REVIEW

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Re: Competition for an Associate Professor position at the Institute of Optical Sciences and Technologies, BAS in professional field 4.2 Chemical Sciences, scientific specialty "Physical Chemistry"

There is only one candidate applying for the Associate Professor position, announced in the State Gazette 41/21.05.2019: Head Assistant Dr. Silvia Emilova Angelova. For the competition the candidate has provided a full set of documents in accordance with the Regulations for the implementation of the Law for development of the academic community in Republic of Bulgaria. Documents have been prepared with great care and precision and provide ample information about the academic activity of Dr. Silvia Angelova.

1. Brief biographical data of the candidate

Dr. Angelova is a graduate from the Faculty of Chemistry of the Sofia University. 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". From 2000 to 2005 she worked as a chemist at the same institute, and in 2005 acquired a Research Associate position in the laboratory of Physical Organic and Computational Chemistry. In 2011 Dr. Angelova was promoted to a Head Assistant Professor in the laboratory of Structural Organic Analysis / Theoretical Chemistry at the Institute of Organic Chemistry with a Centre of Phytochemistry, BAS where she works till now. She has conducted several specializations in the University of Alcala de Henares (Spain) as a postdoctoral researcher or visiting scholar.

2. Description of the application materials

For the competition, the candidate has presented 28 scientific papers (printed after obtaining her doctoral degree), 14 of which are equated to habilitation thesis (set of metrics "V", indicator "4") whereas the rest 14 papers are unified under the set of metrics "G", indicator "7". Additionally, a full list of candidate's publications (62) is provided. Provided are lists of noticed citations, presentations at scientific forums and research grants participation, as well.

The papers, selected for participating in the Associate Professor competition, can be classified as follows:

By type:

- Publications in scientific peer reviewed journals – 28
- Publications in conference proceedings – 0
- Popular science magazines – 0

By importance:

- Papers in journals with quartile Q1 – 7 (papers 3, 5, 13,20, 21, 23 and 51 from the full list of publications);
- Papers in journals with quartile Q2 – 9 (papers 1, 2, 7, 8, 17, 24, 25, 35 and 36)
- Papers in journals with quartile Q3 – 5 (papers 16, 18, 29, 30 and 31)
- Papers in journals with quartile Q4 – 5 (papers 6, 27, 47, 56 and 57)
- Papers in journals without quartile – 2 (papers 33 and 34)

Note that majority of the papers are printed in top journals in the fields of physical and theoretical chemistry (quartiles Q1 and Q2).

By place of publication:

- Publications in refereed journals - 26
- Publications in non-refereed journals – 2

3. Reflection of the scientific production of the candidate in the literature (scientific publications, collective volumes and patents, refereed and indexed in Web of Science / Scopus)

- Total of 98 citations

4. Participation in scientific forums (2016 – 2019)

- Lectures presented by herself or a collaborator: Total 14
- National forums with international attendance: 9
- International conferences/symposiums: 5
- Posters presented: Total 29
- National forums with international attendance: 10
- International conferences/symposiums: 19
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5. Participation in research and educational grants:

- Total: 11
- National: 5
- International: 6

6. Research and pedagogical activity of the candidate

6.1 Research activity

The research activity of Dr. Angelova is in the field of theoretical physical chemistry: quantum chemistry, computational chemistry and molecular modeling. Her scientific contributions can be grouped in the following domains:

I. Application of quantum-chemical calculations for characterization of properties of dyes for photovoltaic applications [23, 27, 29, 30, 33, 34, 36, 47].

II. Application of quantum-chemical calculations for studying the electron structure in both ground and excited states of tautomeric systems [24,25].

III. Application of molecular orbital calculations for studying the electron structure in ground state and physico-chemical properties of fluorescent dyes – biomarkers [35, 51,56,57].

