

REVIEW

of the materials submitted for participation in a competition for the academic position of "professor" in the field of higher education 4. "Natural Sciences, Mathematics and Informatics", Professional field 4.2. "Chemical Sciences" (Inorganic Chemistry), announced in SG, issue. 47 of 04.06.2021 for the needs of the Laboratory "Salt Systems and Natural Resources" Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences

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she fulfills and repeatedly exceeds the national minimum requirements as well as the supplementary ones of the Institute of General and Inorganic Chemistry for occupation of the academic position "professor"

The only candidate in the competition is Assoc. Prof. Dr. DIANA TODOROVA RABADJIEVA. The presented materials are in accordance with the Law for the Development of the Academic Staff in the Republic of Bulgaria (LDASRB), its regulations, Regulations for application of LDASRB in IGIC-BAS.

1. Brief biographical data

Assoc. Prof. Rabadjieva acquired higher chemical education in the period 1981-1986 after graduating from the University of Chemical Technology and Metallurgy, Sofia; with qualification - chemical engineer, Speciality "Technology of inorganic substances". The master's degree is defended with a thesis on "Low-temperature catalysts for the conversion of CO with high Al₂O₃ content." He obtained the scientific and educational degree "Doctor" in 2003 by PhD thesis on "Crystallization processes in marine-type systems and applications."

Assoc. prof. Rabadjieva's scientific career began at IGIC-BAS with admission as a chemist in 1994. She successively acquired academic positions from assistant to associate professor in 2012. In 2017 she was elected head of the Laboratory "Salt Systems and Natural Resources" IGIC-BAS.

Assoc. Prof. Rabadjieva has a successful scientific career, which covers a total of 76 publications, of which 41 in journals with impact factor and 2 book chapters. She demonstrated active project activity with participation in a total of 76 projects. Assoc. Prof. Rabadjieva effectively combines scientific activity with applied chemistry activity by connecting research on nature and waste resources, in particular seawater and lye and their utilization. As a member of the laboratory "Salt systems and natural resources" she is involved in the traditional topics related to thermodynamic modeling and experimental studies of the processes of solubility and

crystallization in water-salt multicomponent systems. Research studies conducted aimed to establish patterns between the composition of solutions and the structure and type of crystallizing solid phases. The idea of this research studies is to achieve targeted synthesis of compounds with certain properties and structure. Her research interests include the application of thermodynamic modeling to estimate the speciation of chemical elements in solutions with different salinity. As a result, a reliable assessment of the chemical/ecological status of transitional waters has been achieved.

2. Description of the submitted materials

The materials that Assoc. Prof. Dr. Rabadjieva has applied are very precisely organized and it might be easily concluded that all formal requirements of LDASRB, the regulations for its implementation as well as the enhanced criteria of the Bulgarian Academy of Sciences and the special requirements of the Institute of General and Inorganic chemistry for the academic position of professor are met. Associate Professor Dr. Rabadjieva has attached a list of scientific papers for her entire scientific period, selecting publications for the award of educational and scientific degree doctor, materials for the award of the academic position of associate professor, materials in this competition and additional materials that characterize her research interests and achievements. She is a co-author of a total of 76 publications, of which 41 have been published in impact factor editions. The number of noticed citations of all scientific publications according to WoS and Scopus database is 275. Twenty publications were submitted for participation in the present competition, of which 17 were published in journals with impact factor (Web of Science), 3 were published in proceedings of international scientific conferences, presented in Conference Proceedings in Thomson Reuters and/or Scopus, 207 citations were declared for the period after the habilitation. About 70% of the publications with which the candidate participates in the competition are from the first Q1 (9) and second Q2 quartile (5). The habilitation paper is based on the results from 6 publications, published mainly in Q1 journals. The h-index of the candidate, according to citations of all articles (Scopus, Web of Science, Google Scholar) is equal to 10. The results of the research studies have been reported at a significant number of national and international forums, more than 30 participations with poster and oral presentations at international forums and more than 16 participations at national scientific forums have been presented. Associate professor Rabadjieva demonstrates high project activity - she has participated in 5 international research projects funded by the EU, NATO and others, she was a leader of one of them. She has been a participant and leader (3) of 14 national projects funded by the Ministry of Education and Science and NSF, a participant in 4 bilateral projects. All submitted materials are related to the topic of the competition. On the basis of the declared publication activity the candidate has attached a reference for the fulfillment of the minimum national requirements and the enhanced criteria of BAS for holding the academic position "Professor" in the scientific field "Natural Sciences, Mathematics and Informatics", professional field "Chemical Sciences". The distribution between indicators is as follows: indicator A - 50 points; indicator B - 135 points (recommended 100); indicator D - 262 points (recommended 220); indicator E - 380 points

