

REVIEW

for obtaining the scientific position of Associate Professor at the Faculty of Chemistry and Pharmacy at Sofia University "St. Kliment Ohridski "in the scientific specialty 4.2. Chemically Sciences (Theoretical Chemistry) in a competition announced in the State Gazette, issue 63 of 30.VII. 2021 with candidate **Julia Ruslanova Romanova, Doctor of Chemistry, Chief Assistant.**

(three names, scientific title, scientific degree, position)

Reviewer: **Ivan Petkov Bangov, Doctor of Chemical Sciences, Professor, University of Shumen, "Episcopo Konstantin Preslavski", retired.**

(three names, scientific degree, scientific title, address)

According to the "RULES FOR THE CONDITIONS AND PROCEDURE FOR ACQUISITION OF SCIENTIFIC DEGREES AND OCCUPATION OF ACADEMIC POSITIONS IN SU" ST. KLIMENT OHRIDSKI "the minimum requirements for the position of ASSOCIATE PROFESSOR

are:

1. To possess an educational and scientific degree "doctor", which for the specialties of the regulated professions must be from the same specialty;

According to the CV of the candidate, Julia Romanova has obtained the degree of Doctor of Chemistry from Sofia University and Université de Haute-Alsace (France) in the period 2007-2011, and her topic was "Influence of the environment on geometry and electronic structure, magnetic and conducting properties of polyaniline (Theoretical and experimental studies of the structure and magnetic properties of conjugated N-containing oligomers) "

2. Not less than two years to have held the academic position of "assistant", "chief assistant".

Candidate Julia Romanova has a very rich background in positions. In 2011 She is a visiting scientist (3 months) at the Leibniz Institute for Polymer Research Dresden, Theory of Polymers, Germany, in 2012-2014 she was a postdoctoral fellow (2.5 years) at the University of Namur, Theoretical Chemistry Laboratory, Belgium, 2014 - 2016 and is a researcher 2 years at the University of Surrey, Advanced Technology Institute, UK, has a maternity leave and since March 19, 2018, she holds the position of "Chief Assistant Professor" in the Department of Chemistry and Pharmacy at Sofia University. All this shows that she has gained a lot of experience in conducting research, and has more than 2 years held the position of Assistant Professor.

3. To have submitted a published monographic work or equivalent publications in specialized scientific publications in the field of the competition or evidence of relevant artistic achievements in the field of arts, which do not repeat the submitted for the acquisition of

educational and scientific degree "Doctor" and for the acquisition of the scientific degree "Doctor of Science".

The total scientific production of the candidate chief assistant Julia Romanova consists of **4** chapters in monographs, **2** studies in conference proceedings and **24** articles in scientific journals. All the works that the candidate Dr. Julia Romanova has presented are in the field of the competition for the position Associated Professor, namely works in the field of theoretical chemistry - application of quantum chemical methods to various molecular systems, most of which have a practical interest. All of her **24** scientific publications are in journals with IF and SJR (all **24** indexed in Scopus), **4** book chapters (1 of them indexed in Scopus, **2** in Web of Science) **2** conference proceedings without IF and SJR (non-indexed), **1** patent, a total of **31** papers, with **10** as the first author and **8** as the corresponding author. Of these, **14** articles and **1** chapter in a monograph, **2** conference studies, and one paper are after obtaining the degree of "doctor".

4. Meet the minimum national requirements for the respective scientific field and / or professional field and the additional requirements of Sofia University "St. Kliment Ohridski".

According to the CV presented to me, the candidate has in group A, indicator 1: Dissertation work for awarding educational and scientific degree "doctor" -**50** points, group B, Indicator 4: Habilitation work - scientific publications-**100** points, group D, Indicator 7: Scientific publications - **217** points and Indicator 8: Published chapter of a book or collective monograph **15** points, group E, Indicator 11: Citations**106** points, group G, 21. h-index-**110** points, participation in scientific projects -**15** points . Thus, she collects a total of **613** points, a fairly high indicator for the position of associate professor, which is **510** according to the minimum requirements for this position in the specialty of chemistry.

5. General characteristics of the research, scientific-applied and pedagogical activity of the candidate.

The importance of the scientific production of the candidate Julia Romanova falls on the research on the diradical character (DRC) and the singlet-singlet splitting of certain organic compounds. Here I want to note that I find this topic very interesting. The stability, emission and Raman spectra, and DRC character of a number of compounds from which singlet-singlet splitting is expected, have been extensively studied (in the English version she uses *singlet fission*, while I would prefer *singlet splitting*, but perhaps this terminology is accepted in this area of science). The elucidation of the mechanisms of singlet-singlet splitting in DRC leads to results useful in practice mainly for determining a strategy for the design of chromophores to be used in solar technologies as substitutes for silicon photovoltaics.

Candidate Julia Romanova presented a habilitation work on "*Handbook for hunting and design of chromophores for singlet splitting.*" (there is a typographical error in the title, it is written chromiphores instead of chromophores), which summarizes the results of her scientific work on this problem and outlines the path for obtaining such *chromophors*, as she writes about "*hunting chromophors*". One work is in the field of theoretical pharmacology, considering the antiproliferative action of gold (i) complexes with n-heterocyclic carbenes or triphenylphosphines with ibuprofen derivatives as effective enzyme inhibitors. Julia Romanova also presented a chapter from a monograph in which theoretically studied homoleptic complexes of metals (M) with pyridine-triazolate ligands (L) and their significance for the molecular design of optical and conductive materials were studied.

