

REVIEW

by prof. Ivayla Nedialkova Pantcheva-Kadreva, DSc,
for a competition for the occupation of the academic position "professor",
field of Higher education 4. Natural Sciences, Mathematics and Informatics,
professional field 4.2. Chemical Sciences (Physical Chemistry)
for the needs of the Institute of Optical Materials and Technologies (IOMT)
"Acad. Jordan Malinowski"
at the Bulgarian Academy of Sciences

The only candidate for the competition announced in the State Gazette (issue 24 of 21.03.2025) for the academic position of "professor" is assoc. prof. Silviya Emilova Angelova, PhD, from the Optical Metrology Laboratory at IOMT-BAS. In accordance with the regulatory requirements, Dr. Angelova has submitted the necessary information in electronic form and has been admitted for participation in the procedure.

1. Brief presentation of the candidate

1.1. Education: Silviya Angelova completed her higher education in chemistry at Sofia University "St. Kl. Ohridski" - Faculty of Chemistry (now Faculty of Chemistry and Pharmacy) and in 2009 she obtained PhD in theoretical chemistry with a defence of a Thesis entitled "Quantum-chemically calculated NMR parameters as a tool for studying tautomeric and conformational transformations" (supervisor Venelin Enchev, DSc). She obtained a qualification in Business Management and Marketing (UNWE, 1990-1995) and is an expert in European technical legislation, safety and quality control of industrial products.

1.2. Work experience: The main work experience of S. Angelova is in two Institutes of the Bulgarian Academy of Sciences (BAS): Institute of Organic Chemistry with Centre of Phytochemistry (IOCCF) – chemist (1996-2005); research associate (2005-2011), assistant/senior assistant professor (2013-2019); IOMT – associate professor (since 2019). Since 2022 she has been the scientific secretary of IOMT-BAS.

2. Research and teaching activities of the candidate

Assoc. prof. Silviya Angelova is a co-author of over 110 publications, 101 of which are found in the Scopus database and 95 – in the Web of Science. After taking up the position of assoc. prof. in 2019, S. Angelova co-authored 46 scientific full-text communications (Scopus). Currently, Dr. Angelova runs one scientific project and is a member of the teams participating in the implementation of 4 ongoing and 14 completed projects funded under various programs

of the National Science Found and the Bulgarian Academy of Sciences. In the period 2020-2025, S. Angelova participated in the work of 20 scientific forums giving a total of 31 scientific presentations (19 oral and 12 poster communications). She was a co-supervisor of 16 graduate students (2014-2024) and is a lecturer of a special course at the Doctoral Training Center at the Bulgarian Academy of Sciences.

3. Evaluation of the materials for participation in the competition for AP "professor" and their compliance with the legislation in force in the Republic of Bulgaria

3.1. General presentation

Dr. Angelova participates in the competition with a total of 19 papers. In line with the current criteria according to the Rules in Bulgaria, the full-text communications are distributed as follows: Q1 – 11 (275 points); Q2 – 6 (120 points); Q3 – 1 (15 points) (Scimago Journal & Country Rank).

3.2. Fulfillment by the candidate of the groups requirements

Indicator A (50 points): The candidate has defended a PhD dissertation (Diploma No. 33406 / 20.07.2009).

Indicator C (165 points): Dr. Angelova presents 7 scientific publications, equivalent to a habilitation thesis, which do not repeat the materials in other competitions for holding academic positions and acquiring scientific degrees. Five of the publications are in journals in the first quartile and two - in the second. The total number of points covers and significantly exceeds the minimum national requirements and those of the IOMT-BAS for the occupation of the AP "professor".

Indicator D (245 points): In this group assoc. prof. Angelova participates with 12 scientific publications (Q1 – 6; Q2 – 4; Q3 – 1; 1 without SJR/Q). The scientific communications are of a quality that meets the established criteria.

Indicator F (150 points): Assoc. prof. Silviya Angelova has participated in the implementation of 13 national and 1 international scientific projects, thereby meeting the national and institutional criteria.

The information provided so far regarding the fulfilment of the various indicators for occupying the position of "professor" at the IOMT-BAS in the professional field 4.2. "Chemical Sciences" (Physical Chemistry) reveals that the candidate is qualified to perform research activities.

3.3. Candidate's research

I accept the author's reference for her contributions. Silviya Angelova conducts fundamental research in the field of advanced materials science, related to the evaluation of

existing processes through new experimental and theoretical protocols and to the study of the physicochemical properties of known and new compounds. Although some of the objects in her scientific publications can be attributed to "crossing" areas of scientific knowledge, the candidate's main contributions relate to two main scientific directions - organic and coordination chemistry.

