

REPORT

by Prof. Ivanka Tsakovska, PhD,

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Member of the Scientific Jury appointed with Order № RD-38-10 from 07.01.2021
of the Rector of Sofia University “St. Kl. Ohridski”

Regarding the call for **Professor Position**, Area of Higher Education 4. *Natural sciences, Mathematics and Informatics*, Professional Field 4.2. *Chemical Sciences (Theoretical Chemistry)* published in the State Gazette, vol. 105 from 11.12.2020.

In the call for the Professor Position announced in the State Gazette vol. 105 from 11.12.2020 there is a single applicant - Assoc. Prof. Dr. Petko Stoev Petkov. The set of materials provided by the applicant are in accordance with the Act on Development of the Academic Staff in the Republic of Bulgaria (ADASRB) and includes all required documents.

The applicant has built a substantial resume with numerous research stays at prestigious European universities, intensive research, teaching, project and organizational activities. He is an Associate Professor at the Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski” (FCP-SU) from 2018 and in an impressively short period of time has accumulated the necessary materials for participation in the call for a professor position.

Dr. Petkov is a co-author of 52 scientific publications, 49 of which are in journals with impact factor, two - in journals without impact factor, and one is a book chapter in the international publisher Elsevier. According to data submitted by the applicant, the scientific publications have 898 citations and his h-index is 13 according to the Scopus database. He participates in the call for a professor position with 20 publications, all in journals with impact factor (total impact factor 155.83), 19 of them in journals in Q1 category. Given that they have been published only recently (in the interval 2017-2021), their response in the scientific community is remarkable (235 citations according to Scopus).

The applicant’s research explores the field of quantum chemical modelling of structures, their electronic properties, as well as important structural interactions.

The habilitation thesis is based on 7 publications, all of which in Q1 category journals with a total impact factor of 74.556. Those publications focus on quantum chemical modelling of metal-organic frameworks with remarkable structural flexibility. A current project in collaboration with TU Dresden has yielded the synthesis of such a polymer and quantum chemical investigations of its dimeric layers have been conducted (publications 2, 13, 14, 17 and 20), which have led to a number of conclusions: the collective flexibility is controlled by the conformational isomerism of the ligands; the spectral investigations on the open and closed forms of the metal-organic framework have shown that the low-frequency vibrations are vital in the process of the phase conversion; the role of non-linear ligands for the breathing phenomena of the explored metal-

organic framework has been shown; the possibility for modifications of the breathing characteristics of the explored metal-organic frame with the help of other metal ions has been demonstrated.

The second direction in the habilitation thesis (publications 3, 12) describes combined experimental and quantum-chemical investigations which clarify the structure, electronic and magnetic properties of bi-layered metal-organic frameworks as important semiconductor materials. A confirmation for the importance of these investigations is the remarkable number of citations of the papers which have been recently published (year 2018-2019) but have already 84 and 28 citations respectively.

Depending on the investigated objects some of the other scientific achievements of the applicant can be summarised as follows:

- A quantum-chemical modelling and analysis of the interactions of drug structures with mesoporous materials and biopolymers applied as drug delivery systems has been conducted (papers 4, 8, 9, 10, 19)
- A quantum-chemical modelling of the spectral characteristics of molecules and clusters in different media has been performed (papers 1, 5, 16, 18).
- Using ab initio molecular dynamics simulations the mobility of ions has been explored. Namely, the theoretical investigations in paper 15 focus on protium transport through the van der Waals gap in bulk layered materials and provide information on the transport and division of hydrogen isotopes. Review paper 6 has been appropriately included alongside because it conducts a systematical comparative analysis of experimental and theoretical approaches for exploring the dynamics and interactions of alkaline and alkaline earth metal ions with RNA and DNA.

In the provided Author's contributions report the applicant has precisely defined his personal contributions to the conducted research. Based on this information, I assess his personal contribution as essential for carrying out the studies. At the same time, the wide professional network of co-authors is undoubtedly a good prerequisite for participation in future international projects and interdisciplinary research of high quality.

Based on the quality of the publications, as well as the fulfilment of the respective scientific indicators for holding the academic position "Professor", I give a high assessment of the research activity of Dr. Petko Petkov.

Another important aspect of the applicant's professional activity is the active teaching, which includes 6 lecture courses, half of which have been developed by him, as well as three seminars. He has been a supervisor of four diploma students, and currently is a supervisor of a postdoctoral fellow in the competitive and prestigious program "Peter Beron. Science and Innovation with Europe" of NSF.

The analysis on the fulfilment of the minimal national requirements for holding the academic position "Professor", as well as the recommended specific criteria of the FCP (SU), shows the following:

Indicator	Minimal national requirements	Recommendations of FCP/SU	Applicant's scores
A	50	50	50
Б	-	-	0
B	100	100	175
Г	200	220	320
Д	100	120	470
E	150	150	250
Ж (recommendations in SU)		120	182
Total	600	760	1447

These data show that the applicant meets and exceeds 2.5 times the minimal national requirements and twice the recommended quantitative criteria of FHF-SU.

As a researcher working in a related scientific field, I know Dr. Petkov personally and I have been following his academic career from the very beginning. I would point out three typical qualities of him: research curiosity, thoroughness and professional attitude. I am pleased to note that he has grown up as a distinguished scientist, with leadership positions and recognition in the scientific community.

Conclusion: The materials submitted for participation in this call meet and / or exceed many times the requirements of the Act on Development of the Academic Staff in the Republic of Bulgaria, the Regulations for its implementation, as well as the Recommended Criteria of the Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski". Dr. Petkov has demonstrated a fruitful research and teaching activities after taking the position of "Associate Professor" and significant contributions in the field of his academic development.

Based on what has been previously said, I give a positive assessment and strongly support the appointment of Assoc. Prof. Petko Stoev Petkov as a Professor in the Professional Field 4.2. Chemical sciences (Theoretical chemistry).

Sofia, 21.04.2021

Member of the Scientific Jury:

(Prof. Ivanka Tsakovska)