(recommended 120) and indicator E - 187.6 points (recommended 150), indicator G - 290 points (recommended 120). It is obvious that the scientific data of Assoc. Prof. Dr. Rabadjieva meet and exceed the required minimum for all requirements under Art. 2b of the Law on Higher Education in the field of higher education 4. Natural sciences, mathematics and informatics in Professional field 4.2. "Chemical Sciences", when holding the academic position of "Professor".

3. General characteristics of the research activity and personal contribution of the candidate. Scientific contributions

All publications of the candidate in the competition are collective.

The main scientific interests and research of assoc. prof. Dr. Rabadjieva are in the field of chemistry of water-salt systems - topic of the laboratory "Salt systems and natural resources", which she develops and enriches within the framework of her scientific career at IGIC-BAS. The scientific topics include a combination of experimental and theoretical approaches for characterization of water-salt systems through phase equilibria, theoretical prediction of species of chemical elements based on appropriate thermodynamic models, thermodynamic modeling of equilibria. The obtained results have been successfully applied for the development of technologies for targeted synthesis of inorganic substances with predetermined properties.

The habilitation work is based on 6 publications and is dedicated to the main directions in the research of Assoc. Prof. Dr. D. Rabadjieva:

Investigations on phase equilibria in multicomponent water-salt systems through thermodynamic modeling, conducting laboratory experiments and developing technologies for targeted synthesis. The conducted researches are a good example of combining theoretical models with experimental application and final technological result. The main aim is to achieve complete characterization of high-salt systems obtained after evaporation of seawater by including additional components. Based on thermodynamic modeling, the conditions for obtaining $\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$ by metastable crystallization are shown and subsequently experimentally proved. The obtained results are applied for development of a new technology for production of large-crystal $\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$ with pharmacopeial purity and good filtration characteristics from waste sea lye, after malting. The developed technology has been confirmed by semi-industrial experiments.

A similar approach has been applied in studies of biomineralization processes, the mechanism of which is not yet fully understood. The idea is to find suitable biomimetic conditions to obtain bone-like materials for use in orthopedic and dental medicine. After thermodynamic modeling of metastable and stable phase equilibria in different systems, experimentally confirmed conditions for metastable crystallization of $\text{CaHPO}_4 \cdot 2\text{H}_2\text{O}$ and amorphous calcium phosphate $\text{Ca}_3(\text{PO}_4)_2(\text{am})$, doped with Mg^{2+} or Zn^{2+} ions depending on the composition of initial solution. The relationship between the composition of the initial simulated tissue fluid and the behavior of the two phosphates - dissolution/crystallization/re-crystallization - has been proved theoretically and experimentally. The recrystallization of $\text{CaHPO}_4 \cdot 2\text{H}_2\text{O}$ and $\text{Ca}_3(\text{PO}_4)_2(\text{am})$ into thermodynamically more stable hydroxyapatite has been predicted and experimentally proven, regardless of the composition of the simulated tissue fluid. The influence of the organic component

in the body fluids as well as the increased content of HCO_3 on the processes of dissolution and production of low-crystalline carbonate apatite was evaluated.