3.3.1. Structures and properties of organic compounds

Dr. Angelova investigated isomerization, tautomerization and/or aggregation processes of various molecule systems: coumarin derivatives [15], aminobenzoimidazole [19], naphthalenes [43, 105], molecular switches based on hydrazones [58, 75], modified crown ethers containing dyes [60], antioxidants and their synthetic analogues [73]. Series of 1,8-naphthalimides alone or as a sensor part in the structure of polymers and dendrimers [68, 69], as well as charged chromophores with potential nonlinear optical properties [85], are other subjects of structural studies.

3.3.2. Coordination chemistry

In addition to the study of the structures and physicochemical characteristics of organic compounds, the candidate is also interested in coordination chemistry in its different aspects varying from "classical" complex compounds through "host-guest" interactions to model systems, an object of bioinorganic chemistry. The studied systems include cyclodextrins – metal cations from groups 1-3 [40, 109], crown ethers – groups 1-2 metal ions [59], ACE inhibitors [70], rhodamine – pyrazole – Cu(II) [84], derivatives of 1,8-naphthalimide with ions of Mg(II), Fe(III) [97], Hg(II) [100], complexes between dyes and cucurbit[7]uril [104].

3.3.3. Habilitation thesis

Assoc. prof. Angelova conducts wide research, which shows the application of quantum-chemical calculations at different levels of knowledge according to the peculiarities of the studied systems. In sync with the presented materials are the publications, summarized as a habilitation thesis (indicator C), which reflect the already discussed scientific interests of the candidate. Here, the introductory part, focused on fundamental issues that show the need to combine experimental research with theoretical developments, makes a very good impression.

3.3.4. Methodology

Dr. Silviya Angelova applies a set of computational protocols, the diversity of which is dictated not only by the nature of the compounds and the environment in which they are studied, but also by the experimental methods used for their characterization. The main DFT functionals are B3LYP, M06, M062X, MN12-SX, etc., and the solvent effect is accounted for by PCM (Polarizable Continuum Model) and SMD (Solvation Model based on Density). Various characteristics are predicted based on the calculations performed - HOMO/LUMO orbital

energies, charges, thermodynamic parameters (enthalpy, Gibbs energy), UV spectra, chemical shifts, etc.

The majority (12, 60%) of the publications submitted for the competition are experimental studies, skilfully combined with appropriate quantum-chemical calculations. Six scientific communications summarize the output of the pure theoretical studies, and one is a review paper containing own results and those of other authors.

3.3.5. Quality of the scientific papers

Assoc. prof. S. Angelova publishes in specialized journals that fully correspond to the research subjects: Journal of Photochemistry & Photobiology A: Chemistry, Dyes and Pigments, Sensors, Beilstein Journal of Organic Chemistry, Physical Chemistry Chemical Physics, Inorganics, Inorganica Chimica Acta, Molecules, ChemPhysChem, etc. The impact factor (IF) varies from 2.3 to 7.0, with an average value of 3.4 for the publications submitted for the competition.

The author teams include colleagues from the Institutes of the Bulgarian Academy of Sciences, Universities in the country (SU, MU), teams from Italy, Russia, Germany, Denmark, Egypt, Belgium, Spain. In one publication, assoc. prof. Angelova is the sole author, in the rest the teams vary between 3 and 13 co-authors, which shows the candidate's ability to teamwork with good communication between the research groups. Silviya is a corresponding author in 45% of the submitted scientific communications.

The Hirsch index for the overall production of S. Angelova is 13 (excluding self-citations of all authors), reflecting the relevance and significance of the research conducted, as assessed by the scientific community.

4. Scientific contributions of the candidate

In the presented publications, Silvia Angelova contributes mainly to planning, conducting and interpreting of the theoretical calculations. In addition to the already mentioned fundamental impact of the most of her research, some of the studied systems also show potential for application as chemosensors, molecular switches, nonlinear optical devices, etc.

4.1. Publications equivalent to a habilitation thesis

The publications under indicator C can be divided into three main groups:

- chemosensors based on 1,8-naphthalimide and rhodamine-pyrazoles;
- "host-guest" complexes between dyes and cucurbit[7]uril;
- D-A⁺ chromophores for application in nonlinear optics.

Main contributions:

4.1.1. New derivatives of 1,8-naphthalimide were synthesized; the geometry, the electronic structure and the solvent effect on their absorption were studied using DFT / TD-DFT methods. Coordination compounds were modelled to explain the observed photophysical characteristics and/or the selective sensing ability under the influence of metal ions (Mg(II), Fe(III), Hg(II), etc.). After confirming the presence of sensing activity, some of the newly obtained dyes were used to obtain fluorescent styrene copolymers.

