REVIEW

on the competition for the academic position "Associate Professor"
in the professional field 4.2. Chemical sciences (Inorganic chemistry),
announced in the State Gazette no. 36 / 03.05.2019
by the Institute of General and Inorganic Chemistry-BAS
for the High Temperature Oxide Systems Laboratory

Reviewer: Prof. Dr. Ekaterina Zhecheva from the Institute of General and Inorganic Chemistry of the Bulgarian Academy of Sciences

1. General information and brief biography of the applicant

One candidate - **Assistant Professor Dr. Albena Dimitrova Bachvarova-Nedelcheva** from IGIC-BAS, participates in the competition for the selection of an Associate Professor in the professional field 4.2 Chemical Sciences (Inorganic chemistry) announced by the Institute of General and Inorganic Chemistry of the Bulgarian Academy of Sciences (IGIC- BAS) in SG No. 36 / 03.05.2019 for the High Temperature Oxide Systems Laboratory at IGIC.

Assistant Professor Dr. Bachvarova-Nedelcheva graduated in the year 2000 from the University of Chemical Technology and Metallurgy in Sofia with a Master degree in Chemical Engineering, majoring in Materials Technology and Materials Science. During her studies, she also obtained the professional qualification "Teacher in general technical and special subjects". As a student, she was specializing in an ERASMUS-SOCRATES project in the year 2000 for 3 months at the University of Aveiro, Portugal, Department of Glass and Ceramics. After finishing her higher education, she was a full-time PhD student at the University of Chemical Technology and Metallurgy under the supervision of Professor Dr.Sc. Yanko Dimitriev. In 2005 she defended her PhD Thesis entitled "Glass and Phase Formation in the Selenite Systems SeO_2-Ag_2O-M_nO_m and SeO_2-CuO-M_nO_m (M_nO_m = B_2O_3, MO_3)". Since 2005 she has been working at the Institute of General and Inorganic Chemistry of the Bulgarian Academy of Sciences, initially as a chemist and since 2010 as an Assistant Professor at the Laboratory of High Temperature Oxide Systems.

2. Description of the submitted documents

Assist. Prof. Bachvarova presented a list of her total scientific output: 61 scientific papers, 56 of which were in Impact Factor IIF) and Impact-Rank (SJR) journals. The journals where she published most often are Journal of Chemical Technology and Metallurgy - 15 papers (a journal with SJR without IF) and Bulgarian Chemical Communications - 13 articles (Q4) .

The candidate participates in the competition for Associate Professor with 28 scientific works, 10 of which are assigned to her habilitation work. All papers included in the

habilitation work are published in specialized international journals with an impact factor. They are distributed in the quartiles (Q) as follows: Q1 - 5 papers (Journal of Materials Science with IF_{2018} = 3.442, Materials Research Bulletin with IF_{2018} = 3.335, Journal of Non-Crystalline Solids with IF_{2018} = 2.600 and two papers in Optical Materials with IF_{2018} = 2.687); Q2 - 2 papers (Journal of Optoelectronics and Advanced Materials and Journal of Materials Science); Q3 - 3 papers (Physics and Chemistry of Glasses, Advanced Materials Research and Optoelectronics and Advanced Materials - Rapid Communications), Q4 - none.

The papers that do not belong to the habilitation work are assigned to the following quartiles: in Q1 - none, in Q2 - 4 papers (Digest Journal of Nanomaterials and Biostructures with IF_{2018} = 0.638, Central European Journal of Chemistry with IF_{2018} = 1.460, European Journal of Glass Science and Technology B with IF_{2018}= 0.857 and Journal of Sol-Gel Science and Technology with IF_{2018} = 1.986), in Q3 - 4 papers, in Q4 - 5 papers, in journals with SJR but without IF - 5 papers.

A list is attached containing the titles of her contributions to scientific forums in Bulgaria and abroad – a total of 62.

307 citations on Mrs. Bachvarova's scientific papers are visible in Web of Science and/or Scopus databases. Her Hirsch index (Scopus) is 9. The citations on the papers submitted to the competition are 206.

In total, the applicant was a team member in 10 projects, one of which was funded under the EU Framework Programs and the rest was nationally funded (National Research Fund and National Innovation Fund). She participates in the competition with 3 projects funded by the National Science Fund.

Mrs. Bachvarova was advising the thesis of 4 master students at the Faculty of Chemical Engineering and Metallurgy, as well as 2 PhD students at the University of Chemical Technology and Metallurgy and one at IGIC-BAS.