Thermodynamic modeling of natural systems, distribution of chemical species of the elements in order to assess their bioavailability and accumulation. Extremely relevant field, in the research of assoc. prof. Dr. D. Rabadjieva, in which on the basis of theoretical modeling, chemical species of the elements have been determined in different types of water bodies. Regardless of the variety of programs for calculating chemical speciation, any new application in this direction is essential, aiming to achieve as higher as possible relevance to environmental conditions. The candidate proposes a new combined model for calculation of inorganic chemical species of the elements in salt and hyper salt waters. In addition to this application, a new database has been developed, including thermodynamic data for the elements Al, Fe, Mn, Co, Ni, Cu, Zn, Cd and Pb and their binary parameters of ionic interaction. It should be emphasized that the new Directive 2013/39/EU introduces an environmental quality standard for lead and nickel content in surface waters taking into account only their bioavailable species, the same approach should be applied when assessing the ecological status based on the elements - copper, zinc, manganese, i.e. the total concentrations measured by standard spectral and mass spectral methods cannot be used to assess surface water quality. In Bulgaria for the assessment of chemical/ecological status condition, i.e. the compliance of the concentrations of lead and nickel, copper, zinc, manganese with their quality standards is performed by applying the model of biotic ligands, but this model is not suitable for salt and hyper salt waters. The candidate's approach for highly saline aqueous solutions provides new information on water bodies of the transitional water type (Atanasovsko Lake and Pomorie Lake, Burgas Bay, Ropotamo River and Aheloy River, which is extremely important for national monitoring. Probably in future plans, the results obtained by the proposed modeling will be compared with the results obtained by analytical methods based on electrochemistry or ion exchange for experimental determination of chemical species. Experimental studies on the assessment of relationship between chemical species of elements and their biouptake revealed new data on the bioavailability of small kinetically labile inorganic complexes. Topic of high importance due to the lack of environmentally relevant experimental data. The relatively new idea is that not only free ions but also small inorganic complexes might be bioavailable. In recent studies the candidate includes in the thermodynamic modeling the concentration of the dissolved organic matter, which further increases the relevance of the obtained results.

Studies related to the possibilities for targeted synthesis of inorganic compounds with a certain composition and properties deserved interest. Based on theoretical models and experimental results, the influence of a number of factors is evaluated, which allows to predict and propose suitable conditions for targeted synthesis.

connection has been established between synthesis - composition - structure for double salts of the type $x\text{Gly}_y\text{ZnX}_2 \cdot z\text{H}_2\text{O}$ ($X = \text{Br}^-$, I^- , $x = 1, 2, 3$; $y = 1, 3$; $z = 0, 2, 4$), structure of the solution - kinetics of crystallization of soluble salts, composition - thermal properties, composition - gelation.

Scientific contributions can be characterized as new scientific results with very good practical application and potential for final realization

The report on the contribution nature of the scientific works of Assoc. Prof. Dr. D. Rabadjieva is comprehensive and very correctly outlines her own contributions, which gives me a reason to conclude that the personal contribution of the candidate in the presented research is undoubted and significant.

4. Reflection in the literature

Assoc. prof. Dr. D. Rabadjieva presented a list of citations of the works with which she participated in the competition and the general conclusion is that the research she has conducted and published has found a serious response in the literature. The articles devoted to the kinetic and thermodynamic studies in biomimetic transformations of amorphous calcium phosphate have a significant number of citations and shows the relevance of the obtained results. The articles characterizing the chemical species of the elements in waters from mining areas have also received a wide response.

5. Pedagogical activity

Assoc. prof. Dr. D. Rabadjieva is the supervisor of a successfully defended doctoral student and is currently the supervisor of a second doctoral student of independent training.

6. Critical remarks

I have no principled critical remarks on the research from the publications of assoc. prof. Dr. Rabadjieva

CONCLUSION

Associate professor Dr. D. Rabadjieva has submitted for participation in the competition detailed information about her scientific activities. The evaluation of the presented materials by a system specified in the Regulations applying the LDASRB, demonstrates that Dr. D. Rabadjieva covers the requirements for the occupation of the academic position "Professor" at IGIC-BAS in the professional field of "Chemical Sciences". The presented documents show that she is a researcher with her own style and original ideas, who successfully combines theoretical approaches with experimental results to solve scientific problems and in addition to reach effective application of the results obtained in practice. A review of the publications shows that she successfully upgraded the achievements of the Laboratory "Salt Systems and Natural Resources" and has a clear perspective for its future development. In this aspect, based on current and promising scientific topics, quantity and quality of scientific papers, responses in the literature, scientific contributions, leadership and participation in scientific projects, I strongly recommend the Scientific Council of IGIC-BAS to vote positively for the award of the academic position " Professor" in professional field 4.2. Chemical sciences, scientific specialty "Inorganic chemistry for associate professor Dr. D. Rabadjieva.

One can see that Dr. Violeta Koleva significantly exceeds the national requirements for the occupation of the academic position “Professor”, the enhanced criteria of the Bulgarian Academy of Sciences and the special requirements of the Institute of General and Inorganic chemistry

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