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PEER REVIEW

Written by Assoc. Prof. Reni Tomova, Ph.D. - Institute of Optical Materials and Technologies “Acad. J. Malinowski” (IOMT) – BAS

on a competition for appointment on academic position "Associate Professor" in the professional field 4.2 "Chemical Sciences", specialty "Physical chemistry", for the needs of IOMT, announced in Newspaper of State No. 41/21.05.2019.

Applicant: Dr. Sylvia Emilova Angelova, Assistant Professor in The Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP)) – BAS.

1. General presentation of the received materials

Subject:

By Order No. 383/19.07.2019 of the Director of IOMT I was nominated as a member of the Scientific Jury of the competition for the occupation of the academic position Associate Professor (area 4: Natural sciences, mathematics and informatics, professional field 4.2: Chemical Sciences, scientific specialty: "Physical chemistry"), declared for the needs of the “Institute of Optical Materials and Technologies"

Only one candidate has submitted documents for participation in the competition - Assistant Professor Dr. Sylvia Emilova Angelova from the Institute of Organic Chemistry with Center of Phytochemistry (IOCCP) - BAS.

The applicant submitted all documents and materials required by the procedure accordance the Art. 13 of the Rules on the application of the Law for the development of academic staff in the Republic of Bulgaria (LDASRB) in IOMT:European curriculum vitae, Doctor of Philosophy Degree, Medical Certificate, Criminal Record Certificate, List and Imprints of Publications, List of Participation in Conferences, List of Participation in projects, List of citations, Certificate of Minimum Five-Year Internship in the Specialty, Certificate of Minimum Two-Year Internship in the Position of Assistant Professor, Reference for covering of the Minimum Requirements in Annex 1, Table 1, Reference for Scientific contributions of the publications submitted in instead of the Monograph, Proof of participation in Projects, Copy of the announcement of the opening of the competition in the Newspaper of State.

The documents allow being done full and accurate assessment according to the requirements of LDASRB: Art. 24., Art. 24. 1., Art. 24. 2a), Art. 24. 3., Art. 2b., and according the Rules of implementation of LDASRB in IOMT - Art. 2., as follows:

•According to LDASRB Art. 24 "Candidates for occupying the academic position" Associate Professor" must meet the following conditions: Art. 24. 1 - “to have a Ph.D.

degree, Art. 24. 2a)"to have worked at least two years at the academic position "Assistant Professor", Art. 24. 3."to have submitted published monograph or equivalent publications in specialized scientific editions which do not repeat these used for the Ph.D. degree".

- The candidate has a Ph.D. degree (a diploma number 33406 / 20.07.2009 from the Higher Attestation Commission) and since 01.01.2011, she has worked as an Assistant Professor in the scientific field of the competition (Certificate of Work Experience). For participating in the competition, Dr. Angelova has submitted 28 publications in specialized scientific editions and separately all 5 publications used in her Ph.D. Tessie.

•According to (LDASRB) Art. 2b. Applicants for the occupation of the academic positions of "Assistant Professor ", "Associate Professor" and "Professor" must meet the minimum national requirements for scientific and teaching activity, Article 2b. 2 in the scientific fields and/or professional fields for the acquisition of each academic degree and the occupation of each academic position shall be determined on the basis of a set of indicators and shall be expressed in the minimum number of points that the candidate must receive in accordance with the individual their visual results on these indicators.

•According to Art. 2. (1) of the Rules on the application of LDASRB in IOMT - "Applicants for scientific degrees and for occupying academic positions should meet the minimum requirements of BAS for field 4 Natural sciences, mathematics, and informatics, professional fields 4.1 Physical Sciences and 4.2 Chemical Sciences according to Appendix 1 (an integral part of these Regulations) and specific requirements of IOMT. Appendix 1, Table 1 gives the minimum requirements of BAS".

- From the data for the fulfillment of the minimum requirements in Appendix 1, Table 1 submitted by Sylvia Angelova is seen that the candidate has a total of 906 points from the required 430 points for coverage of the academic position of Associate Professor.

2. A short biography of the applicant

Sylvia Angelova was born on 28.04.1972. In 1995 she graduated the Sofia University "Kliment Ohridski" as a Master of Chemistry with a specialization in Organic and Analytical Chemistry. In 2009 she defended her Ph.D. degree in the scientific specialty 01.05.01 "Theoretical chemistry" on the topic: "Quantum-chemical calculated NMR parameters as a means of studying tautomeric and conformation equilibriums".