All documents presented by Assist. Prof. Bachvarova fit the topic of the competition. Scientometric data satisfy the requirements specified in the Law for the Development of the Academic Staff of the Republic of Bulgaria and the Regulations for its application for the occupation of the academic position of "Associate Professor" in the scientific field "Natural Sciences, Mathematics and Informatics", professional direction "Chemical Sciences", as well as the Rules on the Terms and Conditions for Acquisition of Academic Degrees and Occupation of Academic Positions at IGIC-BAS (1042 points in total with 500 required).

3. General characteristics of the research activity

The studies of Assist.Prof. Bachvarova cover two modern fields of inorganic chemistry: (i) synthesis and characterization of glasses with the participation of non-traditional glass formers, mainly SeO_2 and TeO_2, and (ii) sol-gel methods for synthesis of nanostructured and nanocomposite materials with functional properties.

The publications of the habilitation work belong to the first field and contain results on the synthesis of selenite glasses and crystalline phases in three- and multi-component selenite systems. In addition to the theoretical aspect, selenite glasses are also of potential practical

interest due to their low melting point, high refractive index and high transmittance in the near infrared region of the spectrum. Due to the specificity of the investigated compositions, different synthesis methods were used (in evacuated quartz ampoules, in autoclave apparatus or in the air), and glass- or glass-crystalline monolithic samples were synthesized in three- and multi-component selenite systems. The compounds obtained are structurally characterized by X-ray analysis and spectroscopic methods (infrared spectroscopy and X-ray photoelectron spectroscopy). Optical properties (transmission spectra in the visible and near infrared region and diffuse reflectance spectra) have been investigated for some compositions. The short- and middle-range order of glass structures, as well as the structural transformations in the amorphous networks, are monitored as a function of their composition.

The articles outside the habilitation work belong to the candidate's second field of scientific interest. Sol-gel techniques for the synthesis of nanostructured and nanosized materials with photocatalytic and antibacterial activity have been adapted. Multicomponent nanocomposites based on TiO_2 - ZnO well as nanocomposite powders containing TeO_2 and TiO_2 from two- and three-component systems were obtained.

4. Major scientific contributions

4.1. Major scientific contributions of publications of habilitation work

Phase diagrams have been studied and new non-traditional selenite glasses have been synthesized in three-component systems, in which, in addition to SeO_2, non-traditional (MoO_3) or classic (B_2O_3) network-former and modifying oxide (Ag_2O or CuO) are involved. The regions of glass formation in the SeO_2-Ag_2O-MoO_3 and SeO_2-CuO-MoO_3 systems were experimentally determined. The short-range order in the glasses consists of SeO_3-, MoO_6- and MoO_4-structural units. The structural features of selenite glasses are determined by the existence of an upper and lower boundary of glass formation. For compositions with a high content of SeO_2, the upper limit of glass formation is determined by the depolymerization of the selenite chains in the presence of the modifying Ag^+ and Cu^{2+} ions, thereby increasing the structural disorder in the amorphous network. At low SeO_2 content, the lower boundary of glass formation is determined by the existence of mainly highly mobile isolated SeO_3 and MoO_4 units, thereby increasing the tendency to crystallize. By increasing the concentration of modifying ions, the number of bridging oxygen bonds between polyhedra decreases and the number of isolated SeO_3 and MoO_4 groups increases.

Replacing MoO_3 with the classic B_2O_3 network former in the SeO_2-Ag_2O-B_2O_3 and SeO_2-CuO-B_2O_3 systems does not improve glass formation, since BO_3 and isolated SeO_3 groups are involved in the formation of the amorphous network of the obtained glasses.

Multicomponent selenite and selenite-tellurite glasses containing other conditional network formers - Nb_2O_5, MoO_3 and V_2O_5, have been synthesized. From a structural point of view, it has been found that the amorphous network of all multicomponent tellurium-selenite glasses is composed of TeO_3, TeO_4 and SeO_3 units connected mainly by bridging oxygen bonds. Depending on their composition, the glasses are differently colored (yellow, orange, red) and are transparent above 400 – 500 nm. The results obtained from the optical

measurements of selenite-tellurite glasses indicate the presence of a sharp absorption edge in their spectra which suggests that these glasses could be used as optical filters.

The thermal stability of multicomponent selenite glasses and the possibility of stabilizing micro-heterogeneous structures with formation of glass-crystalline phases were investigated. SeO_2-rich glasses have been found to be thermally stable up to 300 ° C, while oxide phases crystallize above this temperature. When heating Ag^+ containing glasses at low temperatures (150 °C), micro-heterogeneous structures are formed due to the generation of silver nanoparticles.