4.1.2. A significant contribution to the chemistry of 1,8-naphthalimides is their inclusion in dendrimers of different generations (based on PPA, PAMAM), which results in the formation of new ones possessing interesting properties. Due to the large size of these systems, a fragment was modelled, the geometry of which was optimized. The possibility of participation in hydrogen bonds with the solvent methanol, which are decisive for the 3D structure of the dendrimer, was considered.

4.1.3. A chemosensor based on rhodamine and pyrazole was synthesized, and the geometry of its fluorescent and non-fluorescent forms was optimized using theoretical approaches. Coordination compounds with Cu(II) ions were modelled at different reactants molar ratio, and the ability of various ligating functionalities to participate in the formation of complex species was evaluated.

4.1.4. The ability of cucurbit[7]uril (CB[7]) to be used as a solid matrix for the incorporation of certain fragments of structurally different dyes and/or polymers into its cavity has been investigated. The thermodynamically favourable formation of “host-guest” complexes and the possibility of designing supramolecular polymer hydrogels based on dyes and CB[7] have been evaluated.

4.1.5. Systems containing donor (D, N-heterocycles) and acceptor (A, azonium cation) fragments, which are directly bound without a conjugated system between them, have been synthesized. The electronic structure, linear and nonlinear optical properties of the compounds, as well as the influence of substituents on them, have been studied using theoretical approaches. The result of combining theory and experiment is the rise of a promising strategy to design the synthesis of directly bound D-A organic chromophores with application in nonlinear optics.

4.2. Publications outside the habilitation thesis

The publications under indicator D illustrate a wide range of scientific issues that can be addressed through an appropriate combination of experimental and/or theoretical approaches. Below are presented the candidate's main contributions in the field of phenomena related to objects of organic and bioinorganic chemistry.

4.2.1. The main factors responsible for the interaction of α -, β , γ -cyclodextrins with metal ions from groups 1-3 have been evaluated (DFT/PCM study). It has been found that the small size of the metal ions, combined with their high charge, favours the complexation reactions. The gas phase or solvents with low polarity influence the processes in the same direction.

4.2.2. DFT study has revealed that the small ionic radius of group 1-2 metal ions is preferred to undergo the formation of thermodynamically stable complexes with crown ethers containing Schiff bases. These complex species exist preferentially in acetonitrile, while the coordination of the remaining cations is favoured in the gas phase.

4.2.3. New styryl dyes containing crown ethers have been synthesized and was found to exhibit a higher degree of trans-cis photoisomerization, possessing longer live-time of the higher-energy forms compared to their analogues. The enthalpy of the two isomers and the potential for energy storage by the studied systems have been predicted using the DFT method.

4.2.4. The ability of the antihypertensive drugs captopril and lisinopril to interact with the Zn(II)-containing fragment (HEXXN) of angiotensin-converting enzyme (ACE), leading to their inhibitory effect and their use as antihypertensive agents, was evaluated. The results were compared with those of the tripeptide Val-Pro-Pro, isolated from milk, which shows its significantly weaker affinity for binding to the Zn-HEXXN motif of ACE.

The indicated contributions to the publications outside the habilitation work of Silviya Angelova are only representative of her efforts in solving various scientific issues and do not belittle her achievements in the other communications under indicator D for participation in the competition.

In summary, the candidate's research activity is aimed at using recent and adequate theoretical models to explain the matter properties, and in some cases - to predict them. The presented research is part of Silviya's significant project activity, and her participation as co-supervisor of numerous graduate students demonstrates her ability to guide and support students in their scientific work. The achieved results in the field of organic / coordination chemistry and the relevant contributions meet the criteria of the competition for holding the academic position "professor".

5. Question to the candidate

I am convinced that the advanced trends of the computational protocols lead to the development of methods that are in good enough agreement with (or predict) the characteristics of compounds in their experimental UV-VIS, IR, NMR spectra. A problematic area is the

circular dichroic spectroscopy of small molecules rich in chiral centers and their metal complexes, where to date the theory has rarely been able to explain the experimentally observed phenomena.

My question to the candidate is (of course, if she is familiar with this strictly specific issue) – what is the reason for the shortcomings of quantum chemical calculations in predicting the circular dichroic characteristics of small chiral molecules?

6. Final remarks

From the point of view of the current rules for holding the academic position "professor", Silviya Angelova's scientific production meets the requirements set out in the current Law for acquiring scientific degrees and holding academic positions of the Republic of Bulgaria, in the Regulations for its implementation and in the documents of the IOMT-BAS. The scientometric indicators have been exceeded the criteria for the professional field 4.2. "Chemical Sciences".

From the above, as well as from the overall scientific and professional activity of the candidate, I **support** the election of assoc. prof. Silviya Emilova Angelova, PhD, for the "professor" position in the field 4.2. "Chemical Sciences" (Physical Chemistry) for the needs of the Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, and highly recommend the Scientific Council of IOMT-BAS to approve this decision.

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