In 1996, she started to work at the NMR Spectroscopy Laboratory of the Institute of Organic Chemistry with the Center for Phytochemistry (IOCCF) - BAS. From 2005 to 2011 she has been working as a research associate 3 and 2 degrees at the Laboratory of Physical, Organic and Computational Chemistry and since 2011 to date, she has been occupying the academic position of "Assistant Professor" at the same institute. For the period 2012-2019, she has 5 specializations in Spain: 12 months as a visiting scholar and 6 months as a postdoctoral fellow.

3. General characteristics of the applicant's scientific activity

Dr. Angelova has a significant scientific output well-publicized in international journals and scientific forums. Its total number of publications for the period 2000 - 2019 is 61, 55 of which indexed in the WoS and Scopus database. For the same period, she has h-index 10 (WoS), 9 (Scopus) and 244 citations (Scopus). In the last three years, she has attended a total of 43 international scientific forums (5 of which abroad), where she has presented 5 oral reports and 38 posters. In addition, the applicant has participated in five national projects: three with the FNI and two under the Operational Program "Science and Education for Smart growth" and in 6 international scientific or educational projects (including those under bilateral agreements for scientific cooperation and exchange of BAS) with Macedonia, with the Russian and Polish Academy of Sciences, with the Swiss National Science Foundation (one each) and with Italy (two).

4. General characteristics of the applicant's work

To participate in the competition, Dr. Angelova has submitted 28 scientific publications (26 of which in Q1, Q2, Q3, and Q4 quartiles) divided into 2 groups according to Appendix 1, Table 1:

•Publications equated to habilitation thesis (a group of indicators "B", indicator "4"): 14 pieces (№23-25, 27, 29, 30, 33-36, 47, 51, 56, 57) with 34 citations (from foreign authors outside the team of the candidate).

• Publications according a group of indicators "D", indicator "7": 14 pieces (№1-3, 5-8, 13, 16-18, 20, 21, 31) - with 64 citations (from foreign authors outside of the teams the applicant participates).

Outside the contest, Silvia Angelova has provided another 5 publications (№4, 9-11, 14) used in the acquisition of educational and scientific degree "Doctor" and 28 other (№15, 19, 26, 28, 32, 37-46 , 48-50, 52-55, 58-61) with 146 citations.

5. Basic scientific contributions

Dr. Angelova works in the field of "theoretical chemistry" in one of the first laboratories in the world for quantum chemistry, created at IOCCF - BAS by Prof. N. Tyutyulkov. Current research in this field combines concepts from classical, quantum and statistical mechanics with high-performance computational methods for the study of molecular properties and reactions.

The main subject of research in the candidate's publications [4-7, 9-12, 14-62] is the electronic structure of the molecules and their properties determined by “Ab initio” and DFT methods. The aim of the “Ab initio” (non-empirical) method is to calculate the multi-electron wave function (solution of the Schrodinger equation) using a mathematical description of the orbitals of a molecular system. According to DFT methods, based on the Density Functional Theory, the energy of the molecule can be determined by the electron density in it, instead of the wave function.

5.1. Scientific contributions to publications Indicator group "B", Indicator "4": 14 issues (No 23-25, 27, 29, 30, 33-36, 47, 51, 56, 57)

These publications can be grouped into three main groups:

5.1.1. Application of quantum-chemical calculations for studying the electronic structure in the ground state and the properties of dyes for photovoltaic applications [23,27,29,30,33,34,36,47].

Using quantum-chemical calculations the data on the structure of a series new perylene [23], merocyanine [27,29,36], squaraine [30,34] and croconine dyes [33], were obtained

- ✓ The applied computational protocols reproduce the experimental results, including nonlinear optical (NLO) effects, in good quality. One-step synthesis concomitantly with the spectroscopic, the solvatochromic and the NLO properties define the new perylene dyes as promising candidates for determining the polarity of solvents for photovoltaic and nonlinear optical applications.
- ✓ The study of new merocyanine [27,29,36], squarillium [30,34] and croconium dyes [33] as potential electron-donating components in solar cells with bulk heterojunction is supplemented by quantum-chemical (DFT) calculations that provide information for the geometry of the dyes in the ground state. The calculated energies of the HOMO and LUMO orbitals and the band gap are used to characterize the dyes and to determine their potential for use in solar cells with a fullerene acceptor component [60] PCBM.
- ✓ Symmetrically and asymmetrically substituted model structures of squarillium and croconium dyes have been theoretically investigated as potential electron donors in organic photovoltaic solar cells with an acceptor component [60] PCBM fullerene [47]. The bandgaps of all proposed model compounds are in the order of about 2 eV, values typical for organic semiconductors. For all model compounds, high oscillator power values were predicted, ie. for these dyes are expected a high absorption coefficient. Based on the results of quantum chemical calculations, it is concluded that some of the proposed dyes are suitable for use as components of optoelectronic devices.

