

## REVIEW

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by competition for the academic position of "Professor" in professional field 4.2. Chemical Sciences, scientific specialty "Chemical Kinetics and Catalysis ", in the thematic field "Design of metal and metal oxide systems with application in energy and improving the quality of life", by the competition announced in the State Gazette, issue 82/ 07.10.2025

In the competition announced by the Institute of Catalysis - BAS, mentioned above, for the academic position of "professor", one candidate participated - Assoc. Prof. Dr. Dimitrinka Aleksieva Nikolova.

### **Biographical data about the candidate**

Dr. Dimitrinka Nikolova is an established specialist with over 29 years of experience at the Institute of Catalysis at the Bulgarian Academy of Sciences. She graduated from the Bulgarian Technical University of Technology - Sofia in 1995 as a chemical engineer with a degree in "Inorganic and Electrochemical Production", specialization "Technology of Inorganic Substances. Her professional development has gone through all key academic stages. In 2001, she obtained the ONS "doctor" with a dissertation on the topic "Influence of the addition of potassium on the activity and structure of NiO-MoO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> catalysts for the reaction of conversion of carbon monoxide with water vapor in the presence of hydrogen sulfide ". From a chemist (1996) and a doctoral student, she successively held the positions of chief assistant and associate professor, which position she currently holds.

The presented professional biography and official documentation of work experience certify that Dr. Nikolova fully meets the regulatory requirements for holding the academic position of "professor".

### **Overview of the candidate's research activities**

21 scientific publications, one book chapter and two patents, 1 patent application were submitted for participation in the competition. All scientific works were published after 2016 and the list does not include the publications submitted in the competition for "associate professor".

The scientific output included in the habilitation thesis includes 9 publications distributed in prestigious journals (5 in Q1, 1 in Q2, 1 in Q3 and 2 in Q4). The leading role of the candidate is clearly impressive: in 4 of the articles she is the first author, and in 6 she appears as a corresponding author, which is a clear indicator of her leading participation in the research. The applied nature of the work is complemented by one patent and one patent application (indicator D). The candidate's scientific contributions outside the scope of the habilitation thesis are protected by a solid volume of additional output. It includes 12 scientific articles published in highly ranked refereed journals (of which 5 in the prestigious quartile Q1, 2 in Q2, 1 in Q3 and 4 in Q4), as well as a chapter of a collective monograph. The applied aspect of the research is confirmed by another patent.

The candidate's scientific achievements enjoy wide publicity and recognition in the professional community. The results have been reported at a total of 34 scientific forums, with participation in international conferences prevailing (20). The high number of oral presentations

(24 reports) is impressive, which is a certificate of the personal authority of Assoc. Prof. Dr. Nikolova and her ability to convincingly present the achieved results to an international audience. This includes 1 plenary report at an international forum, 12 reports at international forums, one plenary report at a national forum and 10 reports at national forums.

The scientific output of Assoc. Prof. Dr. Nikolova enjoys a significant resonance among the international research community. The total number of citations noted is 217, and it is striking that over 50% of them (110 citations) are to publications with which the candidate participates in this competition. This is indisputable proof of the relevance and significance of the presented scientific results.

The project activity of Assoc. Prof. Dr. Nikolova is impressive and proves her high organizational qualities. She has participated in the implementation of 10 scientific projects (2 international and 8 national). A key achievement in her career is taking on responsibility as a leader. In the period 2021-2025, she was the leader of three projects between the Israeli company GenCell LTD and the Institute of Catalysis . She is currently the coordinator of the IC-BAS in No. BG16RFPR002-1.014-0009 of 31.03.2025 and the implementation of the Project "Development and Sustainability of the Competence Center HITMOBIL" and led the project "Clean Hydrogen Technology for Green Energy - a Step Forward to Zero Emissions", funded under investment C2.I2: "Increasing the Innovation Capacity of the Bulgarian Academy of Sciences in the Field of Green and Digital Technologies" as part of the National Recovery and Sustainability Plan. Assoc. Prof. Nikolova was also the head of 3 projects on Equivalent Currency-Free exchange - two with the Institute of Chemistry, Technology and Metallurgy, Center for Catalysis and Chemical Engineering, University of Belgrade, Serbia and one with the National Research Center, Giza, Egypt.

GenCell, is extremely impressive. Ltd (Israel). In the period 2012–2023, she participated in the development of innovative anode catalysts from base metals for alkaline fuel cells. The results of this partnership are protected by two patents and one patent application. This clearly shows that Assoc. Prof. Nikolova has valuable practical experience in the industrial implementation of catalysts.

Assoc. Prof. Dr. Nikolova actively contributes to the development of the next generation of researchers, successfully passing on her rich professional and practical experience to young colleagues at the Institute. Under her leadership, two graduate students have successfully defended their bachelor's theses, and she is currently the supervisor of one doctoral student.

