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## OPINION

on the competition for holding the academic position “Associate Professor”  
at the Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski”,  
in professional field “4.2 Chemical sciences”,  
scientific field “Theoretical Chemistry”,  
published in the Bulgarian State Gazette, issue 63 of July 30, 2021

*by Assoc. Prof. Dr. Silvia Emilova Angelova,  
Institute of Optical Materials and Technologies “Acad. J. Malinowski” - BAS,  
member of the scientific jury, appointed by order № RD-38-455 of September 21, 2021,  
of the Rector of Sofia University “St. Kl. Ohridski”*

In the competition for holding the academic position “Associate Professor” in the professional field “4.2 Chemical Sciences” (“Theoretical Chemistry”) at the Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski” (FCP-SU) only one candidate participates – Assist. Prof. Dr. Julia Ruslanova Romanova.

The electronic materials, prepared by the candidate and described in the competition application form, are in accordance with *Development of Academic Staff in the Republic of Bulgaria Act (DASRBA)* and the *Rules on the conditions and procedure for acquiring science degrees and holding academic positions in Sofia University “St. Kl. Ohridski”*, and include all required documents. Assist. Prof. Dr. Julia Romanova is registered in the *Register of the academic staff in the Republic of Bulgaria*, maintained by the National Centre for Information and Documentation (<https://ras.nacid.bg/dissertation-preview/38450>). Data on her academic degree (PhD) and academic position (Assist. Prof.) are available.

After defending a PhD thesis “Influence of the environment on the geometry, electronic structure and magnetic properties of polyaniline” in 2010 and a number of postdoctoral specializations, in 2018 she was appointed to the position “Assist. Prof.” at the Department of Inorganic Chemistry, FCP-SU, and holds the position at present.

Assist. Prof. Dr. Julia Romanova is a co-author of 4 book chapters, 24 publications in scientific journals, 2 publications in full text in conference proceedings and 1 patent. In this competition she participates with 15 scientific papers (14 publications and 1 book chapter), published in the period 2010-2021 - 8 active research years and 2 years of maternity leave. All publications (14) are published in peer-reviewed and indexed journals with impact factor and have not been included in her PhD thesis. 9 publications are in journals of category Q1, 4 publications - category Q2, 1 publication - Q4. The citations of these publications are 53 in total as of the date of preparation of the reference by the candidate. The Hirsch index of Assist. Prof. Dr. Julia Romanova according to data from Scopus and WoS is 11. Assist. Prof. Dr. Julia Romanova is a leader of an ongoing project with Bulgarian National Science Fund (NSF) and a participant in another project with NSF.

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According to the author's reference for the original scientific contributions in the scientific publications, out of fifteen scientific papers, thirteen include research on "Contemporary Materials" (Papers № 1-9 and 12-15), and the other two are dedicated to the study of spectroscopic characteristics (Raman spectra) of molecules (Papers № 10-11). According to the systems studied, the candidate's publications can be divided into two groups and are dedicated to open-shell organic molecules (Papers № 1, 2, 4, 8, 10, 11, 12, 13) and to organometallic complexes (Papers № 3, 5, 6, 7, 9, 14 and 15). In 6 of the presented studies the candidate is the first author (№ 5-7, 10, 11, 15) and in 5 she is the corresponding author (1-5).

For participation in the competition, the candidate has prepared a habilitation paper, written on 44 pages, with the attractive title "Handbook for hunting and design of chromophores for singlet fission". The introduction to the habilitation work is an overview of modern solar technologies written in a fascinating way and in comprehensible language. She states that one of the promising strategies for increasing the efficiency of solar cells is the use of a photophysical process called singlet fission (SF). The introduction also explains the basics of this process and the thermodynamic conditions that a chromophore must meet in order to be used in a photovoltaic cell working on the SF principle. Approaches for creating chromophores with intermolecular SF and strategies for overcoming the situation "A Needle in a Haystack", highlighting the advantages of a multidisciplinary approach, representing the intersection of theoretical/quantum chemistry, machine learning, statistics and data science, are summarized. The candidate's scientific contributions to this topic have been published recently (2020 - publication №4; 2021 - publication №1) or are to be published. In these studies, there is a tendency to increase the number of chromophores studied - potential SF materials in an attempt to find a fast and reliable approach to screening large groups of compounds:

- For the first group of studied systems - 14 diboron-doped anthracenes and phenanthrenes, the calculations are performed at a high theoretical level: the geometries are optimized at MP2/aug-cc-pVDZ level, the diradical character of the compounds is studied by the PUHF/6-31G \*\* method, multi-configuration calculations are performed with the RASPT2/aug-cc-pVDZ method;

- For the second group of tested compounds (quinone methides, 21 in number) the calculation protocol includes optimization of the geometry of the molecules at the B3LYP/6-31G\* level of theory, study of the diradical character of the compounds at the PUHF/6-31G\*\* level of theory, and chemometric analysis to develop a classification model for laboratory stability of quinone methods;

- In the third study of the candidate nearly 2000 molecules are extracted from a database (PubChem PM6 - a database of 221 million molecules with optimized molecular geometries and electronic properties) and subjected to processing by quantum chemical and chemometric methods to develop an algorithm, based on machine learning, which can quickly and without consuming many resources predict whether a molecule has a non-zero diradical character, i.e. is potential chromophore for singlet cleavage.

The candidate applies in her research a wide range of theoretical methods and is even familiar with methods developed recently, which makes an excellent impression. The obtained results contribute to a deeper understanding of the structure/properties dependence of various

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chemical systems. The topic of the habilitation thesis shows that the candidate has focused on an interesting and challenging area.

I have no critical remarks on the materials submitted for evaluation.

#### CONCLUSION

From the information on fulfillment of the minimal requirements (groups of indicators A-E) and the additional requirements of Sofia University (group of indicators G), it can be seen that for each of the indicators Dr. Romanova has the required number of points. The total number of scientific papers co-authored by Dr. Romanova (27) is almost twice as large as the number of papers submitted for the competition (15). The scientific achievements of Assist. Prof. Dr. Romanova are high and fully meet the topic of the competition. She has the necessary scientific qualification to continue to develop extremely successfully in the promising field in which she works thoroughly and systematically.

The scientific papers submitted for participation in the competition, the number of citations, participation in projects and project management by the candidate exceed the requirements for holding the academic position “Associate Professor” according to *DASRBA*, the *Regulations for application of DASRBA*, and additional requirements of the relevant Rules of Sofia University. I give a positive assessment to the candidate and recommend to the members of the Scientific Jury and the Faculty Council of FCP-SU to elect Assist. Prof. Dr. Julia Romanova as an “Associate Professor” in professional field “4.2. Chemical sciences” (“Theoretical chemistry”).

Sofia

November 9, 2021

/Assoc. Prof. Silvia Angelova, PhD/