R E V I E W

by Prof. Dr. Mihail Mihaylov – IGIC–BAS, member of the Scientific Jury

for the competition announced in the State Gazette, issue 55 of June 27, 2023, for the position of "Associate Professor" in the professional field 4.2 "Chemical Sciences," scientific specialty "Chemical Kinetics and Catalysis," thematic direction "Synthesis and Characterization of Catalytic Materials for the Abatement of Volatile Organic Compounds" for the needs of the Laboratory of "Catalysis for Energy and Environmental Protection," Institute of Catalysis, Bulgarian Academy of Sciences

In the competition for the position of "Associate Professor", only one candidate is participating - Asst. Prof. Dr. Petia Tsvetanova Petrova, currently employed in the Laboratory of "Catalysis for Energy and Environmental Protection" at the Institute of Catalysis, Bulgarian Academy of Sciences.

1. Review of the Candidate's Documents

For her participation in the competition, Dr. Petrova has presented all the necessary documents: (i) application; (ii) a copy of the announcement in the State Gazette; (iii) curriculum vitae; (iv) diploma for the educational and scientific degree of "Doctor"; (v) certificate of work experience in the specialty as "Assistant Professor"; (vi) a list, reprints, abstracts, translation of abstracts, and a list of citations of scientific papers for participation in the competition; (vii) a general list of scientific papers; (viii) reference of fulfilment of requirements for occupying the academic position "Associate Professor" in the Institute of Catalysis; (ix) author reference for scientific contribution of the works included in the habilitation and non-habilitation works.

2. Brief Biographical Data about the Candidate

Asst. Prof. Petia Petrova graduated from the University of Chemical Technology and Metallurgy in Sofia in 2003 with a specialization in "Inorganic Substances Technology." In the same year, she started working as a chemical engineer at the Institute of Catalysis, Bulgarian Academy of Sciences, in a laboratory then titled "New Catalytic Materials and

Nano-sized Catalysts." The following year, she enrolled as a Ph.D. student, and in 2009, she successfully defended her dissertation on the topic of "Gold-Molybdenum Catalysts Supported on CeO_2 and CeO_2-Al_2O_3 for the Complete Oxidation of Benzene," earning her the educational and scientific degree of "Doctor."

In 2010, Dr. Petrova was appointed as an Assistant Professor. From 2011 to 2018, she underwent several short-term specializations at Bilkent University in Ankara, Turkey, the Royal Institute of Technology in Stockholm, Sweden, and the Institute of Nanomaterials in Palermo, Italy.

Since 2017, alongside her research work at the Institute of Catalysis, she has been working as a teacher in "Chemistry and Environmental Protection," most recently in some of the most prestigious high schools in Sofia, including the First English Language School and the 91st German Language School. She is frequently engaged by the Ministry of Education and Science to evaluate textbook projects for "Chemistry and Environmental Protection" for the eleventh and twelfth grades.

3. Overall Assessment of the Candidate's Scientific Activity

Dr. Petia Petrova has co-authored a total of 47 publications, which have been cited over 360 times by other authors. Her overall H-index according to Scopus is 14.

In the competition, she has participated with 25 papers related to the competition's topic, of which 8 have been published in Q1 journals, 7 in Q2 journals, 4 in Q3 journals, 1 in a Q4 journal, and 5 in open-access journals and conference materials without a Q category. These articles have been published in reputable specialized journals such as Applied Catalysis B: Environmental (IF 24.319, 2 publications), Chemical Engineering Journal (IF 16.744, 1 publication), Fuel (IF 8.035, 1 publication), International Journal of Hydrogen Energy (IF 7.139, 1 publication), Catalysis Today (IF 6.562, 2 publications), Applied Catalysis A: General (IF 5.723, 1 publication), among others. Dr. Petrova is the first author in 4 publications and the second author in 12, demonstrating her significant contribution to the conducted research. The publication of results in peer-reviewed journals excludes any elements of impropriety or plagiarism in the materials submitted for the competition.