## **Analysis of the main scientific achievements**

### **Habilitation report (indicator B).**

As noted, the habilitation work is based on nine publications, one patent and one patent application. The scientific interests and activities of Dr. Dimitrinka Nikolova are characterized by a clear focus. They are focused on the development and study of the properties of new nanoscale metal and metal oxide materials for reactions related, on the one hand, to environmental protection by obtaining environmentally friendly clean fuel (hydrogen), and on the development and study of non-noble electrocatalysts for the production of green energy through hydrogen fuel cells and green hydrogen for solid oxide fuel cells; alkaline fuel cells; and electrolysis.

The main method for producing hydrogen is still from fossil fuels, and after the reforming process, the processes of water gas shift reaction (WGSR) follow to reduce the CO content in the

mixture and selective oxidation of CO. The production of hydrogen on an industrial scale through the WGS carried out in two stages at different temperatures and with the participation of two types of catalysts: High-temperature WGS in the temperature range 350–450 °C with Fe<sub>2</sub>O<sub>3</sub>-Cr<sub>2</sub>O<sub>3</sub> catalyst and low-temperature WGS in the temperature range 180–250 °C with CuO-ZnO-Al<sub>2</sub>O<sub>3</sub> catalyst to a residual CO content below 0.5%.

Conventional catalysts for this process are unsuitable for low-temperature systems due to operational drawbacks (pyrophoricity, sensitivity to poisons, complex activation) and the need for intercooling. Therefore, efforts are directed towards the development of highly efficient compositions for a single-stage process optimized for hydrogen fuel cells.

In the direction related to development of rhenium-containing catalytic systems for WGS and in WGS the presence of sulfur compounds, the main achievements are the following:

- Two critical directions are identified for optimizing catalytic activity in Re (Mo) systems promoted with K and Co: Precision stoichiometric design - modeling of the composition to achieve an optimal balance between the redox couples Re<sup>4+</sup>/Re<sup>7+</sup>, Co<sup>2+</sup>/Co<sup>3+</sup> and Mo<sup>4+</sup>/Mo<sup>6+</sup>) and modification of the electronic properties of the surface; Optimization of precursor activation: Determination of a specific reducing agent and precise temperature-time regime to unleash the full potential of the active centers.

The CoRe configuration was demonstrated, achieving 94% CO conversion at 260 °C and a space velocity of 4000 h<sup>-1</sup>.

- Re as an economical alternative to gold (Au) has been studied. Ni-Al layered double hydroxides (LDHs) with a molar ratio of Ni<sup>2+</sup>/Al<sup>3+</sup>=2.5 were used, on which 3 wt.% Re was impregnated. Key results are: The addition of CeO<sub>2</sub> improves the structural characteristics and slightly increases the catalytic activity compared to the system without cerium. It has been found that the catalytic efficiency can be refined by adjusting the ratio between the oxidation states in the redox couple Re<sup>4+</sup>/Re<sup>7+</sup>, and subsequent optimization of the system composition. Although the gold analogue Au/CeNiAl shows higher initial activity, the rhenium catalyst demonstrates excellent deactivation resistance.
- Development of K, Co and Ni -promoted rhenium sulfide catalysts for WGS in the presence of sulfur:

The trimetallic catalyst KCoRe has established itself as a stable, sulfur-resistant system for the purification of gas mixtures from CO. The high efficiency is due to the uniform application of the active components, which ensures maximum access of the reagents to the catalytically active centers. The key to the activity is the maintenance of a specific balance between the sulfide ReS<sub>2</sub> and the oxide ReO<sub>x</sub>S<sub>y</sub> forms of rhenium (the ratio Re<sup>4+</sup>/(Re<sup>7+</sup>+Re<sup>6+</sup>)). It has been found that simultaneous doping with K and Co optimizes the redox state of rhenium, fixing the Re<sup>4+</sup>/Re<sup>7+</sup> ratio close to the value of 2. This specific configuration ensures high activity and stability of the KCoRe catalyst.

The stress test conducted confirms the ability of the KCoRe system to fully restore its high conversion. This remarkable stability is due to the resistance of the active phases against the oxidative effects of water vapor and CO<sub>2</sub>, even in the absence of H<sub>2</sub>S. The results clearly demonstrate the reliability of the catalyst under potential emergency conditions.