IV. Combined theoretical-experimental studies of tautomerisation and isomerization of organic molecules [1-3, 5-8, 13, 16-18, 20, 21, 31]

More specifically, the following results have been achieved for domain I:

- Employing molecular-orbital calculations, structural and thermodynamic data is obtained for large series of perylene, merocyanine, squaraine and croconine dyes. Theoretical results are in very good agreement with the available experimental data. Molecular characteristics derived (first hyperpolarizability, intramolecular charge transfer, HOMO-LUMO energy gap, oscillator strength) define the studied molecules as appropriate candidates to be used in the non-linear optoelectronics.
- The most appropriate theoretical approach (various DFT and TDDFT methods) has been determined for evaluating structural and spectral characteristics of different classes of dyes with potential use as donor components in photovoltaic devises. It has been convincingly proven that applying the approach developed by Dr. Angelova allows for pre-screening of candidates for donor systems thus saving costs for synthesizing and experimentally characterizing their physico-chemical properties.

Domain II:

- Molecular orbital calculations have been employed in studying the full set of possible tautomeric forms, in both ground and first excited singlet state of the newly synthesized 3,6-bis(4,5-dihydroxyoxazo-2-yl)benzene-1,2-diol. The calculations performed, although computationally challenging, shed light on the mechanism of the double proton transfer in excited singlet state which is of paramount practical importance in using such molecules as photostabilizers, laser dyes and metal sensors.
- The quantum chemical calculations conducted demonstrate that they can be reliably used in predicting the behavior of complex tautomeric system under the influence of a static external electric field. It has been found that alterations in the strength and directionality of the electric field result in stabilizing different tautomeric forms. Thus, it has been suggested that by changing the parameters of the external electric field, it is possible to modulate the tautomeric equilibrium at will.

Domain III:

- Quantum-chemical calculations have been used in characterizing the geometry and electron structure of a series of new monomethine cyanine dyes – potential candidates as DNA biomarkers. Correlation has been found between the chemical character of the substituent group and the optical properties of dyes under study.
- Theoretical calculations have been employed in following the processes of dimerization of monomethine cyanine dyes, which allows for deriving information about the structure and behavior of the molecular aggregates formed in solution. Comparison between experimental and theoretical data revealed that in solution the dye exists as a mixture of monomeric and dimeric forms.

Domain IV:

- Large spectrum of quantum-chemical methods (B3LYP, X3LYP, OLYP, B3PW91, LC-BLYP, B2PLYP and mPW2PLYP) in combination with experimental techniques has been used in studying the physico-chemical aspects of processes taking place in solution (mainly tautomeric and conformational transformations). The effect of solvent polarity has been studied on the conformational/tautomeric equilibrium, as well as on the chemical reactivity of studied molecules. In a number of papers the theoretically evaluated ^{13}C chemical shifts have been employed in solving structural or spectroscopic problems.

6.2. Work with students

Over the years, Dr. Angelova has been actively participating in student educational programs. She has acted as a student mentor in the framework of "Student Internship Programs", where she has supervised over 50 students from Sofia University and University of Chemical Technology and Metallurgy in the areas "Computational chemistry", "Design of new molecules/materials" and "Applied computational chemistry". As a result of the program fulfillment, the students have deepened their interest and knowledge in the field of computational chemistry which enabled them to prepare reports presented at scientific conferences, writing diploma theses and publishing research papers in scientific journals. Dr. Angelova has co-supervised 4 B.Sc. and 4 M.Sc. successfully graduated students.

7. Conclusion

Scientific publications presented by the applicant fall into the scope of the announced competition and represent original scientific investigations with substantial contribution to the field of theoretical physical chemistry. The application materials enable me to believe that the candidate is a well-known scholar in her field possessing deep knowledge and practical skills in applying a large spectrum of theoretical approaches for characterizing organic/bioorganic molecules and reaction processes. The results obtained by the candidate are innovative and belong the category of innovations in the scientific field. They provide basis for future research in the realm of theoretical modeling of systems of interest to electronics, photonics, biomarking and sensing. Applicant demonstrates creative thinking and

maturity in selecting tasks of relevance to science and practice. In conclusion, as a result of the foregoing, I believe that with her scientific and educational activities Dr. Silvia Angelova fully complies with all the requirements of the Law for the occupation of the academic position "Associate Professor".

In connection with the above, I propose Head Assistant Professor Dr. Silvia Emilova Angelova to be elected Associate Professor in the professional field 4.2 Chemical Sciences, scientific specialty "Physical Chemistry" for the needs of the Institute of Optical Materials and Technologies, BAS.

25.08.2019

Reviewer:

(Prof. Todor Dudev)