-1 Sensors for the Safety Assessment of Lithium-Ion Batteries via Early Detection of Vapors Produced by Electrolyte Solvents. ACS Appl Mater Interfaces 13, 32363–32380 (2023). <u>https://doi.org/10.1021/acsami.3c03564</u>.
- Santos-Carballal D., Lupan O., Magariu N., Ababii N., et al.: Al<sub>2</sub>O<sub>3</sub>/ZnO composite-based sensors for battery safety applications: An experimental and theoretical investigation. Nano Energy 109, 108301 (2023). <u>https://doi.org/10.1016/j.nanoen.2023.108301</u>.
- 7. Brinza M., Schröder S., Ababii N., Lupan O., et al.: Biosensors 13(5), 538 (2023). https://doi.org/10.3390/bios13050538
- 8. Postica V., Vahl A., Dankwort T., Lupan O., et al. ACS Appl. Mater. Interfaces 1131452–31466 (2019). https://doi.org/10.1021/acsami.9b07275.