

REVIEW

on the competition for the occupation of the academic position "Professor"
at the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski"
in the field of chemical sciences, code 4.2. (Physical chemistry)
declared in the State Gazette, issue 21/15.03.2022

Candidate (sole): Assoc. Prof. Dr. Vesselin Kostadinov Petrov

Review: Prof. Dr. Vanya Bogdanova Kurteva, IOCCP-BAS; Member of the Scientific Jury,
appointed by Order RD-38-174 from 01.04.2022

Assoc. Prof. Dr. Vesselin Petrov presented all required documents in hard copy and electronic form, which are in accordance with the Act for the Development of the Academic Staff in the Republic of Bulgaria (ADASRB), the Regulations for the application of the ADASRB, the Regulations for the terms and conditions for acquiring academic degrees and occupying academic positions of the Sofia University "St. Kliment Ohridski" and the Recommendations on the criteria for acquiring scientific degrees and occupying academic positions at the Sofia University for the professional field "Chemical Sciences", related to the procedure for occupying the academic position "Professor". The documentation submitted has been prepared correctly, transparently and in accordance with all requirements.

I. Personal and professional data of the applicant

Assoc. Prof. Petrov has over 20 years of work experience in the specialty at IOCCP-BAS (1998-2000) and at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kl. Ohridski" (since 2013). In the period 2000-2004 he was a doctoral student at the University of Forestry in Sofia, and in 2006 the High Attestation Commission awarded him the educational and scientific degree "Doctor" in the scientific specialty 02.22.01. "Ecology and ecosystem protection". Since 2013 he has held the positions of guest researcher at Sofia University „St. Kl. Ohridski“, Faculty of Chemistry, under the project "Beyond Everest", chief assistant in the Department of Physical Chemistry at FHF-SU, and in 2018 acquired the academic position of "Associate Professor". In the period 2000-2001 he completed a postdoctoral qualification at the Free University of Amsterdam, the Netherlands, and in the period 2006-2014 he was a visiting researcher at the New University in Lisbon, Portugal.

Assoc. Prof. Petrov carries out intensive expert work. He is a reviewer of scientific communications for many renowned scientific publishers such as RSC, ACS, Elsevier, Wiley, MDPI, LDD, etc.

Assoc. Prof. Petrov has impressive computer knowledge and skills. Uses at an expert level a wide range of standard and specialized software products and has a thorough knowledge of computer hardware.

II. General characteristics of scientific, applied and pedagogical activity and their reflection in the scientific literature

Assoc. Prof. Petrov has presented for the current competition a list of scientific publications for his entire creative period, a list and copies of scientific publications with which he participates in the current competition, habilitation work entitled “Molecular metamorphoses”, and author’s query. A check up of compliance with the national requirements is presented. The breakdown of indicators is as follows: indicator A - 50 points; indicator C - 135 points; indicator D - 275 points; indicator E – 222.87 points; and indicator E - 128 points. As can be clearly seen, the contributions of Assoc. Prof. Petrov exceed the national requirements. The presented list of scientific publications for the entire creative period includes 45 scientific papers, of which 42 in international journals with impact factor. In this competition Assoc. Prof. Petrov participates with 18 scientific publications in refereed and indexed journals. The distribution of scientific reports according to the rank of the journal in which they are published is as follows: 11 in journals with rank Q1 (61.1%), 6 with rank Q2 (33.3%) and 1 with rank Q3 (5.6%). The fact that almost all scientific publications (94.4%) were published in the two highest categories of journals, Q1 and Q2, makes an excellent impression. According to indicator C, Assoc. Prof. Petrov presented 6 scientific publications in journals with rank Q1 and Q2, 3 of each category, and according to indicator D he participated with 12 publications, 8 in journals with rank Q1, 3 with rank Q2 and 1 in Q3. It should be noted that of the scientific publications presented under indicator D, 1 cannot be recognized as an article (Pina, F.; Petrov, V.; Laia, C. A. T., Photochromism of flavylum systems. An overview of a versatile multistate system, *Dyes and Pigments* **2013**, 99, 256), as it is the *Corrigendum* of another article with which Assoc. Prof. Petrov participated in the competition (Pina, F.; Petrov, V.; Laia, C. A. T., Photochromism of flavylum systems. versatile multistate system. *Dyes and Pigments* **2012**, 92, 877-889), and for one article (Petrov, K.; Avdeev, G.; Petrov, V., Revision of the crystal structure and cation distribution of $\text{LiMn}_{2-y}\text{TiyO}_4$ ($0 \leq y \leq 1.0$) spinels. *Solid State Sciences* **2022**, 123, 106781) are given 15 points, while the article is published in a journal with rank Q2 according to the *Web of Science* and *Scopus* databases, therefore it is reported with 20 points.

