ACADEMIA ROMÂNĂ
SCOSAAR

Anexa nr.6

ABSTRACT OF THE HABILITATION THESIS

TITLE: Oxide semiconductor structures with adjustable properties for environmental protection and energy applications

Habilitation domain: *CHEMISTRY*

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The habilitation thesis, entitled "***Oxide semiconductor structures with adjustable properties for environmental protection and energy applications***", highlights the major scientific contributions achieved after the doctoral thesis defense (2012), with particular emphasis on the progress made over the last 12 years. This work is structured into three main chapters, each reflecting consolidated research directions, original results obtained, and their impact in the field of chemistry and materials science, with applications in several areas of current interest. Thus, the thesis provides a coherent and integrated overview of the evolution of the research career, the scientific maturity achieved, and the ability to lead research projects and to develop new research directions in these fields.

Chapter I (Professional and Academic Achievements) summarizes the most relevant contributions from the analyzed period, focusing on published scientific articles and on the roles undertaken within research projects, while highlighting high-impact results. It also presents the awards received, citation metrics, editorial activity, as well as the involvement in the training and supervision of doctoral and postdoctoral researchers. Over the 12 years of scientific activity following the PhD defense, I have published ***74 scientific papers*** (***52 as first and/or corresponding author), 6 articles in conference proceedings, and delivered 70 presentations*** at national and international scientific events (***7 invited lectures, over 30 oral communications, and more than 30 poster***

presentations). I have coordinated ***3 research projects*** and participated as a team member in an additional ***7 national and international projects***. The published works are visible in high-impact journals indexed in the Web of Science.

At present, my ***Hirsch index is h = 25*** (cumulative as Pascariu P. or Dorneanu P.), and my publications have been cited in **1948 ISI-indexed articles** (**1767** excluding self-citations), in the Web of Science database. According to Scopus, my ***Hirsch index is 27***, with a total of ***2258 citations***.

In 2023, I was included in the ***Top 2% Scientists Worldwide 2023 Stanford University*** ("Updated science-wide author databases of standardized citation indicators," https://doi.org/10.17632/btchxktzyw.6).

Chapter II (Scientific Contributions Achieved over the Last 12 Years) represents the core section of the thesis, highlighting the main research directions in the field of oxide semiconductor materials and polymer/inorganic nanostructure composites. This chapter is structured into three subchapters, corresponding to applications of major interest, namely photocatalysis, energy storage, and humidity sensors.

Subchapter ***II.1*** (***Inorganic Oxide Semiconductor–Based Materials Used in Photocatalytic Processes***) presents the results obtained regarding the development and optimization of ZnO- and TiO_2-based oxide semiconductors, both in pristine form and doped with lanthanide, noble metal, and transition-metal ions, synthesized via an electrospinning approach followed by calcination. The photocatalytic activity of these materials was evaluated for the degradation of relevant organic pollutants (dyes and antibiotics), and the influence of the dopant nature and reaction parameters was systematically analyzed. A representative result is the 0.1 % Pr-doped ZnO material, which induced complete degradation of oxytetracycline, superior kinetic parameters, and good stability over multiple reuse cycles. In parallel, hybrid nanostructured membranes based on ZnO or TiO_2 integrated into polymer matrices (PVDF, PVDF/GO) were developed to facilitate catalyst recovery. These membranes exhibited remarkable photocatalytic efficiencies, ranging from 93–100 %, and good stability even after ten reuse cycles. Part of these results was validated within the TE project (PN-III-P1-1.1-TE-2019-0594), demonstrating significant contributions to the design of advanced photocatalytic materials with high potential for sustainable applications in contaminated water treatment.

Subchapter ***II.2 (Inorganic Nanostructures and Polymer/Inorganic Nanostructure***

Composites for Energy Storage Applications) systematizes the contributions to the development of nanostructured materials for energy storage, with an emphasis on oxide semiconductors and hybrid polymer/inorganic nanoparticle composites. The use of two fabrication methods, electrospinning and electropolymerization, enabled the formation of one-dimensional porous structures with high active surface areas, favorable for charge–discharge processes in supercapacitors.

Three systems were investigated: pristine and Cu-doped TiO_2, p–n NiO–SnO_2 heterojunctions, and PTh/Ni nanocomposites. Cu ions doping of TiO_2 significantly enhanced the pseudocapacitive response with 0.5 %, the Cu composite exhibiting the best electrochemical performance. For NiO–SnO_2, the optimal 75:25 ratio generated the most efficient synergy between structure and electrochemical characteristics, yielding high specific capacitance and superior stability. The PTh/Ni nanocomposites showed a substantial increase in the number of active sites and in capacitance due to the incorporation of metallic nanoparticles.

The final subchapter, II.3 (Ceramic Fibers Based on Oxide Semiconductor Materials for Humidity Sensor Applications), systematizes the contributions made to the development of oxide semiconductor nanostructures for humidity detection, focusing on two representative systems: NiO–SnO_2 composite nanofibers and ZnO nanostructures doped with 1 % lanthanides. Both types of materials were obtained via electrospinning followed by calcination, a method that yields porous one-dimensional architectures with high specific surface area, favorable for water-vapor adsorption–desorption processes.

NiO–SnO_2-based nanofibers exhibited a well-defined granular structure and high humidity sensitivity, manifested by a rapid decrease in electrical resistance and very good response and recovery times, particularly for composites with high NiO content. This behavior is attributed to the synergy between the p-type semiconductor (NiO) and the *n*-type semiconductor (SnO_2), as well as to the high porosity of the fibers.

In the case of lanthanide-doped ZnO, XRD and XPS analyses confirmed the formation of doped materials and an increased degree of surface hydroxylation, with dopants influencing the microstructure, defect density, and morphology. From an electrical standpoint, lanthanide doping leads to an increase in relative dielectric permittivity, a one-order-of-magnitude decrease in resistivity, and a reduction in response times from 98 s (pristine ZnO) to 62–89 s for the doped materials. Ce-doped samples exhibited the highest sensitivity coefficients (≈83 % at 33 % RH), confirming the role of multivalent Ce^{3+}/Ce^{4+} ions in the generation of active sites.

Chapter III, entitled Future Research Directions, outlines a development plan for advanced materials based on oxide semiconductors, hybrid polymer-inorganic membranes, and one-dimensional nanostructures, with applications in areas such as water purification, energy storage, sensors, and biomedical fields. A major priority is the design of photocatalysts capable of efficient responses under visible light, through strategies such as metal and non-metal doping, the formation of *p–n* heterojunctions, and the integration of carbon-based components. In parallel, the development of recoverable composite membranes with enhanced stability for wastewater treatment is envisaged, along with the design of laboratory-scale photocatalytic reactor prototypes.

Another major research direction to be pursued involves the development of hybrid polymer/oxide semiconductor materials for energy applications, particularly next-generation supercapacitors, using electrospinning and electropolymerization as the main synthesis methods. At the same time, one-dimensional ceramic nanofibers remain a strategic research direction, targeting applications in gas and humidity sensing/detection, supported by previous results and sustained collaborations with national and international institutes.

Complementary to these directions, emphasis is placed on promoting scientific excellence, attracting research funding, strengthening international collaborations, and training a new generation of researchers capable of contributing to advances in emerging fields of chemistry and materials science.

The habilitation thesis concludes with a list of bibliographic references, presenting the main literature sources consulted during the preparation of this work.