1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Fabrication and characterization of oxide/polymer nanocomposites thin films

1.1. Project goals

The proposed project aims to discover new composite inorganic-organic materials with potentially useful physical properties, particularly with projected applications in sensing, thermoelectric or photovoltaics. These materials will be fabricated as thin films using wet chemical and physical deposition techniques.

1.2. Outline

Semiconductor metal oxides such as CuO, Cu_2O and ZnO have many advantages, including good chemical and thermal stability, nontoxicity, abundant resources, and convenient low-cost preparation. The application of nanomaterials, including these compounds, is significantly expanded by combining them with polymer materials, allowing for the final composites' tunable properties. Creating more complex materials for many applications, such as photovoltaics, thermoelectric, optoelectronics, and sensing, is crucial. Therefore, increasing interest is in developing new composite systems based on predominantly conductive polymers (e.g. PEDOT:PSS) thin layers. Such nano-composites can exhibit tunable structural, optical, electrical and optomechanical properties. The project emphasizes developing convenient, economically, and ecologically advantageous methods of obtaining, which are also transferable from the laboratory to the industrial scale. The production of nano/micro oxide structures will be carried out using the simple co-precipitation method or chemical treatment of previously deposited by physical methods metallic layers. Polymer layers will be deposited using spin- and dip-coating methods. The project can extend the methodology and materials design process to fabricate new low-dimensional oxide-polymer structures (e.g. copper oxide, zinc oxide). Understanding the relationship between the structure and physicochemical properties will underpin this study.

1.3. Work plan

a) Development of chemical methods of oxide low-dimensional structures synthesis with a specific morphology (nanoparticles, nanorods, nanocrystalline layers and finally, nanocomposites).

The homogenous precipitation/reduction process will be used to synthesise nanoparticles. The development of stable dispersions of such structures in selected conductive and non-conductive polymers such as PEDOT:PSS, PVK or PMMA will result in the obtaining of thin composite layers.

In the second approach, oxides will be produced as thin three-dimensional coatings by chemical treatment of thin metallic layers, leading to nano-structure growth. Mentioned layers will be deposited using thermal evaporation, a common method of physical vapour deposition (PVD). In the final stage, the polymer will be deposited on the resulting oxide layer to modify the opto-physical properties.

When planning synthetic methods, using soft substrates for described composite layers will be crucial, which implies avoiding drastic processing conditions. Therefore, one of the scientific problems will be developing soft synthesis processing.

b) Materials will be first structurally and compositionally characterized by SEM/EDX, TEM, AFM, X-ray diffraction, IR, Raman, and XPS.

c) During project implementation, we will also focus on examining the optical properties of these films using UV-Vis spectroscopy, UV VIS DRS, ellipsometry, and photoluminescence measurements. In the application context, measuring thermal and electrical conductivity provides information about fabricated materials. According to the literature, copper oxides have the properties of being used as sensors, which will also be tested for CO_2 and other gases.

c) The selected composite layers will ultimately be used to produce functional devices based on them.

d) The project results will be published in high IF journals and presented at international and domestic scientific conferences. PhD students will attend at least two international conferences. We also intend to organise for PhD student a short-term visit to Prof. Duncan Gregory's laboratory at the University of Glasgow.

1.4. Literature *(max. 10 listed, as a suggestion for a PhD candidate)*

1. *Yinhua Lin, Jiexin Zou, Wenliang Wang, Xingyue Liu, Junning Gao, Zhenya Lu, High-performance self-powered ultraviolet photodetector based on PEDOT:PSS/CuO/ZnO nanorod array sandwich structure, Applied Surface Science, 599, 2022, 153956,* https://doi.org/10.1016/j.apsusc.2022.153956

2. *Abas, A., Sheng, H., Ma, Y. et al. PEDOT:PSS coated CuO nanowire arrays grown on Cu foam for high-performance supercapacitor electrodes, J Mater Sci: Mater Electron 30, 10953–10960 (2019).* https://doi.org/10.1007/s10854-019-01469-9

3. *Paneru, S., Sweety & Kumar, D., CuO@PEDOT:PSS-grafted paper-based electrochemical biosensor for paraoxon-ethyl detection. J Appl Electrochem 53, 2229–2238 (2023).* https://doi.org/10.1007/s10800-023-01909-9

4. *Wen Cai Ng, Meng Nan Chong, Organic-inorganic p-type PEDOT:PSS/CuO/MoS2 photocathode with in-built antipodal photogenerated holes and electrons transfer pathways for efficient solar-driven photoelectrochemical water splitting, Sustainable Materials and Technologies 38 (2023) e00749.* https://doi.org/10.1016/j.susmat.2023.e00749

5. G. Prunet *et. al., A review on conductive polymers and their hybrids for flexible and wearable thermoelectric applications, Materials Today Physics 18 (2021) 100402.* https://doi.org/10.1016/j.mtphys.2021.100402

6. *Nara Kim et. al., Elastic conducting polymer composites in thermoelectric modules, NATURE COMMUNICATIONS, (2020) 11:1424.* https://doi.org/10.1038/s41467-020-15135-w

7. Petr Krcmar *et. al., Fully Inkjet-Printed CuO Sensor on Flexible Polymer Substrate for Alcohol Vapours and Humidity Sensing at Room Temperature, Sensors 2019, 19(14), 3068;* https://doi.org/10.3390/s19143068

8. Ścigała Aleksandra, Szłyk Edward, Rerek Tomasz , (…), Robert Szczęsny, Copper nitride nanowire arrays: comparison of synthetic approaches, Materials, 2021, vol. 14 (3), 1-14. https://www.mdpi.com/1996-1944/14/3/603

9. Optical and morphological properties of ZnO and Alq3 incorporated polymeric thin layers fabricated by the dip-coating method Sypniewska Małgorzata, Szczęsny Robert, Skowroński Łukasz et. al., Applied Nanoscience, 2023, vol. 13 (7) 4903-4912. https://link.springer.com/article/10.1007/s13204-022-02647-8

10. Radtke, A. Photocatalytic Activity of Nanostructured Titania Films Obtained by Electrochemical, Chemical, and Thermal Oxidation of Ti6Al4V Alloy—Comparative Analysis. *Catalysts* **2019**, *9*, 279. https://doi.org/10.3390/catal9030279

1.5. Required initial knowledge and skills of the PhD candidate

PhD candidate:
- should be skilful and familiar with the basic methods of synthesis and analytical methods for the characterization of nanomaterials; and semiconductor chemistry
- have creative thinking
- should possess a willingness to increase competence in the field of material engineering and inorganic chemistry
- should have a good command of English in writing and speaking due to planned extensive scientific cooperation

- should be able to work in a team.

1.6. Expected development of the PhD candidate’s knowledge and skills

The PhD student will acquire interdisciplinary knowledge of material chemistry and instrumental analysis methods to characterize the materials' structure, morphology, and opto-electrical properties. Additionally, the skills in interpreting analytical and statistical data will be developed during PhD study. PhD students also will develop soft skills like organising work, working with scientific literature, and preparing publications and conference presentations.