The personal contribution of Assoc. Prof. Petrov in the scientific communications presented at the competition is clear from his leading role in a part of the articles. In 6 of the scientific publications (33.3%) the candidate is an author for correspondence; 4 in journals with rank Q1 (36.4% of the articles in journals with rank Q1; 4 out of 11) and 2 with journals with rank Q2 (33.3% of the articles in journals with rank Q2; 2 out of 6). The distribution of these reports by indicators is 2 in journals with rank Q1 on indicator C and 4 in journals with rank Q1 and Q2, 2 of each category, on indicator D. These data clearly show that the scientific reports of Assoc. Prof. Petrov fully covers the additional recommended criteria in the Recommendations for the criteria for acquiring scientific degrees and holding academic positions at Sofia University for the professional field "Chemical Sciences", related to the procedure for holding the academic position "Professor": 6 (recommended 5) publications in which the candidate is the first author or author for correspondence, and 275 (recommended 220) points on indicator D.

The articles Assoc. Prof. Petrov have found a wide response in international literature. A list of noticed citations in refereed and indexed in *Web of Science* and *Scopus* journals is presented, including 102 citations (recommended 60) after his election as an associate professor in 2018, of which 89 of the articles with which he participated in the competition. A search in *Scopus* data base shows that Assoc. Prof. Petrov possesses Hirsh index of 9 excluding self-citations.

The reference for the scientific contributions for the scientific contributions is written concisely and clearly outlines the achieved results and the personal contributions of Assoc. Prof. Petrov. It covers 27 scientific communications published in the period 2010-2022, which have been cited more than 250 times in the last 5 years. The achieved results are divided into 3 thematic directions: 1. synthesis and properties of flavylum salts; 2. synthesis and properties of inclusion complexes in cyclodextrins and cucurbiturils; and 3. synthesis and properties of rare earth metal complexes.

According to indicator "C", Assoc. Prof. Petrov participated with 6 articles in journals with rank Q1 and Q2, described above. A habilitation thesis entitled "Molecular metamorphoses" is also presented, designed on 44 pages as a view article summarizing results on the topic published in 51 literary sources and supported by 28 figures. The literary sources include 13 scientific reports co-authored with Assoc. Prof. Petrov. The preparation of this material is of undoubted benefit to the candidate and I would recommend that it be updated with the latest results and published in a suitable high level journal.

According to indicator "F", Assoc. Prof. Petrov presented participation in scientific projects and attracted funds, supported by relevant documents, with a total score of 192.87 points, not 264 as written in the minimum requirements reference. He is a participant in 4 national scientific projects; National Center of Excellence "Mechatronics and Clean Technologies", project

"Achieving an optimal environment for training, research, innovation and sustainable development of human potential in the field of chemical sciences: Adapting education today for tomorrow", funded by the Ministry of Education and Science under Operational Program "Science and Education for Intelligent Growth", which was incorrectly indicated by the candidate as international, and in 2 projects of the FNI at the Ministry of Education and Science, DFNI K02/15 on the topic "Creation of a specialized electronic library for research and identification of art artefacts with the aim of preserving the Bulgarian cultural heritage" and KP-06- H39/2 entitled "Machine learning in structure-property correlation estimation: on the hunt for singlet cleavage chromophores". He is also a participant in 2 international scientific projects funded by the European Commission: Beyond Everest - REGPOT-ST-2011, on the topic "Development of the research staff of the Faculty of Chemistry at Sofia University in the field of modern functional materials for successful participation in scientific research at the world level within the framework of the European Union", financed within the frame of the 7th Framework Program, and Materials Networking 692146 entitled „Enhancing the scientific capacity of the Faculty of Chemistry and Pharmacy at Sofia University as leading regional research and innovation centre in the area of advances functional materials“.

