

# REVIEW

by Prof. Vassil Borissov Delchev, DSc,

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Competition for the academic position “professor” at the University of Sofia

*Field of higher education:* 4: Natural sciences, mathematics and informatics

*Professional area:* 4.2. Chemical sciences

*Scientific field:* Theoretical chemistry

*Candidate:* associate professor Petko Stoev Petkov PhD,

Faculty of chemistry and pharmacy, University of Sofia

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Announcement of the Competition: **State Gazette No 105 / 11.12.2020.**

Rector's order for the constitution of the Scientific jury: **РД-38-10/07.01.2021r.**

Decision of the first meeting of the Scientific jury: **to write an academic review.**

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The documents for the competition are available on the electronic platform of the University of Sofia named *Elearn*. They consist of the next files: 1) a standard *Curriculum Vitae*; 2) a diploma for higher education and a PhD diploma; 3) a certificate for the academic position “associate professor” at the Faculty of chemistry and pharmacy; 4) a certificate for academic positions at the Faculty of chemistry and pharmacy; 5) a list of all publications and a list of publications participating in the current competition; 6) lists of citations and contributions; 7) a habilitation thesis; 8) a file with a scan of the announcement of the competition published in *State Gazette*.

## **Biographic information**

In 2002 assoc. prof. Petkov has graduated the University of Sofia with a bachelor's degree. According to the CV enclosed the subject of the bachelor program is “Physical chemistry and theoretical chemistry”. Two years later (in 2004) assoc. prof. Petlov has finished his master's level study in “Computational chemistry” at the Faculty of chemistry and pharmacy of the University of Sofia, defending a master's thesis. In 2009 Dr. Petkov defended successfully a PhD thesis at the Chemical faculty of the University of Sofia. The title of the thesis is: “*Influence of non-metal atoms on the properties and reactivity of small nickel clusters – a DFT level investigation*”; scientific field: theoretical chemistry. The defence of the PhD thesis has been carried out to a Specialized scientific council at the former Higher attestation commission. Among the enclosed documents I did not find the name of the scientific supervisor of the applicant; however the check up in the database of the National center for information and documentation revealed that the scientific supervisor is prof. DSc G. Vayssilov from the Faculty of chemistry and pharmacy of the University of Sofia.

In 2018 the applicant has been promoted to an academic position “associate professor”, and he holds this position until now. In the period 2009 – 2018 the applicant has passed gradually through the university positions “assistant professor” and “chief assistant professor”. The appointments to these positions are certified with a document issued by the Human resources department at the University of Sofia. There is one systematic and gradual development of assoc. prof. Petkov in the academic carrier which makes him a complete academic person, highly prepared and motivated to perform deep scientific research and teaching in a serious academic institution like the Faculty of chemistry and pharmacy of the University of Sofia.

## Scientific activity

Indicator	A	Б	B	Г	Д	E	Ж
1	50	-	100	220	120	150	120
2	50	-	275	320	470	210	182

1 – According to the Minimal national requirements in the professional area.  
2 – Assoc. prof. PhD Petko Stoev Petkov

### Scientific works

The applicant assoc. prof. Petkov participates in the competition for the academic position “professor” with 20 scientific papers. Nineteen from them are published in scientific journals with quartiles Q1. One publication is in a journal with a quartile Q2. Seven publications are included in indicator B in accord with the minimal national requirements of the professional area for the academic position “professor”. All of them have quartiles Q1 and their total impact factor is 74.556. The total number of points for this indicator is 175. I have to point out that the applicant has enclosed a habilitation thesis among the documents which should be valued with 100 extra points! Thus the total number of points for indicator B has to be 275. I suppose that the applicant has given only 175 points since the publications included in indicator B are also involved in the reference list of the habilitation thesis. Nevertheless I think that 100 extra points should be added to indicator B! The habilitation thesis comprises 38 pages, in English. It is entitled: „*Computational modeling of the framework flexibility and electronic properties of metal-organic frameworks*”. The number of references is 58, nine of them – self-publications of the applicant. Two publications are not given in indicator B.

For indicator Г the applicant presents 13 scientific publications. Ten of them have quartiles Q1 and only one is with a quartile Q2. The total impact factor of the journals with publications of assoc. prof. Petkov is 81.277. It is known that the deep impact factor of a journal is a consequence of its high prestige. No doubt that all this is a proof for the high significance of the scientific investigations of assoc. prof. Petkov. Most of the publications have many co-authors which shows that the results published are based on many-vector research. In the applied documentation the applicant has declared that his personal contribution is connected with the computational study of structures and interactions between molecular systems.