In the direction related to the development and research of non-noble electrocatalysts for green energy production through hydrogen fuel cells and green hydrogen, the research activity is focused on the synthesis of innovative electrocatalytic systems for solid oxide (SOFC) (publ. No. 2,5, 12, 13) and alkaline fuel cells (AFC). The significance of the developments in the field of alkaline systems is confirmed by a patent (Patent US 12,230,809 B2/2025 and patent application EP 4046217 A1/2022). The research is in full harmony with the global transition to a low-carbon economy, and also includes the design of bi-functional electrocatalysts for efficient generation of green hydrogen (publ. No. 20). The main achievements here can be formulated as follows:

- Yttrium -doped barium cerate,  $\text{BaCe}_{0.85}\text{Y}_{0.15}\text{O}_{2.925}$  (BCY15), has been developed . The developed energy-saving approach for liquid-phase reduction in ethylene glycol media allows the preparation of Ni /BCY15 catalysts with excellent performance characteristics. The new methodology eliminates the need for industry-standard mixing, sintering , and reduction in hydrogen. The final product is a Ni-cermet anode for SOFC with proton conductivity, which demonstrates better stability of the active surface and resistance to degradation, optimizing the production of green energy.
- Development of catalyst systems for alkaline fuel cells. Research in this area is the result of long-term projects between GenCell Ltd and IK-BAS. Innovative noble metal-free (PGM- free ) anode catalysts for alkaline fuel cells have been developed and implemented. The multicomponent system NiMoReW/C exhibits electrochemical activity and stability equivalent to those of platinum Pt/C and palladium NiPd/C analogues at 70 °C in a highly alkaline environment (operating conditions of liquid electrolyte 6.6M KOH@70°C). The high reliability of the catalyst has been confirmed by long-term operation (1800 hours) in a real 375 W module, demonstrating stable anode potential over multiple load cycles. The technology is protected by patents in the USA (US 12,230,809 B2) and Europe (EP 4046217 A1) and has been successfully transferred to mass production.
- Bi -functional electrocatalysts for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in water electrolysis. The electrolytic deposition method, a relatively simple synthesis method suitable for practical implementation and scaling, was used for preparation. Commercially available conductive materials were selected as supports , including 3D-structured Ni -foam (NF) and 2D-structured Fe -steel sheet (FS), suitable for applications as electrodes. The best results were shown by the Ni<sub>50</sub>Co<sub>50</sub>P/ Fe -steel configuration, which demonstrated extremely high bifunctional activity ( $\eta_{\text{HER}} = 23 \text{ mV}$  and  $\eta_{\text{OER}} = 400 \text{ mV}$  at  $10 \text{ mA cm}^{-2}$ ), comparable to Pt- based catalysts, as well as high stability at industrially relevant current densities ( $100 \text{ mA cm}^{-2}$ ). These exceptional properties are the result of the unique 3D microstructure obtained by cost-effective co-electrodeposition on a steel substrate. The analysis identifies as a determining factor the unique 3D-like architecture of the  $\text{Co}_{3.6}\text{Ni}_{0.4}\text{P}_4$  alloy, which is composed of discrete spherical particles with a size of over 1  $\mu\text{m}$ , whose morphology favors a high concentration of active centers and optimized diffusion processes.

Author reference (index I).

In this part, the scientific achievements are presented in 12 publications in refereed international journals, distributed by quartiles as follows: 5 in Q1, 2 in Q2, 1 in Q3 and 4 in Q4. The list is supplemented by 1 book chapter and 1 patent.

The research is of a fundamental-applied nature and is aimed at the design of innovative metal and metal oxide systems. The main contributions are focused on two strategic directions: protecting human health and improving the quality of life, as well as application in energy. Three directions are being formed here:

1. Development and research of effective catalysts for the production of healthy foods
2. Development and research of effective catalysts for the production and purification of fuels and the production of clean energy;
3. Development and research of effective catalysts for clean and safe industry, including removal of synthetic dyes from industrial wastewater and air purification through catalytic ozone degradation.

The first research direction is focused on the synthesis and characterization of highly efficient Ni -containing catalytic systems. They are designed for partial hydrogenation processes of vegetable oils, aimed at the production of modified fats with optimized parameters (increasing hydrogenation activity, reducing harmful *trans*-fatty and saturated fatty acids in the reaction products) for the needs of the food industry. Synthetic silicate supports such as silica gels were chosen as carriers for these catalyst systems, thus eliminating the disadvantages of natural silicate sources (differences in composition between individual batches and content of different metals, which requires procedures of mechanical, chemical, thermal, etc. treatments). By introducing specific modifying additives (M, Ag, CeO<sub>2</sub>) precise control over the hydrogenation kinetics was achieved. This allows for optimization of selectivity towards the target *cis* -isomers and effective minimization of the synthesis of unwanted *trans*-fatty acids, which is of critical importance for the quality of food products.