In this sense, it is noteworthy that in the chapters of monographs in which she is a co-author, the tendency for theoretical research on systems with practical application is clearly visible. They are in the field of low-carbon energy for transport and everyday life (RDC chromophores), in the series of Critical Analysis, Storage and Conversion of Renewable Energy, both in the field of theoretical pharmacology of anti-cancer drugs on graphene-surface and in the field of molecular design of organometallic materials. Here I want to emphasize this symbiosis in the application of theoretical quantum chemical methods to problems that are of great practical interest are characteristic of the articles of Chief Assistant Julia Romanova. The last chapter in the monograph is a purely theoretical development on the influence of the degree of protonation on the geometry and electronic structure of emardin oligomers. All **14** papers submitted for the competition and **1** chapter in a monograph are in renowned European and American journals with impact factor (SCOPUS), such as Symmetry, MDPI-Molecules, Applied Organometallic Chemistry, Journal of Physical Chemistry Letters, Journal of Physical Chemistry A and C, Chemistry - An European Journal, Angewandte Chemie-International Edition, Physical Chemistry Chemical Physics, Chemical Papers, Synthetic Metals, European Journal of Inorganic Chemistry. **53** citations were noted for these articles, as only the article "The role of substituent effects in tuning metallophilic interactions and emission energy of bis-4-(2-pyridyl)-1,2,3-triazoloplatinum (ii) complexes" published in Angewandte Chemie-International Edition received **34** citations. In **6** of these articles he is the first author and in **10** the corresponding author. Chief Assistant Julia Romanova has a high **h-index = 11**, reached in **13** years of research career. With such an index, one usually applies for a professor.

All this speaks of a high quality of the scientific production of the candidate Julia Romanova. Taking a look at the articles on doctoral studies, we understand that Romanova is already an established researcher. This is evidenced by the high h-factor mentioned above.

In conclusion, I would like to emphasize that the scientific production of Chief Assistant Julia Romanova is united around a major subject, which I believe she will continue to develop in his position as associate professor. We do not have a thematic fragmentation that we often see in many other candidates.

6. Evaluation of the pre-pedagogical preparation and activity of the candidate for the requested title: level of textbooks and teaching aids and developments created by him, experience as a lecturer, leader of exercises, seminars, scientific circles, etc .; work on training young scientific staff (graduate students, assistants, graduates, etc.).

Candidate Julia Romanova has significant experience as a lecturer and as a supervisor and consultant of doctoral dissertations and bachelor's theses. In 2018/2019. it had an auditorium of **222** hours and a total employment of **244.40** hours, in 2019-20220, respectively an auditorium employment of **413** hours and a total employment of **446.90** hours, in 2020/2021, respectively an auditorium employment of **295** hours and a total of **360.2** hours. She has supervised one doctoral student within a research project (NSF-SU: № 80-10-22 / 22.03.2021) and the management of 4 students within research projects (NSF-SU: (80-10-3 / 18.03.2020) .; FNI: KP-06-N / 39/2 dated 19.12.2019; FNI-SU: № 80-10-168 / 16.04.2019). She was a scientific consultant for **1** doctoral dissertation and **1** bachelor's thesis.

7. Participation in projects, conferences and symposia.

Here the research activity of the candidate Julia Romanova is extremely impressive. She has participated in a total of **25** projects, mainly with the National Research Fund (I may be wrong here because I could not read what FNI-SU and only FNI means), **7** of which are abroad, and in **5** of which she is a manager. In **4** of these projects she has led students. This shows that she can propose and manage projects, holding the position of ASSOCIATE PROFESSOR.

8. What, in particular, is the significance of contributions to science and practice? Is there already realized social (scientific, economic or other useful for society) effect: use and citation by other authors at home and abroad, the amount of direct economic effect, improvements in various spheres of economic and social life. Presented documentation on these claims.

The scientific production of the candidate Julia Romanova is theoretical so that it cannot have a direct contribution to the practice and have an economic effect. But as I noted above, most of her theoretical work is on objects of economic interest, such as low-carbon energy for transport and everyday life (study of radicals, potential photovoltaics) and as in the field of theoretical pharmacology of anti-cancer drugs . The valuable thing in her contributions is that all her publications are in renowned international journals having a high impact factor, and have a good citation from other authors at home and abroad, which speaks of a high scientific level of her

publications. So, the contributions of the candidate Julia Romanova represent a serious scientific contribution.

Based on the documentation presented to me about the scientific achievements and scientific activity of Chief Assistant Julia Ruslanova Romanova, my opinion is that she grew up as a well-educated scientist with extensive practice in both research and teaching. . My opinion is also that on the basis of the requirements in the RULES FOR IMPLEMENTATION OF THE LAW ON THE DEVELOPMENT OF THE ACADEMIC COMPOSITION IN THE REPUBLIC OF BULGARIA, as well as on the basis of the minimum requirements for the position of **Associate Professor** of Sofia University , for which I appeal to the committee I respect, this position to be granted to Julia Ruslanova Romanova.

Date: 26.11.2021

Reviewer:

(signature)