

OPINION

by Prof. Dr. Nikolay Georgiev Vassilev, IOCCP – BAS

of the materials submitted for participation in the competition to hold the academic position of
professor in Sofia University "St. Kliment Ohridski"
professional field 4.2 Chemical sciences (Theoretical chemistry)

In the competition for professor, announced in the State Gazette, issue 105 of 11.12.2020 for the needs of the Faculty of Chemistry and Pharmacy of Sofia University "St. Kl. Ohridski" as the only candidate participates Associate Professor Dr. Petko Stoev Petkov from the Faculty of Chemistry and Pharmacy of Sofia University "St. Kl. Ohridski".

1. General presentation of the procedure and the applicant

Associate Professor Dr. Petko Petkov graduated from the University of Sofia "St. Kl. Ohridski" in 2004 with a professional qualification Master in Computational Chemistry. He defended his doctoral dissertation on "Influence of non-metallic atoms on the properties and reactivity of small nickel clusters - a study with the theory of the density functional" in 2009 at the Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski". His career began at the same faculty in 2004 as a chemist, from 2009 as an assistant professor, then senior assistant professor. From 2018 until now he is an associate professor at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kl. Ohridski".

2. General characteristics of the applicant's activities

Associate Professor Dr. Petko Petkov has included in the documents a list of a total of 49 scientific publications in peer-reviewed and peer-reviewed journals and one chapter of a book. From this list in the competition for the academic position "professor" he participates with 20 scientific publications, of which 7 scientific publications are equated to habilitation work (publications № 2, 3, 12, 13, 14, 17, 20), and 13 are scientific publications with which he fulfills the requirements for the academic position of "professor". The distribution of the 7 scientific publications included in the habilitation work according to the category of scientific

journals is as follows: all are in scientific publications with Q1. The distribution of the 13 scientific publications with which he fulfills the requirements for the academic position of "professor" according to the category of scientific journals is as follows: 12 are in scientific journals with Q1 and one is in a scientific journal with Q2. According to the attached report, the number of citations of scientific publications submitted for participation in the competition is 235. According to the Scopus database, the candidate's h-index is 13. This value is indicative of high scientific productivity combined with a wide response in the literature.

The attached report shows that Associate Professor Dr. Petko Petkov meets the minimum national requirements for holding the academic position "Professor" (indicator A fulfills the national requirement, indicator B is 175 at a minimum value of 100, indicator D is 320 at a minimum value of 200, indicator E is 470 with a minimum value of 100 and indicator E is 210 at a minimum value of 150). According to the recommended criteria for acquiring scientific degrees and holding academic positions at Sofia University "St. Kl. Ohridski" for professional fields 4.2 "Chemical Sciences" the candidate has according to indicator G 320 at a recommended value of 220, according to indicator D has 470 at a recommended value of 120 and according to indicator G has 182 at a recommended value of 150.

The research of Associate Professor Dr. Petko Petkov in the publications included in the habilitation paper is applications of quantum chemical calculations to clarify the structure and properties of Metal-organic networks (MOF) - coordination polymers composed of organic ligands and metal ions forming a system of pores of different sizes. The combined use of theoretical and experimental methods provides a comprehensive insight into the nature of the flexibility of the studied MOFs, as well as explains their properties as semiconductors.

The research of Associate Professor Dr. Petko Petkov in the publications on a group of indicators "D" is a theoretical modeling of the structure and electronic properties of coordination polymers, molecules, clusters and ions in different environments:

- 1) Modeling the structure and electronic properties of coordination polymers and organic polymers;
- 2) Modeling the interaction of drug molecules with mesoporous materials and biopolymers;
- 3) Quantum chemical modeling of spectral characteristics of molecules or clusters in different environments;
- 4) Study of ion mobility by the method of ab-initio molecular dynamics.

In these groups of publications, the systematic research and the selection of an appropriate quantum chemical approach for a correct description of the studied processes stand out.

Scientific papers of Associate Professor Dr. Petko Petkov are at a very high scientific level, meet the theme of the competition and are in the field of computational theoretical chemistry. In most of the scientific publications experimental data are used to verify the theoretical characteristics of the studied systems. The conducted research can be referred to the categories of novelty for science, as well as enrichment of scientific knowledge, clarifying the structure and properties of various molecular systems and describing the processes in which they participate.

3. Teaching and project activity

As a lecturer at FHF - Sofia University "St. Kliment Ohridski" Associate Professor Dr. Petko Petkov has developed three courses and is a lecturer of 6 courses, has led practical classes in "Organic Chemistry" for bachelor students from all specialties of the Faculty of Chemistry and Pharmacy and the Faculty of Biology, and for the specialty Pharmacy in English, being adapted in English by the applicant. The practical classes on Introduction to Linux Shell Programming, Molecular Modeling of Materials, Applied Quantum Chemistry and Quantum Chemical Modeling of Organic Systems have been developed by the candidate. Associate Professor Dr. Petko Petkov is the research supervisor of a post-doctoral student in the program "Peter Beron i NIE" (2021-2022) and has supervised 4 defending graduates. His teaching load in the last 4 years is significantly above the required minimum.

Associate Professor Dr. Petko Petkov has participated in a total of 18 research projects: national projects funded by the Bulgarian National Science Fund and various Operational Programs to the Structural Funds of the European Union and international projects funded by DFG (Germany) and the European Commission. The candidate was the leader of a project funded by the Bulgarian National Science Fund and was the leader of the Bulgarian team in an international project. Associate Professor Dr. Petko Petkov has two specializations at the Technical University of Munich, three at the Jacobs University in Bremen (Germany), and was a postdoctoral fellow at the same university as at the University of Leipzig (Germany). In 2018 he was a guest lecturer at the Technical University - Gdansk (Poland).

CONCLUSION:

Associate Professor Dr. Petko Stoev Petkov fully complies with the regulations for the implementation of the academic staff in the Republic of Bulgaria and the regulations adopted by the Council of Ministers, as well as with the requirements of Sofia University "St. Kl.

Ohridski” for the occupation of the academic position "Professor". The valuable scientific production presented for participation in the competition is sufficient in volume, has been published in renowned scientific journals and has found a wide echo in the literature. Based on the above, I am convinced to give my positive assessment and to propose Associate Professor Dr. Petko Stoev Petkov to be elected to the academic position "Professor" in professional field 4.2. Chemical sciences (Theoretical chemistry).

21.04.2021 г.

Writing the opinion:

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