5.1.2. Application of quantum-chemical calculations for studying the electronic structure in the ground and excited state of tautomeric systems [24,25].

- ✓ The DFT and TDDFT calculations confirmed and clarified the mechanism of double proton excitation at the excited singlet state (ESIPT) in all three tautomeric forms of the newly synthesized compound 3,6-bis (4,5-dihydroxyoxaz-2-yl) benzene- 1,2-diol [24]. The reactions of proton transfer in excited states are a computational challenge and have immense practical importance, because the compounds with such ESIPT find application as photo stabilizers, laser dyes, sensors for metal ions, etc.
- ✓ It has been proved that can be predicted the influence of a static external electric field on the behavior of a system of 3 tautomeric forms of the model compound

2-(5-(benzo[d]oxazol-2-yl)-6-hydroxypyridin-2-yl)-3-hydroxy-1H-inden-1-one [25]. It was found that the change of the power and direction of the electric field, stabilize the different tautomeric forms of the molecule. Systems similar to the studied model system can be used in the design of new molecular electronic devices.

5.1.3. Application of quantum-chemical calculations for studying the ground state electron structure and properties of fluorescent dyes - biomarkers [35,51,56,57].

- ✓ On the base of quantum-chemical calculations was obtained the information of the ground-state structure of the novel monomethine cyanine dyes [35,51,56,57], analogs of the Thiazole Orange commercial product, synthesized by a new ecological procedure. The DFT and TDDFT calculations were used in analyzing the relationship between chemical structure and optical properties of the chromophores [51,56,57] and for obtaining the information on the structure of the different types of aggregates existing in the solution. In two of the cases [35,57], a hypothesis for the presence of a monomer-dimer equilibrium was confirmed by a comparison of the simulated absorption spectra of the possible monomeric and dimeric species and experimental spectra of the compounds.

5.2. Scientific contribution in publications in indicator group "G", indicator 7 - 14 броя (№1-3, 5-8, 13, 16-18, 20, 21, 31).

The publications [1-3,8,13] refer to the application of experimental methods on investigating the structure and properties of organic compounds and complexes.

The publications **(**[5-7,16-18,20,21,31]**),** include either only theoretical models [5,16]**,** or a combination of theoretical methods and more experimental techniques for solving structural and/or spectroscopic problems and predicting the molecular properties. In the quantum-chemical calculations a wide range of DFT functionals has been used: B3LYP [17,18,21,31]**,** X3LYP [20], OLYP [20,21]**,** B3PW91 [21]**,** LC-BLYP [21]**,** B2PLYP [21] and mPW2PLYP [22]**.**

Mostly studied are processes of tautomerization [5-7,16,20,21,31], isomerization [17] and conformational equilibrium [18]. The described processes are often achieved in the solution, so the research related to the influence of the solvent on the equilibrium has significant importance because of the structure (and the reactivity) of the molecule can differentiate a lot in different solvents.

Calculated ^{13}C chemical shifts are used to solve structural or spectroscopic problems in a series of publications: [5,7,16,20,31], which is a continuation of the topic of the candidate's Ph.D. thesis (publications [4,9-11,14].

6. Assessment of the applicant's contribution

The publications presented by the candidate are collective works involving several authors. Nevertheless, given the well-structured and formulated contributions, I believe that Dr. Angelova has a significant personal contribution to the obtained results and layout of the paper.

I have no critical remarks and recommendations regarding the applicant's work.

CONCLUSION

Documents and materials presented by Assistant Professor Dr. Sylvia Emilova Angelova meet all requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria (LDASRB), the Rules for the implementation of the LDASRB and the Rules for the implementation of the LDASRB in the IOMT.

The candidate submitted a sufficient number of scientific articles, published after the defense of her Ph.D. degree. The evidence meets 906 points, which exceeds twice the minimum requirements of BAS and the additional requirements of IOMT. there is no doubt that there are sufficient scientific contributions to guarantee the successful future development of the research activity started.

All mentioned above is a reason to give my positive assessment and to recommend to the Scientific Jury to provide a report proposal to the IOMT Scientific Council for the election of Dr. Sylvia Emilova Angelova in the academic position of Associate Professor, field 4. Natural Sciences, professional field 4.2. Chemical Sciences, scientific specialty "Physical chemistry", IOMT - BAS.

Sofia,

12.09.2019

Reviewer: .....

Assoc. Prof. Dr. Reni Tomova