In the next direction, nickel-based catalysts, namely NiAl and NiMgAl layered double hydroxides (LDH), modified with Au and CeO<sub>2</sub> for the WGS, are again used. Studies confirm that the efficiency of the catalysts in the WGS is a function of the Ni concentration, the presence of Mg and the Au content. NiAl -based systems with the maximum gold content exhibit the highest activity due to the increased density of active centers. An optimization methodology has been defined by precisely controlling the Ni–Mg–Al ratio, and the role of magnesium in the LDH structure has been identified as critical for achieving a balance between CO activation and water vapor dissociation. The modification of NiAl LDH with CeO<sub>2</sub> leads neither to an improvement in the reducibility nor to an increase in the efficiency of the catalyst, but the simultaneous presence of gold and cerium has a beneficial effect, and the optimal amount of CeO<sub>2</sub> has been found, which provides the highest dispersion of gold particles in the Au / CeNiAl catalyst.

The Ni-Al layered double hydroxides have also been used as precursors of catalysts for CO<sub>2</sub> methanation (an efficient method for conversion and utilization of carbon emissions) and have been found to be a successful alternative to conventional nickel catalysts. The effect of the type of divalent metal (Ni or Co) on the structure, phase composition, thermal stability and reducibility of co-precipitated Ni-Al LDH and Co- Al LDH at a molar ratio of  $M^{2+}/Al^{3+} = 3.0$ , where  $M^{2+} = Co^{2+}$  or  $Ni^{2+}$ .

I would like to pay particular attention here, again, to research with a strong applied focus, namely the creation of a non-platinum catalyst composition, NiPd, for the anode in

GenCell products Ltd , Petah Tikva). Two NiPd catalysts have been developed and implemented in production , with the second composition being optimized to achieve a reduced price. The catalyst compositions and synthesis methodology are protected by patent US 10,522,844 B2 dated 31.12.2019. Technological procedures for the synthesis of industrial batches of catalyst with a mass of 1, 2 and 3 kg have been developed and validated . The two catalysts are part of the company's commercial products.

According to the above-defined Direction 3. Development and research of effective catalysts for clean and safe industry, research is focused on: *development and research of catalysts for the removal of synthetic dyes from industrial wastewater and development and research of catalysts for air purification by catalytic ozone degradation.*

The catalytic potential of Co-Al<sub>2</sub>O<sub>3</sub> has been investigated oxide systems synthesized by sol - gel method and calcined at high temperatures (1000 °C and 1100 °C). The catalysts were applied for the decomposition of the dye Orange G in the presence of Oxone ® and textile dyes Orange G ( anionic ) and Basic blue 41 ( cationic ) in the presence of Oxone ®, a precursor of sulfate anion radicals, which are the main reactive oxygen species. It has been found that the oxide Co- Al<sub>2</sub>O catalysts are effective in the degradation of other dyes studied: Methylene Blue , Basic Blue 41 and Remazol Brilliant Blue R. Found that they can also be used for simultaneous degradation processes, Orange G in binary mixtures of dyes.

In conclusion, the habilitation and author's report of Dr. D. Nikolova reveals in an indisputable way her significant contribution to all published scientific results. Her personal merits in the design of new nanoscale metal and metal oxide catalysts with desired and controlled characteristics and catalytic properties, in clarifying the relationship between structure and activity in reactions for obtaining alternative ecological fuels, environmental protection and improving the quality of life, are beyond doubt. The results of the research are an important stage in building the scientific foundations for the selection of catalysts, a major part of the development of innovative technologies.

### **Personal qualities of the candidate**

I have known Assoc. Prof. Dr. Nikolova since she joined the institute and have personal observations of her overall scientific activity. For the last year, we have been working together on the implementation of the project "Pure Hydrogen Technology for Green Energy - A Step Forward to Zero Emissions", funded under investment C2.I2: "Increasing the Innovation Capacity of the Bulgarian Academy of Sciences in the Field of Green and Digital Technologies" as part of the National Recovery and Resilience Plan, and also within the framework of the HITMOBILE Center. I am impressed by her activity and purposefulness, precision, ambition and drive to expand scientific research, her relationships with colleagues and her ability to work in a team.

### **Conclusion**

The scientific research of Assoc. Prof. Dr. Dimitrinka Aleksieva Nikolova fully meets the topic of the announced competition for the award of the academic position of "professor". The publication activity, the citations of the published results, the participation in projects fully meet all the requirements of the Academic Staff Development Act and the Regulations on the terms and conditions for acquiring scientific degrees and occupying academic positions in the EC - BAS.

I strongly recommend that the Scientific Jury and the National Board of the IC-BAS vote "YES" for the appointment of Assoc. Prof. Dr. Dimitrinka Aleksieva Nikolova to the academic position of "Professor" in the professional field 4.2. "Chemical Sciences", scientific specialty "Chemical Kinetics and Catalysis ".

06/02/2026

Sofia

Reviewer:

/Prof. Dr. Silvia Todorova/