

OPINION

of Assoc. Prof. Dr. Violeta Koleva
from Institute of General and Inorganic Chemistry – BAS

on the competition for occupation of the academic position “Associate Professor” in professional field 4.2. "Chemical Sciences", scientific specialty "Chemical Kinetics and Catalysis" for the needs of the Institute of General and Inorganic Chemistry (IGIC), Laboratory "Reactivity of Solid Surfaces", announced in Newspaper of State, issue 36, dated 03.05.2019

Assist. Prof. Dr. Stanislava Andonova is the only candidate in the announced competition. All the documents, required and specified by “The Regulations for the Terms and Rules for Occupation of Academic Positions in IGIC” have been duly submitted.

The research activity of the applicant comprises 32 scientific works, of which: 24 articles in journals with impact factor, one article in a journal without impact factor, 4 articles as conference papers and 3 patent applications. Assist. Prof. Andonova participates in the present competition with 22 scientific works (which do not repeat the ones presented for science degree PhD) published in the period from 2009 to 2019, of which 19 articles and 3 patent applications on the same topic.

It is noteworthy that all the papers have been published in reputable international journals with high impact factor: 15 papers (80%) are in journals having impact factor above 4.5, respectively being of the highest category Q1, and the other 4 - in journals with impact factor between 2 and 3 (category Q2). The significant role of Assist. Prof. S. Andonova in the joint research is confirmed by the fact that she is the first author in 10 articles and 3 patent applications, as well as a corresponding author of one of the articles. All the papers are co-authored by leading foreign scientists on the topic (or together with scientists from IGIC), the cooperation being established during the long-term specialization of the applicant abroad. Research results have been presented in 16 international and 2 national scientific events as the number of applicant's oral presentations is impressive - 11. She is participant in 3 international and 3 national projects.

The overall research activity of Assist. Prof. Andonova is entirely in the field of synthesis and characterization of catalysts and adsorbents for specific purposes. She has started these studies as a PhD student at the Institute of Catalysis (BAS) and continued them in co-operation with scientists from Bilken University in Turkey, the Center for Catalysis Competence in Sweden, etc., and from IGIC since 2013.

The studies involved in the competition are mainly related to environmental protection issues and can be summarized into two thematic directions: 1) Development and investigations of efficient catalysts for reducing nitrogen oxides emissions from automobile engines; 2) Investigations on metal-organic frameworks for CO₂ capture and separation.

The majority of research (80%) is focused on solving one of the serious air pollution problems caused by nitrogen oxide emissions. Two different catalytic approaches have been applied: use of NO_x storage-reduction (NSR) catalysts and selective catalytic reduction (SCR) of NO_x with

ammonia which determine the nature of the studied catalysts. A part of the studies on this topic (8 papers and one patent application) are included in the Habilitation Work. A common feature of these investigations is the adequate combination and thorough use of a variety of methods such as IR spectroscopy of adsorbed NO₂, NO, NO+O₂, CO and H₂ molecules with isotope exchange technique (OH/OD and H₂/D₂) that allows a correct interpretation of the observed spectral pictures; dynamic adsorption/desorption measurements; temperature programmed desorption/reduction; powder X-ray diffraction, X-ray photoelectron spectroscopy, energy dispersive spectroscopy, scanning and transmission electron microscopy, catalytic tests at different regimes, and in some cases microcalorimetry and Raman spectroscopy. The valuable information derived from the different characterization methods provides a deep understanding of the fundamental aspects of NO_x storage and reduction in order to increase the activity, selectivity, thermal stability and tolerance to poisoning of the catalysts.

The promoting role of the additives of metallic Rh as well as CeO₂ and ZrO₂, in pure and mixed state, to modify properties of conventional NSR catalyst Pt/BaO/γ-Al₂O₃ has been elucidated in details. NO_x storage and reduction behavior have been also studied in FeO_x/BaO/γ-Al₂O₃ and Ag/γ-Al₂O₃ catalytic systems at low temperatures. The scientific achievements of these studies are related to acquisition of new knowledge and confirmatory data in respect to: nature of the active sites; composition, oxidation state, coordination and the thermal stability of the surface species; multilateral interactions at the catalyst surface; mechanism of adsorption and reduction of NO₂.

The significant effect of TiO₂ on the increased NO_x storage and resistance to SO₂ poisoning of BaO/TiO₂/γ-Al₂O₃ catalyst has been clarified based on thorough comparative study on binary and ternary oxide systems, TiO₂/γ-Al₂O₃ and BaO/TiO₂/γAl₂O₃. The well-dispersed TiO₂ has been found to create additional active NO_x storage sites in the form of bridged and bidentate nitrates as well as to enhance surface dispersion and mobility of BaO clusters which ensures suppressed growth of the large BaSO₄ domains and facile regeneration of the small BaSO₄ clusters.

Regarding the selective catalytic reduction of NO_x with NH₃, the development of a new type of Fe-exchanged SAPO-34 zeolite, characterized by increased activity at high temperatures and significantly improved hydrothermal stability as compared to the commercial Cu/CHA zeolite, is an undisputed contribution. A combined catalytic system, Fe/SAPO-34 + Cu/CHA, with high activity for NO_x reduction over a broad temperature range has been also proposed. Valuable information on the mechanism of deactivation of the zeolites Cu/BEA with phosphorous and Cu/SAPO-34 with SO₂ has been obtained.

The scientific achievements in the investigations on CO₂ capture and storage are mainly related to elucidation by means of IR spectroscopy of various aspects of the interactions of this gas with metal-organic frameworks such as the role of the hydroxyl groups to form different CO₂ species and to increase the adsorption capacity. IR spectroscopic approaches have been proposed for the differentiation of monomer and dimer CO₂ species as well as for more precise determination of the hydroxyl group acidity by comparing the spectroscopic data for the shift of the stretching OH vibrations at adsorption of CO и N₂ used as probe molecules.

An objective assessment of the value of the scientific achievements in the applicant's works is the significant number of the independent citations – 384, of which 315 reflected in WoS and Scopus database. On the publications submitted to the competition 215 citations were noticed. The H-index of the applicant is 10 based on all the papers, accordingly 9 on the topic of the competition.

I would also like to note the following: In my opinion it is not correct a patent application on the same topic to be considered as three separate scientific works, although from standpoint of the national patent law such distinction is permitted in the case since the patent application is registered in different countries. The consideration of the patent application as a single scientific work would not reduce either the scientific contributions or sufficiently high scientific indicators of the applicant.

Conclusion: Assist. Prof. Dr. Stanislava Andonova is highly qualified researcher in the field of synthesis and characterization of catalysts and adsorbents of ecological importance. The research performed is of a high level and fully corresponds to the theme of the competition. The Applicant covers and exceeds all required scientific indicators under the ZRASRB and the Regulations for its Implementation, as well as the Regulations of IGIC for the acquisition of academic position "Associate Professor". In view of the value of the scientific contributions and the scientific metrics achieved, I convincingly recommend the members of the Scientific Jury and the Scientific Council of the IGIC to award to Assist. Prof. Dr. Stanislava Andonova the academic position "**Associate Professor**" in the professional field 4.2. Chemical Sciences, scientific specialty "Chemical kinetics and catalysis".

Member of the Scientific Jury:

Date 02.08.2019

/Assoc. Prof. Dr. Violeta Koleva/