Assoc. Prof. Petrov is the head of a project funded by the European Commission, NanoPaInt – 955612 entitled "Dynamics of dense nanosuspensions: a pathway to novel functional materials". The project has a budget of 211 586.40 euros.

Assoc. Prof. Petrov's pedagogical activity is significant. Leads lecture courses and exercises for bachelor students in 5 specialties at the Faculty of Chemistry and Pharmacy at SU "Kl. Ohridski". His lecturing activity is 354 hours per year and includes 4 lecture courses from the compulsory program (234 hours per year) and 2 elective courses (120 hours per year). Compulsory courses include "Physical Chemistry and Colloid Chemistry" Parts I and II, "Chemical Informatics" and "ICS", and electives "Non-Equilibrium Thermodynamics" and "Near Infrared (NIR) Spectroscopy". It is important to note that the two elective courses were introduced by Prof. Petrov. Leads also exercises with a total annual workload of 315 hours in the disciplines "Physical Chemistry" Part I and II, "Information Technologies", "PDP & NIT", "ICS", "Non-Equilibrium Thermodynamics" and "Near Infrared (NIR) Spectroscopy".

According to indicator "G", Assoc. Prof. Petrov participated in activities with a total score of 128 points. According to the *Scopus* database, the Hirsch index of the articles with the participation of Assoc. Prof. Petrov is 9 excluding self-citations, which gives him 90 points. Apparently, the candidate reported an h-index of 14 including self-citations, leading to the increase in points in the reference for minimum requirements. The above mentioned 2 lecture courses, introduced by Assoc. Prof. Petrov, carry 20 points. Also included are 2 scientific

communications of the candidate (18 points), which were not used in previous procedures; articles 29, 41 and 42 of the list of all publications of the applicant.

III. Basic scientific contributions

Assoc. Prof. Vesselin Petrov is a pronounced spectroscopist with extensive knowledge in theoretical and computational chemistry. His scientific developments fall into three main directions:

- ✓ Synthesis and properties of flavylum salts;
- ✓ Synthesis and properties of inclusion complexes in cyclodextrins and cucurbiturils;
- ✓ Synthesis and properties of rare earth metal complexes.

The study of the *properties of flavylum salts* occupies a central place in the scientific developments of Assoc. Prof. Petrov. The *equilibria in natural and synthetic anthocyanins*, representatives of the family of flavylum salts, are investigated, and the main thermodynamic and kinetic parameters were determined. Adducts and dimers of anthocyanins are studied with spectral methods and a complete mathematical system is developed for entire characterization of the compounds in a thermodynamic and kinetic aspect. Synthetic derivatives of the flavylum cation have been shown to possess interesting photochemical properties and have potential applications as optical recording media, neural networks, ionic liquids, in photovoltaic cells, etc. Complex equilibria related to dimerization and aggregation that may be involved in the reaction chain of the flavylum cation and related forms are investigated, and a complex mathematical model encompassing all possible reactions and forms of the flavylum compounds is derived, which allows easy realization of computer programs. The process of converting 2-hydroxy substituted flavyls into flavonoids, compounds important for humans, animals and plants, has been proven for the first time with kinetic studies.

Substantial attention has been devoted to researching the applications of synthetic flavylum salts and their forms in *nanocrystalline dye-sensitized solar cells* as alternative to Ru(II) complexes sensitizers. A distinction is made between synthetic flavylum salts and natural anthocyanins, which are identical from a physicochemical point of view. The design of effective sensitizers is carried out by varying the type and position of the substituents in the molecule, and a group of 7 compounds is synthesized and studied thermodynamically and kinetically. It has been shown by theoretical methods that the largest dipole moments occur when the electron-donating groups align with the bridging catechol moiety, thereby increasing electron injection into the semiconductor.

The behaviour of *host-guest complexes* of organic compounds with cyclic molecules with suitable cavities, cyclodextrins and cucurbiturils, is studied. The kinetic process of adduct formation between flavylum compounds and β -cyclodextrin is examined and the concept of cyclodextrin cavity emptying under the action of light is illustrated. It is found that synthetic flavylum cations form with cucurbit[7]uril 1:1 complexes and that their stability depends on the size, shape and type of substituents and on the hydrophobicity of the molecule.