Furthermore, the publications submitted for the competition have received 240 citations (excluding self-citations), mainly from foreign authors, which undeniably confirms the relevance and high quality of the research conducted with Dr. Petrova's participation.

The evaluations of the candidate by indicators, according to the minimum requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria and the rules for its implementation, as well as the increased criteria of the Bulgarian Academy of Sciences and the Institute of Catalysis, are presented in Table 1. An analysis of the quantitative results of the candidate's research activities demonstrates that Dr. Petrova exceeds the minimum requirements, especially regarding the citations of her scholarly works. The reference has been completed accurately and reflects the candidate's performance across all criteria.

Table 1. Evaluation of the candidate according to the indicators according to the requirements at the Institute of Catalysis.

Indicator	Points required	Points candidate
A. PhD Dissertation	50	50
B. Habilitation Work	100	150
D. Scientific Publications Outside the Habilitation Work	220	262
E. Citations	60	480
Total	430	942

4. Analysis of the Main Scientific Contributions

Ten of the publications with which the candidate participates are included in her habilitation work, while the results from the remaining 15 publications are summarized in her author reference. These scientific publications primarily focus on the field of environmental catalysis and investigate significant aspects such as the influence of the material synthesis method and relationship between the composition, structure, textural characteristics, redox properties, and catalytic activity.

4.1. Habilitation Work

All publications included in the habilitation work (publications No. 1-3, 5, 15, 19-22, 24) fully correspond to the thematic direction of the competition and are related to the development of efficient materials for the neutralization of volatile organic compounds through catalytic combustion. As a model reaction, complete oxidation of the stable molecule benzene has been

primarily studied. In some cases, oxidations of formaldehyde (publication No. 1), methanol, and CO (publication No. 20) have also been investigated. The objects of study are catalysts based on gold, cobalt, and cerium oxide. Interest in gold as a catalyst has grown rapidly since the surprisingly high activity of nanosized gold particles in the low-temperature oxidation of CO was reported. The mixed-valent cobalt (II, III) oxide with a spinel structure among transition metal oxides exhibits relatively high activity in the catalytic combustion of volatile organic compounds. The use of CeO_2 as a catalytic component is mainly due to the easy conversion between Ce^{3+} and Ce^{4+} without changes in its fluorite structure.

The main scientific contributions in the habilitation work can be summarized as follows:

In publications No. 3 and 5, it was established that CeO_2 promotes the catalytic activity and stability of Co_3O_4 in the complete oxidation of benzene (COB). Moreover, it was demonstrated that when the precursors of both oxides are mechanochemically mixed in a specific ratio (30 wt.% CeO_2), the best results are achieved due to the formation of strained structures of Co_3O_4 and CeO_2 with an increased concentration of defects and Co^{3+} on the surface.

Publication No. 2 noted that doping Co_3O_4-CeO_2 with potassium leads to a decrease in reducibility, texture deterioration, and therefore a drop in catalytic activity in COB.

Publications No. 1, 2, 15, 19-22, and 24 are dedicated to nanoscale gold catalysts (2-3 wt.% Au) supported on CeO_2, usually combined with cobalt oxide due to the synergy between the redox properties of the two oxides.

Key factors for high activity in catalytic combustion have been identified, including the size of the gold particles, the presence of active oxygen in the catalyst, and the activation of the benzene molecule.

It has been established that doping the CeO_2 support with transition metal oxides such as Fe_2O_3 and MnO_x leads to the suppression of catalytic activity in COB, despite increased reducibility. The lack of correlation between the reduction and catalytic behavior in this case is explained by the decisive role of benzene activation.

It is shown that doping Au/CeO_2 with Co_3O_4 leads not only to an increase in catalytic activity in COB but also to the obtaining of catalysts showing high activity in low-temperature combustion of methanol and CO.

