

Attitude of Reviewer

By Prof. Dr. Nikolay Georgiev Vassilev, IOCCP - BAS

Of the materials submitted for the competition for the occupation of the academic position

Associate Professor at IOMT-BAS

Professional field 4.2 Chemical Sciences (Physical Chemistry)

In the competition for the academic position, Associate Professor, announced in the State Gazette, issue 41/19.07.2019 for the needs of the Institute of Optical Materials and Technology (IOMT) "Acad. Jordan Malinowski" at the Bulgarian Academy of Sciences (BAS) as sole candidate Head Assistant Professor Dr. Silvia Emilova Angelova from the Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP) at BAS.

1. General presentation of the procedure and the applicant

Head Assistant Professor Dr. Silvia Angelova is a graduate from the Faculty of Chemistry of the Sofia University "St. Kliment Ohridski". She obtained her M.Sc. degree in 1995 in the field of Organic and analytical chemistry. In 2009 she, under the supervision of Prof. V. Enchev, successfully defended a Ph.D. thesis at the Institute of Organic Chemistry with a Centre of Phytochemistry, BAS entitled "Calculated quantum chemical NMR parameters as a tool for studying tautomeric and conformational transformations". In 1996 she began her working career as a chemist in laboratory of NMR Spectroscopy at the IOCCP-BAS, but her research career is mainly related to the laboratory of Physical Organic and Computational Chemistry and the laboratory of Theoretical Chemistry at the same institute. In 2011 she was promoted to a Head Assistant Professor in the laboratory of Structural Organic Analysis at the Institute of Organic Chemistry with a Centre of Phytochemistry, BAS where she works till now.

2. General characteristics of the applicant's activities

Head Assistant Professor Dr. Silvia Angelova fulfills the minimum required points of the IOMT-BAS Regulations for the implementation of the Law on the Development of the Academic Staff in the Republic of Bulgaria by groups of indicators for the academic position "Associate Professor", as can be seen from the attached reference. The candidate submitted a list of 62 scientific papers, one of which was accepted for publication. From this list, 14 scientific publications are equated to habilitation thesis (publications No. 23-25, 27, 29, 30, 33-36, 47, 51, 56, 57), 14 are sci-

entific publications with which she participates in the competition for the academic position "Associate Professor" (publications No. 1-3, 5-8, 13, 16-18, 20, 21, 31), 5 scientific publications were submitted for the Ph.D. thesis (publications Nos. 4, 9-11, 14), and 28 were other publications not included in this procedure (publications Nos. 15, 19, 26, 28, 32, 37-46, 48-50, 52-55, 58-61). The distribution of the 14 scientific publications equated to habilitation thesis according to the rank of scientific journals is as follows: two are in scientific publications with Q1, four are in scientific publications with Q2, two are in scientific publications with Q3 and four in scientific publications with Q4. The distribution of the 14 scientific publications with which she participates in the competition for the academic position of "Associate Professor" according to the rank of scientific journals is as follows: five are in scientific publications with Q1, five are in scientific publications with Q2 and three are in scientific publications with Q3 and one in scientific publications with Q4. According to the attached information, the total number of citations is 98, with 34 being the citations of 7 publications equated to habilitation thesis and 64 being the citations of 8 publications presented in group "D". According to the Scopus database, the candidate's h-index is 9. This value is indicative of high scientific productivity combined with wide echoes in the literature.

The scientific studies of Dr. Silvia Angelova in publications, equated to habilitation thesis, are applications of quantum-chemical calculations for the study of:

- The ground state electronic structure of dyes for photovoltaic applications [publications No 23,27,29,30,33,34,36,47];
- The ground state electronic structure and excited state of tautomeric systems [publications No 24,25];
- The ground state electronic structure and properties of fluorescent dyes - biomarkers [publications No 35,51,56,57].

In these scientific studies, quantum chemical (DFT and TDDFT) calculations are applied to calculate the energies of the HOMO and LUMO orbitals, as well as the differences between them, which are used to characterize dyes or tautomeric systems.

Dr. Silvia Angelova's scientific research in publications presented in group "D" represents:

- Experimental study of the structure and properties of organic compounds and complexes by NMR spectroscopy [publications No 1-3, 13].
- Experimental [Publications No 8], Theoretical [Publications No 5,16], and Combined Theoretical and Experimental Research [Publications No 6,7,17,18,20,21,31] on the structure and properties of various molecular systems.

In these scientific studies, the transformation of the candidate's scientific interests from the application of spectral techniques (mainly NMR spectroscopy) to the application of computational methods to study the structure and properties of molecular systems can be traced chronologically.

Scientific Works of Dr. Silvia Angelova are at a very high scientific level, fulfill the subject of the competition and are in the field of computational theoretical chemistry, which can be considered as a part of Physical Chemistry. In most of the scientific publications, combined experimental and theoretical characterizations of the systems studied have been used. The studies carried out can be categorized as novelty for science as well as enrichment of scientific knowledge by clarifying the structure and properties of various molecular systems.

The postdoctoral specialization in Spain under supervision of Professor Obis Castagno in the period 03.2012 - 03.2013 has had a beneficial effect on the scientific progress of Dr. Silvia Angelova.

3. Assessment of the applicant's personal contribution

I know the candidate personally from the recruitment and employment at IOCCP-BAS and have followed her scientific development. Therefore, her personal contribution to the research presented here is indisputable to me.

CONCLUSION

Dr. Silvia Emilova Angelova fully complies with the regulations for the implementation of the academic staff in the Republic of Bulgaria and the regulations adopted by the Council of Ministers and BAS, as well as with the requirements of IOMT-BAS for the occupation of the academic position "Associate Professor". The value of scientific production presented for participation in the competition is sufficient in volume, has been published in reputable scientific journals and has found wide echo in the literature. Based on the above, I am convinced of my positive assessment and suggest Head Assistant Professor Dr. Silvia Emilova Angelova to be elected to the academic position of "Assistant Professor" in the professional field 4.2 Chemical Sciences (Physical Chemistry).

Sofia, 13.09.2019

Writing the reviewer attitude:

Prof. Dr. Nikolay Vassilev