Inclusion complexes of *medicinal substances* with limited water solubility in β -cyclodextrin are synthesized and characterized, leading to a significant increase in the solubility of the medicinal form. A synthetic methodology has been developed for obtaining a complex with ibuprofen, a non-steroidal anti-inflammatory agent, which achieves complete formation of a 1:1 complex. The method has also been successfully applied to obtain a complex of the anti-inflammatory medicinal substance naproxen with β -cyclodextrin. Two models for the structure of the obtained complexes are proposed and the binding energies and stability constants are determined. The complexes of naproxen with β - and γ -cyclodextrin are investigated by physical methods and the position of the drug in the cavity of the host molecule is determined. It has been shown by computational methods that the stability of the complexes is strongly dependent on the orientation of the drug molecule. Naproxen is found to enter the cyclodextrin cavity with its carboxyl group oriented toward the narrower edge of the cyclodextrin and form hydrogen bonds with its hydroxyl groups.

Complexes of 1,10-phenanthroline with rare earth metals were obtained and characterized. A simple two-step procedure for the functionalization of hydrophobic silica aerogel with Eu(III) ions and phenanthroline is proposed. The resulting complex is shown to exhibit red emission under UV excitation, while the phenanthroline-only functionalized aerogel exhibited blue emission. A complex of 1,10-phenanthroline with Ho(III) ions is also obtained. A hyperchromic effect with increasing temperature is observed and a new model is proposed to describe the observed broadening of the spectral bands.

The structure of ***LiMn₂-yTiyO₄ spinels***, compounds with applications as electrodes in lithium-ion batteries, is analysed and the absence of tetracoordinated titanium is proven. Two literature models for the valence states and distribution of 3d-cations in spinels are analysed and rejected.

3. Critical remarks and suggestions

I also have some critical notes. A number of inconsistencies are noted between the data specified in the minimum requirements table and the rest of the documents. As stated above, for 1 article, which is a *Corrigendum* of another article with which Assoc. Prof. Petrov participated in the competition, 25 points are illegally awarded, for another article 15 points are given, while

the article is published in a journal with a rank Q2 according to the databases *Web of Science* and *Scopus*, therefore the points should be 20, and 1 project "Achieving an optimal environment for learning, research, innovation and sustainable development of human potential in the field of chemical sciences: Adapting education today for tomorrow', financed by the Ministry of Education and Science under the Operational Program "Science and Education for Smart Growth", is wrongly indicated by the applicant as international. Regardless of the fact that indicator "G" has been introduced in the Regulations for the terms and conditions for acquiring academic degrees and occupying academic positions of the Sofia University "St. Kliment Ohridski" and is valid only for scientist from SU, it is mandatory. It was proper that the data on this indicator were filled in the table for the minimum requirements and that the members of the scientific jury did not have to look for them in the presented documents. However, these notes do not in any way affect the overall positive impression of the scientific output presented.

CONCLUSION

It is undisputed for me that Assoc. Prof. Dr. Vesselin Petrov is a productive researcher with established qualities and a promising career. Analysing the candidate's scientific achievements, the relevance and perspective of the topics, active teaching and his personal qualities and skills, I think that the candidate meets all requirements of the Act for the Development of the Academic Staff in the Republic of Bulgaria, the Regulations for the application of the ADASRB, the Regulations for the terms and conditions for acquiring academic degrees and occupying academic positions of the Sofia University "St. Kliment Ohridski" and the Recommendations on the criteria for acquiring scientific degrees and occupying academic positions at the Sofia University for the professional field "Chemical Sciences", related to the procedure for occupying the academic position "Professor", and I strongly recommend that the Faculty Council of the Faculty of Chemistry and Pharmacy at Sofia University award to

Associate Professor Dr. Vesselin Kostadinov Petrov

the academic position of "Professor" in the field of higher education 4. Natural sciences, mathematics and informatics, professional field 4.2. Chemical Sciences (Physical Chemistry).

Sofia, July 11, 2022

Prepared the appraisal

(Prof. Dr Vanya Kurteva)