Based on the enclosed scientific papers in indicators B and Г, assoc. prof. Petkov has summarized the next major contributions:

1) *Geometry structure and electron properties of coordination and organic polymers.* The structures of breathing metal-organic frameworks of polymers with organic ligands and metal ions have been proposed. They have pores which can change their shapes and size depending on the external conditions. The results are described in papers No 2, 13, 14, 17 and 20 (the paper numbering follows that from the list of publications). The carried out investigations are together with the experimental group of prof. S. Kaskel from the TU-Dresden. They have been performed within a joint project between the two groups which goes on at present. In paper No 2 it has been shown that the low-frequency vibration modes play a crucial role on the phase transformation process of flexible metal-organic frameworks. In paper No 12 with the help of the Density functional theory it is proven that the collective flexibility of pores is controlled by conformational isomerism of the ligands. The free energy of conformational changes of the ligands and the consequences from these processes have been estimated by means of methadynamics calculations. Applying *ab initio* molecular dynamics, it has been proven that the low-frequency Raman vibration modes of some structures, e. g. for the structure DUT-8(Ni), are connected with vibrations along the diagonals of pores of the lattice, which is in a direct dependence with the open / closed form of the lattice.

The electron structure and the magnetic properties of some two-dimensional metal-organic frameworks have been established by experimental (in the group of prof. X.

Feng - TU-Dresden) and quantum chemical computations. The results are described in papers No 3 and 12. Semiconductive properties have been found for one of the structures. In one of the researches (paper No 11) the authors have proposed the molecular structure of quasi-two-dimensional film of polyaniline. The structure has been found at the DFT level. The results have shown a  $\pi$ - $\pi$ -stacking at the areas of overlap (the edges) of the polymer chains.

2) *Theoretical investigations on the interactions of drug molecules with mesoporous materials and biopolymers.* The interactions of drug molecules like quercetin, curcumin, verapamil, miltefosine, doxorubicin with mesoporous materials and biopolymers as carriers have been investigated with theoretical methods. They are based on experimental observations carried out at the Institute of Organic chemistry – Bulgarian academy of sciences. Some features (bonding way, bonding energy etc.) connected with the better absorption of drugs in organisms have been proposed.

3) *Theoretical investigations of spectral features of molecules and clusters in different surroundings.* The spectral properties and the excited states of some molecules and clusters have been studied. For example the study of the system  $\text{Ba}(\text{ClO}_4)_3 \cdot 3\text{H}_2\text{O}$  has shown that the information from the *steady-state* and *time-resolved* spectroscopy of crystal systems in combination with theoretical methods can contribute to the clarification of the main relaxation processes (paper No 5). For 3-diethylphosphonocoumarin it has been proven that the first singlet excited state lifetime depends on the nature of the halogen atom at the sixth position (paper No 16). A new classification of the surface nitrates has been proposed for the process of adsorption of  $\text{NO} + \text{O}_2$  on  $\text{CeO}_2$  surface (paper No 18).

4) *Investigation of ion mobility with ab initio molecular dynamics.* The bonding way of alkali and alkaline earth metals with ionized groups of RNA has been investigated theoretically in water medium. It has been found that the  $\text{Na}^+$  ions are much more movable than  $\text{Mg}^{2+}$  during the process of bonding to the phosphate groups of RNA. The results are summarized in the review paper No 6. Furthermore the diffusion mechanism of protons and protium in layer materials like  $\text{BN}_3$  and  $\text{MoS}_2$  has been revealed. It has been found that the mechanisms involve transportation of protium predominantly through the interlayer space, which is in accord with experimental observation (paper No 15).

In addition to the scientific contributions it should be noted that 18 heterogeneous catalytic systems with metals Pd, Pt, V, Co, Cu etc. have been also investigated. A classification of metals and their salts has been proposed in regards to their toxicity for life forms as fishes, seaweeds and rats. It has been found that the most life-friendly components of the catalytic systems are Ru, Fe and Mo.

