R E F E R E N C E S T A T E M E N T

within the call for **Professor position** in 4.2 Chemical sciences (Theoretical Chemistry)
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by Prof. Dr. **Anela Nikolova Ivanova**
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chair of the scientific jury appointed with Order № RD 38-10 from 07. 01. 2021
of the Rector of Sofia University

There is a single applicant for the position – Assoc. Prof. Dr. Petko Stoev Petkov. He has been employed at Sofia University, Faculty of Chemistry and Pharmacy (SU, FCP) since 2009 and has occupied an "Associate Professor" position for the last two academic years. All required documents are available, together with information on additional criteria related to the selection procedure.

Dr. Petkov is a co-author of 51 scientific articles, 49 of which published in international peer-reviewed journals (Source: Web of Science), and of 1 book chapter. He has submitted for the selection procedure 20 publications (all are articles published in international peer-reviewed journals). None of these has been used for the position of Associate Professor or for the PhD degree. Hence, in line with Art. 29, Sec. 1, P. 3, 4 of the Law for promotions in academia in Bulgaria (LPAB), they are eligible for evaluation of the scientific contributions of the candidate. All articles are published in journals specialized in the area of the study, some of them being especially renowned in the scientific community: Nature Communications (2 papers), Nature Materials (1 paper), Angewandte Chemie International Edition (1 paper), Small (1 paper), materials science and catalysis journals (3 papers). The publications submitted for assessment have been cited >290 times in international peer-reviewed journals. The total number of independent citations of the publications of Dr. Petkov is 897 (Source: Scopus). The applicant participates in the coordination of 1 European research projects, is a work package leader in 1 national project and a visiting professor in 1 bilateral research project. He has had long-terms post-docs abroad for 4 years and 7 more short-term specializations. Dr. Petkov has supervised 2 and co-supervised 2 more successfully defended diploma theses. He also hosts a post-doctoral fellow. He is the recipient of 1 national award in 2003. Dr. Petkov has presented his results at 20 scientific events as 12 oral presentations and 8 posters. He is a lecturer of 6 and an assistant professor of 4 courses at Sofia University, 4 of the disciplines being in the area of the call. His average teaching load for the past 4 years is 517 hours/year.

Dr. Petkov presents the following achievements to fulfill the minimum national criteria and the additional requirements of SU, FCP for occupying the Professor position:

- indicators group A - defended PhD thesis - 50 points out of minimum required 50;

- indicators group C – 7 publications in Q1 standing for a habilitation thesis, devoted to theoretical study of structure, relative stability, and properties of metal-organic frameworks (MOF) - 175 points out of minimum required 100;

- indicators group D - 13 publications not included in the habilitation thesis, 12 of which in Q1 and 1 - in Q2 - 320 points out of minimum required 220;

- indicators group E - 235 citations of the publications submitted for evaluation - 470

points out of minimum required 120;

- indicators group F – supervision of 1 post-doc, coordination in 1 international project and participation in 10 national and 3 international projects (with secured third-party funding) – 250 points out of minimum required 150;

- indicators group G – h-index, supervision of 2 and co-supervision of 2 more successfully defended diploma theses, 2 publications with SJR not included in the previous groups – 172 points out of minimum required 150.

It is evident from the above summary that the applicant either fulfills or goes beyond the minimum national requirements in all groups of indicators. The overall scientific metrics is in compliance with the general requirements of LPAB, the statutes for its application, and the additional recommendations of SU, FCP.

The publications submitted for assessment may be classified mainly in two groups. The first one contains studies focused on the structure and its relation to function of metal-organic frameworks (papers 2, 3, 12-14, 17, 20) or other solid-state materials (papers 1, 5, 7, 11, 15, 18). The theoretical modelling of MOFs is also the topic of the habilitation thesis of the applicant. Structures characteristic of an open and a closed form of the MOF DUT-8 are modelled and it is shown how the shape of organic ligands and the type of inorganic ions affect them. A transition mechanism between the two forms is suggested. The specifics of the band structure of a new MOF are revealed and it is elucidated how they are related to its superparamagnetic and enhanced carrier mobility features. Stable structures are identified also for the materials different than MOF and an explanation of various (vibrational, electronic, X-ray) experimentally observed spectral characteristics is provided. The second group of publications (papers 4, 8-10, 19) addresses the capacity of mesoporous nanomaterials for drug delivery. The theoretical contributions within these works concern quantification of the interactions between functional groups of drug molecules and carriers, the latter being functionalized nanoparticles. Stable intermolecular configurations complying with observed experimental data are put forward. The remaining two publications study interactions of inorganic ions with RNA fragments (6) and the excited state behaviour of coumarins (16). The former work offers an explanation of the specifics of interaction between Na^+ and Mg^{2+} and RNA sequences, while the latter one seeks a molecular-level interpretation of the lifetimes of halogen-substituted coumarins. The applicant has contributed to the theoretical elucidation of the structure and some properties of the investigated materials. The publications have received sizeable short-term response in the community.

The works employ computational methodology based exclusively on Density functional theory. Both static and quantum molecular dynamics calculations are performed in order to obtain a more comprehensive description of the modelled components of materials or phenomena. All computations are carried out at high level of expertise. Incorporating the theoretical predictions into experimental studies is an advantage. The successful collaboration of the applicant with colleagues from other research groups in Bulgaria and abroad for all studies should be underlined.

The habilitation thesis and summary clearly highlight the scientific findings of the applicant, contributing predominantly to interpretation of experimental observations and enabling molecular-level explanation of measured properties.

Overall, during the last decade the applicant has specialized very profoundly in the direction of the call and I am convinced that he has the required scientific competence to continue advancing in the perspective research areas mentioned above. His h-index of 13 (Source: Scopus) is in support of this.

In summary, the materials submitted for the evaluation comply with all requirements of the law and with the additional recommendations of SU, FCP for a Professor position. This motivates me to assess positively the applicant Associate Professor Dr. Petko Petkov and to vote for his appointment as a Professor.

April 19, 2021 Chair of the scientific jury:

/ Prof. Dr. Anela Ivanova /