The advantages of mechanochemical mixing compared to co-precipitation in obtaining a support with a composition of 10 wt.% Co_3O_4-CeO_2 have been demonstrated. This is related to the presence of two phases - cobalt-modified CeO_2 and a separate phase of cobalt oxide.

The latter favours both the reducibility of the support and the small size of the gold particles, which explains the high activity of the catalyst in COB.

Publication No. 2 shows the potential for practical application of a gold catalyst supported on mechanochemically obtained Co_3O_4-CeO_2 (30 wt.% CeO_2). This catalyst is synthesized by an easy and environmentally friendly method and exhibits high stability and complete conversion of benzene to CO_2 and H_2O at relatively low temperatures, without generating side air-polluting products.

In publication No. 1, it is established that combining high hydroxyl coverage and defect concentration when mixing aluminum oxyhydroxide (boehmite) and cerium-cobalt oxide leads to obtaining a suitable support for gold catalysts for total formaldehyde combustion at low temperatures, slightly above room temperature.

4.2. Publications outside the habilitation work

Some of the publications outside the habilitation work are also dedicated to the catalytic combustion of hydrocarbons, including benzene (publications No. 4,7,11,1214,17) and propene (publication No. 12), with the research extended to Pd and bimetallic Au-Pd catalysts. In general, the contributions in these cases are related to clarifying the influence of the type, quantity, and method of doping of the support and the nature of the supported mono and bimetallic catalysts on their structural, redox, and catalytic properties.

Most of the remaining articles are also about catalytic reactions related to environmental protection, such as the selective oxidation of CO for the fine purification of hydrogen for fuel cells (publications No 6,8-10,13,18). Of significant interest are the following results:

The addition of yttrium to CeO_2 in certain small amounts improves the selectivity of the supported gold catalysts and their stability in the presence of water and CO_2. The studies show that impregnation with yttrium has an advantage over co-precipitation, as it results in the surface coverage of CeO_2 with nanoparticles of Y_2O_3 and a decreadse in its basicity. Additionally, the use of Al_2O_3 as a support for such compositions demonstrates the potential to obtain catalysts for practical applications.

Doping Au/CeO_2 with praseodymium leads to decreased CO conversion in the operating temperature range of fuel cells (80-120°C) due to hindered reoxidation of the surface, associated with praseodymium oxide segregation.

Publication No. 16 relates to the development of gold catalysts for the reduction of nitrogen oxide with CO that can be used during the “cold start” period of the engines. A gold catalyst supported on Fe_2O_3-modified CeO_2 has been obtained, which shows high activity, stability, and selectivity towards N_2. Furthermore, the studies show that iron doping favors NO conversion but increases selectivity towards N_2O.

Publication No. 25 investigates catalysts for the cyclization of 1,4-butanediol as a step in the production of antitumor drugs. The study demonstrates that adding approximately 0.5 wt.% palladium to the Co_3O_4/SiO_2 catalyst enhances the reducibility of cobalt oxide, improves dehydrogenation, and significantly increases the yield of 2,3-dihydrofuran.

5. Conclusion

Dr. Petia Petrova's scientific research represents a significant contribution to the development of catalysts for environmental applications based on a scientifically grounded approach. The results have been published in prestigious journals and are highly cited, demonstrating their relevance and importance. The analysis of the quantitative indicators of the candidate has shown that they exceed the requirements of the Law on the Development of Academic Staff in the Republic of Bulgaria and the Regulations of the Institute of General and Inorganic Chemistry - BAS. Therefore, with confidence, I provide my positive evaluation and recommend to the Scientific Jury and the Scientific Council of the Institute of Catalysis - BAS to vote "YES" for the appointment of Asst. Prof. Dr. Petia Petrova to the academic position of "Associate Professor" in the professional field 4.2. "Chemical Sciences," scientific specialty "Chemical Kinetics and Catalysis."

October 3, 2023 Member of the Scientific Jury:

Sofia /Prof. Dr. Mihail Mihaylov/