4.2. Major scientific contributions of non-habilitation publications

Various sol-gel techniques have been used to prepare powders of nanosized (about 20 nm) ZnO - TiO_2 with different component ratios. Based on them, composite materials were obtained with the participation of the natural zeolite clinoptilolite, as well as multicomponent nanocomposite materials containing ZnO, TiO_2, SiO_2 and reduced graphene oxide, which exhibit good antimicrobial activity. A scheme for the synthesis of a complex composite containing three active phases Ag, TiO_2 and ZnO is proposed, for which a strong bactericidal effect towards E. Coli has been demonstrated. The crystalline phase $ZnTiO_3$ was synthesized and found to have good photocatalytic properties against the organic dye Malachite green, as well as good antibacterial properties towards high concentrations of E. Coli.

Transparent homogeneous and monolithic gels were synthesized in a wide concentration range by the sol-gel method in the three-component TiO_2-TeO_2-SeO_2, TiO_2-TeO_2-B_2O_3 and TiO_2-TeO_2-ZnO systems and the regions of gel formation have been identified. The resulting organic-inorganic hybrid networks are stable up to about 300 ° C. At higher temperatures and depending on the composition, simultaneous presence of different crystalline phases (TiO_2 - anatase, α-TeO_2, $TiTe_3O_8$, $ZnTeO_3$, $ZnTiO_3$, Zn_2TiO_4) and an inorganic amorphous part are found, the short-range order of which is determined by the structural units TiO_6, TeO_n, SeO_3, BO_3, BO_4 and ZnO_6. The nanocomposite materials obtained in the TiO_2-TeO_2-SeO_2 system exhibit good antibacterial activity towards E. Coli bacteria as result of a synergistic effect.

5. Impact of publications in the literature.

As already mentioned, Assist. Prof. Bachvarova submitted a list of citations on the papers for the competition - 206 citations appearing in the Web of Science and / or Scopus databases. For the publications included in the habilitation work, 39 citations were noticed, and for those beyond the habilitation work - 167 citations. For the habilitation work, the papers with the highest number of citations are those on glass formation in the SeO_2-Ag_2O-B_2O_3 system and on the structure of selenite-tellurite glasses (papers numbered 5 and 9 from the list of publications in the habilitation work with 14 and 15 citations, respectively). In addition, there is a strong impact in the literature of the set of publications beyond the habilitation work, which are focused on the preparation of ZnO-TiO_2 based nanocomposite materials having photocatalytic and bactericidal properties – more than 150 citations have been noted.

6. Critical notes and recommendations for the applicant's scientific work.

I have no general objections to the documents presented.

7. Evaluation of the applicant's personal contribution and impressions

All of Assist. Prof. Bachvarova's publications for the competition are with co-authors. The average number of co-authors of the 10 papers included in the habilitation work is 3.8, with the candidate being a correspondent author in 8 publications, the first author in 8 publications and the second in the other 2. In non-habilitation papers, studies on the photocatalytic and antimicrobial activity of nanocomposite materials required an increase in the number of co-authors, but the candidate is the first author in 5 publications, the second - in five and the corresponding author in 11 publications. These data, as well as the thematic homogeneity of Mrs. Bachvarova's publications and my personal impressions, lead to conclude that Mrs. Bachvarova's contribution to these studies is clearly significant.

I have known Mrs. Bachvarova since she was starting work at IGIC and I have witnessed her academic progress. In addition to her excellent professional skills, she is impressive with her purposefulness and efficiency, which is the basis of her successful research work.

CONCLUSION

Assistant Professor Dr. Albena Bachvarova-Nedelcheva participates in the competition with an asset that fulfills, and in most cases far exceeds, the requirements for occupying the academic position of Associate Professor at the Institute of General and Inorganic Chemistry - BAS. Based on all of the above, and namely well-outlined and topical studies, the number and the quality of her papers and their impact in the literature, the scientific contributions as well as my personal impressions, I strongly recommend Assist. Prof. Dr. Albena Bachvarova-Nedelcheva to be appointed at the academic position of Associate Professor in the professional field 4.2. Chemical Sciences (Inorganic Chemistry) at the Institute of General and Inorganic Chemistry - BAS.

Reviewer:

Prof. Dr. Ekaterina Zhecheva

Sofia, 28.08.2019