

## REVIEW

on the competition for the academic position "Professor" in the professional field 4.2 Chemical Sciences (Theoretical Chemistry) at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kliment Ohridski ", published in the State Gazette no. 105 of 11.12.2020, with candidate Assoc. Prof. Dr. Petko Stoev Petkov

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Only one candidate participates in the competition for Professor in the professional field 4.2 Chemical Sciences (Theoretical Chemistry) at the Faculty of Chemistry and Pharmacy of Sofia University - Assoc. Prof. Dr. Petko Stoev Petkov. To participate in the competition, the candidate has submitted a complete set of documents in accordance with the requirements of the Regulations for implementation of the Law on the Development of Academic Staff in the Republic of Bulgaria and the Regulations on the conditions for obtaining scientific degrees and holding academic positions at Sofia University "St. Kliment Ohridski ".

### **Biographical reference**

Associate Professor Petko Petkov is a graduate of the Faculty of Chemistry at Sofia University "St. Kliment Ohridski ", where in 2002 he received a bachelor degree in Physical Chemistry and Theoretical Chemistry, and in 2004 - a master degree in Computational Chemistry. In 2009, under the supervision of Prof. G. Vaissilov, he successfully defended his Ph.D. dissertation on "Influence of non-metallic atoms on the properties and reactivity of small nickel clusters - a density functional theory study". He started his professional career in 2009 as an assistant at the Department of Organic Chemistry, Faculty of Chemistry, Sofia University, where he successively grew to chief assistant (2010) and associate professor (2018). He has specialized in renowned research centers such as the Technical University of Munich, Germany (2004 and 2006), Jacobs University, Bremen, Germany (several specialisations between 2009 and 2016), the University of Leipzig, Germany (2016/2017). ) and the Technical University of Gdansk, Poland (2018).

### **Scientometric data**

For the competition, Assoc. Prof. Petkov presented 21 scientific papers, of which 20 publications in specialized journals, on which 235 independent citations were noticed, and 1 habilitation paper. All articles, which have not been used by the candidate in the earlier competition for associate professor, are published in referenced international journals with a high impact factor (total IF = 155.83) which, with the exception of one work, fall into quartile 1. It is worth noting the articles published in Nat. Mater. (IF = 31.03), Nat. Commun. (IF = 12.12), Angew. Chemistry - Int. Ed. (IF = 11.73), Small (IF = 11.46) and J. Mater. Chem. A (IF = 11.30). The vast majority of publications (18) have been produced in collaboration with foreign scholars. In total, Assoc. Prof. Petkov is

a co-author of 52 publications (in 8 of them he is the first author), the results of which are cited 912 times in the scientific literature. The candidate's Hirsch index is 13. The results of Assoc. Prof. Petkov's research were presented (with oral reports and posters) at 20 national and international scientific forums. He has led / leads research teams in the Bulgarian-French-Japanese consortium, funded by the EIG CONCERT-Japan program, in the MOF-Switches project, funded by DFG, Germany, and the project BG05M2OP001-2.009-0028 funded by the operational program "Science and Education for intelligent growth" of the European Structural and Investment Funds of the EU. He has participated as a member of the organizing committee of several national and international scientific conferences. From the reference made by the candidate it can be seen that he meets the minimum national requirements (and in several cases exceeding them) for the academic position of professor under the Law for scientific field 4. Natural sciences, mathematics and informatics, professional field 4.2. Chemical sciences, as well as the recommended criteria of Faculty of chemistry and pharmacy.

### **Scientific contributions**

Assoc. Prof. Petkov's research is focused on the theoretical modeling of the structure, electronic properties and spectral behaviour of chemical / biochemical objects of interest to electronics, pharmacy and medicine. They can be summarized in the following areas:

1. *Modeling of the structure and electronic properties of coordination and organic polymers.* A series of articles and the habilitation thesis are devoted to studies of the structure and properties of metal-organic frameworks (MOFs), forming complexes with pores of different sizes and shapes. The emphasis is on MOFs with a flexible crystal lattice ("breathable" MOFs), which have the ability to open and close their pores upon changing external conditions. The detailed analysis performed using the methods of density functional theory on the recently synthesized object DUT-8 (Ni) by German scientists demonstrates that the pore dynamics is determined by the conformational isomerism of the ligands (naphthalene dicarboxylate ligands) in the complex. The thermodynamic parameters of the transitions between open and closed pore shape have been evaluated. The obtained results show that the structural design of closed metal-organic frameworks, in which the nonlinear shape of the ligands leads to maximizing the dispersion interactions between them, can be used as a tool for rational design of MOF with high flexibility in the crystal lattice. Subsequent spectral studies have demonstrated that the low-frequency vibrations of the lattice play a crucial role in the process of phase transformation of "breathable" MOFs. The effects of various metal cations and organic ligands on the dynamics of the pores in the studied structures have been also studied.

The object of theoretical modeling has been also the electronic properties of a series of conjugated two-dimensional MOFs with electrically conductive properties. The construction of three-dimensional structures as a result of joining between the two-dimensional ones is a determining factor for the manifested electrical conductivity. Quantum chemical calculations have shown the way the two-dimensional layers are joined. The band structure and the density of the states in the system, which are in good agreement with the experimental observations, have been calculated. The effective mass of the charge carriers has been also determined. The work outlines layered conjugat-

ed MOFs as a class of semiconductor materials with promising potential applications in spintronics, which determines the publication of scientific results (Articles 3 and 12) in the prestigious journals of Nature.

Quantum chemical calculations have also been used to elucidate the structure of a quasi-two-dimensional layer of polyaniline. Theoretical modelings, in combination with available experimental data, have determined at the atomic level the most probable structure of the studied objects.

*2. Modeling the interaction of drug molecules with mesoporous materials and biopolymers.* The research, through a combined use of experimental and theoretical methods, has been devoted to the study of the interaction between drugs (curcumin, quercetin, doxorubicin, verapamil, mylethphosine) and carrier materials of the active substance (mesoporous nanoparticles and biopolymers). Various factors that influence the thermodynamics of the interaction between the partners have been studied. The parameters that favor the recognition between the drug molecule and the carrier have been outlined to the greatest extent.

*3. Quantum chemical modeling of spectral characteristics of molecules or clusters in different environments.* The spectral and photophysical properties of a series of molecules / clusters have been studied with a set of theoretical approaches. The intramolecular mechanisms responsible for the observed spectral properties have been established (in detail).

*4. Study of ion mobility by the method of ab-initio molecular dynamics.* Simulations have been performed with the methods of molecular dynamics in order to monitor at the atomic level the mechanisms of the interaction of biogenic cations ( $\text{Na}^+$  and  $\text{Mg}^{2+}$ ) with RNA. The mobility of metal ions has been evaluated, as well as their coordination sites and affinity for RNA.

### **Teaching activity**

Assoc. Prof. Petkov is an established and respected lecturer at the Faculty of Chemistry and Pharmacy with a high reputation among students and colleagues. He has developed and leads lecture courses in Molecular Modeling of Materials, Hybrid QM/MM Methods, Introduction to Programming the Linux Shell, Quantum Chemical Modeling of Organic Systems, as well as seminars/exercises in Organic Chemistry I and II, Applied Quantum Chemistry, Molecular modeling of materials, and Quantum chemical modeling of organic systems. He has been the scientific supervisor of 4 successfully defended graduates and one post-doctoral student (current).

### **Conclusion**

The publications and habilitation thesis presented by the candidate are on the topic of the competition and represent original scientific works with a significant contribution in the field of theoretical chemistry and molecular modeling. The presented materials give me reason to believe that the candidate is a leading scientist in his field with deep knowledge and practical skills in theoretical chemistry. Demonstrates excellent mastery of a set of state-of-the-art computational approaches, which allows him to study at a high scientific level complex molecular systems with non-trivial structure and thermodynamic characteristics. The obtained results are innovative (evidenced by the series of publications in high-impact journals) and can be classified as novelties in scientific

research. The candidate demonstrates maturity, creative thinking and the ability to successfully select and solve problems with a high impact for science and practice.

In conclusion, as a result of the above, I believe that with his research and teaching activities Assoc. Prof. Dr. Petko Stoev Petkov fully meets all the requirements of the Law for the academic position of "Professor". I propose that Assoc. Prof. Dr. Petko Stoev Petkov be elected Professor in the professional field 4.2 Chemical Sciences (Theoretical Chemistry) at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kliment Ohridski".

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