STATEMENT

from Prof. DSc Sonia Varbanova Ilieva,
Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski"
on the materials submitted for the competition for the academic position of **'Professor'**
in the **Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski",**
higher education professional field **4.2. Chemical Sciences (Theoretical chemistry)**

In the competition for the academic position 'Professor' announced in the State Gazette, issue 105/11.12.2020, **Assoc. Prof. Dr. Petko Stoev Petkov** from the Faculty of Chemistry and Pharmacy, Sofia University is the only candidate.

The materials submitted by Assoc. Prof. Petko Petkov **meet and exceed the requirements** of the Law for the Development of the Academic Staff in the Republic of Bulgaria and the relevant regulations for its implementation (including those of Sofia University and Faculty of Chemistry and Pharmacy). The applicant meets the criteria (minimum requirements) of the Faculty of Chemistry and Pharmacy for the academic position "Professor".

Associate Professor Petkov has published **a total of 52 scientific papers** (49 in peer reviewed journals, 2 - in journals without impact factor, 1 book chapter, more than 900 citations, h index 13) and for the participation in this competition he has submitted **20 publications in scientific journals**, which do not repeat the ones presented in other competitions for occupying academic positions and obtaining scientific degrees. It is worth mentioning here that of the 20 publications submitted for participation in the competition, 19 fall into quartile Q1 and one - in Q2.

The candidate has submitted a **habilitation thesis** *"Computational modelling of the framework flexibility and electronic properties of metal-organic frameworks"* and a **report for the scientific contributions** of the research work. The main scientific contributions of Assoc. Prof. Petkov are discussed in the report in a concise and clear manner. I would like to recommend that when creating a list of publications, the leading author (corresponding author) should be marked (for example with a star symbol) as accepted in the scientific literature.

P. Petkov graduated as a Master of Sciences in Theoretical Chemistry at the Faculty of Chemistry, Sofia University "St. Kl. Ohridski" in 2004. In 2009 he defended his doctoral thesis on the topic *" Influence of non-metal atoms on the properties and reactivity of small nickel clusters - a DFT study"*. Then he continued his scientific work at the Faculty, Department of Organic Chemistry as an Assistant and subsequently Chief Assistant (2009-2018). Since 2011 he has held the academic position of Associate Professor in the same laboratory. Therefore, the professional and scientific experience gained is fully linked to the announced competition.

Assoc. Prof. Petkov has conducted a number of specializations, short-term and long-term scientific visits to foreign research groups as guest researcher, postdoctoral student, assistant, guest professor that undoubtedly has significantly enriched his research experience. He has participated in a number of national and international scientific events (congresses, conferences) and research/educational projects. His teaching activity is rich and diverse and is expressed both in the management of graduates, training of PhD students, and in regular teaching activities at the Faculty of Chemistry and Pharmacy.

The applicant's overall **scientific activity** is in the field of theoretical chemistry that is completely in line with the announced competition. The scientific publications submitted for participating in the competition reflect the work of Assoc. Prof. Petkov in the field of theoretical chemistry – computational chemistry methods' development and their application to study the structure and properties of porous materials (zeolites, metal-organic frameworks, etc.), modeling of spectroscopic characteristics of molecules, clusters and materials, study of the dynamics of chemical processes.

It is evident from the presented publications that P. Petkov has established fruitful **cooperation** with research groups from the University of Leipzig - Wilhelm-Ostwald-Institute of Physical and Theoretical Chemistry, TU Munich, TU Dresden, Jacobs University, Bremen, Germany, University of Barcelona, Spain, Faculty of Pharmacy, Medical University, Sofia, BAS. The scientific papers published reflect the results from the research studies on the following topics:

- Modeling of structures and manipulation of properties of "breathing" MOFs - studies were conducted jointly with the experimental group of Prof. Kaskel, TU Dresden in the framework of a current research project;
- Rational design of MOFs with high framework flexibility;
- Investigation of the dynamics of the crystal lattice of DUT-8 (Ni) with Raman spectroscopy and MD simulations;
- Tuning of the gating phenomenon in DUT-8(Ni) MOF using different metal ions;
- Studies of layered MOFs with structural mobility of the crystal lattice with potential application in electronics and spintronics, published in Nature materials and Nature communications;
- Determination and characterization of the structure and stacking of layered MOFs by quantum chemical calculations, exploration of the changes in the electronic structure and the magnetic state of the metal-organic structures in the presence of different stacking interactions;
- Modeling of the interaction of drug molecules with mesoporous materials and biopolymers - the research was conducted in collaboration with the experimental group of Prof. Margarita Popova ((IOCCP-BAS). Characterization of the type, stability and local structure of the adsorbed on the carrier drug molecules by quantum chemical calculations;
- Modeling of spectral characteristics of molecules and clusters in different environments by quantum chemical computations and MD simulations. Based on theoretically calculated vibrational spectra, the first spectral evidences from photodissociation spectra in the infrared region (IRPD) for the high internal mobility of the two rings in the $B13^+$ cluster were obtained. Due to the significance of the fundamental conclusions resulted from the research, the work was accepted in *Agewandte Chemie Int Ed.* and the publication is featured on the journal cover page as a VIP article.

The 20 scientific papers submitted for the competition have been published since 2017 in extremely renowned international journals with a markedly high impact factor. The mean impact factor of the publications is about 8, ranging from 2.73 (*J. Drug Deliv. Sci. Technol.*) to 31.03 (*Nature Materials*). In most cases, they are a result of the work of a large international team that of course is directly related to the multidisciplinary nature of the research work. Assoc. Prof. Petkov is a co-corresponding author in one of these publications. The main contribution of P. Petkov in the presented publications is the conducting of quantum chemical calculations and MD simulations. I believe that he is an established specialist in the

field of theoretical chemistry: the scientific developments and publications in which he has participated are the strongest evidence of his continuous scientific growth, and in this sense the professor position is a natural result in his development.

The research carried out and the published results have **scientific as well as applied contributions** in the relevant fields of science. These contributions can be formulated as: substantiations of significant new sides of already existing scientific fields, problems, theories, hypotheses by means of new methods and approaches; creating new methodologies for analysis; getting new facts.

These contributions are corroborated by reputable international scientific journals in which the articles have been published, as well as by **citations** in the scientific literature. The total number of citations is above 900, 235 of which are on the publications submitted for this competition. Therefore, the research work of Assoc. Prof. Petkov is in extremely topical areas of scientific knowledge, with issues that are widely recognized in the scientific community, and the results achieved have high impact scientific contributions. The scientific results have been disseminated through more than 20 participations in national and international scientific forums with posters and oral presentations. Assoc. Prof. Petkov has participated in 11 national and 3 international research / educational projects, and has been the leader of 2 research projects.

The educational and pedagogical activity of the candidate is quite rich and diverse. He is a lecturer in *Organic Chemistry* - for students of two specialties, Bachelor degree, Faculty of Biology, Sofia University; *Molecular modeling of materials* - Bachelor program in Chemical Engineering and Contemporary Materials, Faculty of Chemistry and Pharmacy; *Hybrid QM/MM methods*, *Introduction to programming "Linux" shell, Quantum-chemical modeling of organic systems* - for Master degree programs in Computational Chemistry and Modern Methods of Synthesis and Analysis of Organic Compounds, FCP. He participates in the teaching activities of the faculty as a supervisor of practical classes as well. He was the supervisor of 4 diploma theses. Although he was not a supervisor, he trained two PhD students (Stefan Kolev from FCP-SU and Yun An from the University of Leipzig) in the theoretical foundations and details for performing ab-initio molecular dynamics and metadynamics. He is currently the head of a postdoctoral fellow under the National Scientific Program “Petar Beron i NIE” (P. Beron).

CONCLUSION

According to the submitted materials and scientific papers, the above analysis of their importance and scientific contributions, as well as my personal opinion about the candidate as a highly erudite scientist, I am convinced in my **positive assessment** and I vote **“yes”** for the election of **Assoc. Prof. Dr. Petko Stoev Petkov** for the academic position **'Professor'** in the professional field **4.2. Chemical Sciences (Theoretical Chemistry)** at the Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski".

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Prof. Sonia Ilieva