#### Citations

The applicant participates in the competition for the academic position “professor” with 235 citations excluding self-citations of all co-authors. Listed by papers they are: paper No 1 – 46 citations, paper No 2 – 14 citations, paper No 3 – 84 citations, papers No 4 and 14 – 5 citations each, papers No 5 and 15 – 1 citation each, paper No 6 – 11 citations, papers No 10 and 13 – 2 citations each, paper No 7 – 3 citations, paper No 8 – 9 citations, paper No 9 – 7 citations, paper No 11 – 17 citations, paper No 12 – 28 citations. All the citations appear in the SCOPUS database. The citations are for the last several years, which shows that they do not repeat those used in previous procedures of assoc. prof. Petkov. Thus for indicator B are collected totally 470 points. According to SCOPUS the Hirsch index of the applicant is 13.

#### Participations in scientific events and projects

Assoc. prof. Petkov has reported the results of his investigations on 20 scientific forums. He has presented 12 oral section reports and 8 posters. It would be better if more information about the conferences was provided – which of them are national and which are international.

For indicator E the applicant provided a list of projects, in which he has been a member of the research teams or a project leader. According to the list, Dr. Petkov is a member of the

research teams of 12 projects, most of them funded by the National Science Fund. Three of the projects are funded by operational programs of the European Union. The applicant has declared three participations in international projects as a member of the research teams. Dr. Petkov is a project leader for the Bulgarian team of a bilateral project with Japan. The total financial support of the projects is 150 000 BGN. I did not see any participations of the applicant in ERASMUS initiatives supported by the European Union.

### **Teaching activity**

The provided information by assoc. prof. Petkov concerning his teaching activity shows that the applicant is a long-standing university lecturer at the Faculty of chemistry and pharmacy of the University of Sofia. The teaching activity of the applicant comprises lecture courses, seminars and laboratory practices. The applicant has proposed three new lecture courses: "Molecular modeling of materials", "Introduction to the programming in Linux shell", and "Quantum chemical modeling of organic systems". He has been also a lecturer of the courses "Organic chemistry" and "Hybrid QM/MM methods".

Assoc. prof. Petkov has been a leader of the seminars and laboratory practices in "Organic chemistry" I and II part and the practical exercises in "Introduction to the programming in Linux shell", "Molecular modeling of materials", "Applied quantum chemistry" and "Quantum chemical modeling of organic systems". The last two practical courses have been proposed by the applicant. All this is a notable teaching activity, which according to the teaching certificate enclosed to the documents, started from the beginning of the academic carrier of the applicant (in 2009 as an assistant professor) at the Faculty of chemistry and pharmacy of the University of Sofia. In support of this is the enclosed document with annual teaching hours of the applicant. It shows on the average 500 academic hours per academic year. For the current academic year the applicant has declared 680 academic hours.

Assoc. prof. Petkov has been a scientific supervisor of two diploma students, who have carried out their investigations in the research area of the applicant – in the field of theoretical chemistry. Together with prof. DSc. G. Vayssilov and prof. T. Heine, Dr. Petkov has been a co-supervisor of two more diploma students. These are the diploma theses of Iskra Koleva and Radu Bors. The last thesis has been presented and defended at the Jacobs University, Bremen, Germany. Despite the fact that the applicant has not been a supervisor of any PhD students, he fulfils the recommended criteria to hold the academic position "professor" at the Faculty of chemistry and pharmacy of the University of Sofia since he applies for the position with an equivalent number of diploma students. All this is marked in indicator Ж of the minimal national requirements. For indicator Ж the applicant provides also two papers with a methodological purpose. They are published in the "Chemistry" journal.

I would recommend to assoc. prof. Petkov in near future to be engaged with PhD students under his supervision. With the experience and the international contacts that the applicant has, I'm sure that a lot of successful PhD theses in the field of theoretical chemistry could be realized.

Among the documents enclosed I did not find information concerning any published text-books, academic manuals etc. (on paper or electronically) by assoc. prof. Petkov. Therefore I would recommend him to be more active in this aspect.

### **CONCLUSION**

The materials provided for the competition for the academic position "professor" are in agreement with the Law for development of the academic staff in Republic of Bulgaria, the Rules for its application as well as with the recommended criteria of the Faculty of chemistry and pharmacy of the University of Sofia. The candidate covers all the criteria in the professional area. He is a complete scientist and lecturer in the professional area and I have

no doubt that his successful carrier will go on in future. In this aspect I give my **positive vote** for the candidature of the applicant and I recommend to the Scientific jury to propose to the Faculty council of the Faculty of chemistry and pharmacy of the University of Sofia to elect associate professor Dr. Petko Petkov to the academic position “professor” in a field of higher education: 4: Natural sciences, mathematics and informatics; professional area 4.2. Chemical sciences; scientific field “theoretical chemistry”.

05.04.2021

Plovdiv

Reviewer: