STATEMENT

on the competition for the occupation of the academic position "Assoc.Prof. "
in the professional field 4.2 "Chemical Sciences", scientific specialty "Physicochemistry",
published in the Newspaper of State no. 41/21.05.2019, by the Institute of Optical Materials and Technologies (IOMT) "Acad. J. Malinowski", Bulgarian Academy of Sciences
a single candidate Assist. Prof. Ph.D Silvia Emilova Angelova
Member of the Scientific Jury: Prof. DSc Nikola Malinowski - IOMT, BAS

1. General characteristics of the materials presented

The overall scientific production of the only candidate for the competition Assis. Prof. Silvia Emilova Angelova includes 62 scientific papers. She has participated in the competition with 28 publications, which are different from the works included in the Ph.D. thesis. They have been published in peer-reviewed and indexed scientific journals in the field of theoretical chemistry and materials science, all co-authored.

The scientific papers for participation in the competition are distributed as follows: 12 publications in journals, refereed and indexed in the Web of Science and Scopus databases, are submitted as substituting the habilitation thesis , 2 of which are published in Q1 ranked journals (J. Phys. Chem. C and Beilstein J. Org. Chem.), 4 - in Q2 ranked journals (ChemPhysLett., Comput. Theor. Chem., Color. Technol., Aust. J. Chem.) , 2 - in Q3 ranked journal (J. Phys.: Conf. Ser.), 4- in the Q4 ranked journal (Bulg. Chem. Commun.) and 2- in refereed journal without IF and SJR rank (Nanoscience & Nanotechnology). According to the Implementing Regulations of the DASRB and the Rules of the IOMT-BAS, these publications collect a total of 208 points with the minimum required 100 points for the respective group of indicators.

Outside the papers substituting the habilitation thesis, 14 articles were presented in refereed and indexed in *Web of Science and Scopus* editions, 5 of which were published in Q1 ranked journals (Tetrahedron, Phys. Chem. A, J. Alloys Compd., Dyes Pigm.), 5 - in Q2 rank journals (J. Chem. Res., J. Mol. Struct., Acta Cryst. E), 3 - in Q3 rank journals (Struct. Chem., Arkivoc, J. Struct. Chem.) and 1 in Q4 rank journal (Bulg. Chem. Commun.). They collect a total of 282 points with the minimum required 220 points in this group of indicators according to the IOMT-BAS Rules.

The reference provided by Ph.D. Sylvia Angelova presents a total of 101 citations reflected in the *Web of Science* and *Scopus* databases, which is a good certificate for the level of her research and the relevance of the thematic areas in which she works. From them, 37 citations were noted for 7 of the papers substituting the habilitation thesis and 64 citations for 8 papers outside it. They accumulate 196 points with the required minimum of 60 points on this indicator according to the IOMT-BAS Rules.

The analysis of the applicant's scientometric indicators achieved shows full compliance and exceeding the requirements for occupying the academic position of Associate Professor, set out in the Rules of IOMT-BAS for applying DASRB.

In addition, Silvia Angelova has participated in the implementation of 5 scientific projects, of which 3 are ongoing, funded by the Bulgarian National Science Fund, and 6 projects under various national and international programs with the Swiss National Science Foundation, Polish, Russian and Macedonian Academies of Sciences, CNR Italy.

The presentation of the candidate's research results is also impressive. Silvia Angelova has 10 oral and 33 poster reports at international and national scientific forums according to the attached reference list. It should be noted that she was also the supervisor of 8 graduates, 2 postgraduate students and numerous student practices which is a good proof for her active pedagogical activity.

2. Assessment of the applicant's research activity.

The main object of the candidate's research publications is the study of the electronic structure of the molecules and their resulting physicochemical properties. Quantum-chemical (ab initio and DFT) methods have been also used to study intermolecular interactions and evaluate the relative thermodynamic parameters of various chemical and biological objects and reactions at the microscopic level using model reactions.

The major scientific contributions of publications substituting the habilitation thesis can be described as applications of quantum-chemical calculations to study the electronic structure of a ground state and the properties of dyes for photovoltaic applications and of fluorescent dyes - biomarkers as well as the study of the electronic structure of the basic and excited state of tautomeric systems.

Another major part of the applicant's research is devoted to theoretical methods or a combination of theoretical methods (DFT, HF, post-HF: MP2 and CCSD (T)) and one or more experimental techniques for solving structural and/or spectroscopic problems and prediction of molecular properties. A wide range of DFT functionals has been used in quantum-chemical calculations like the popular B3LYP, X3LYP, OLYP, B3PW91, LC-BLYP, B2PLYP, and mPW2PLYP. A number of publications have used computational 13C chemical displacements to solve a structural or spectroscopic problem, which is a continuation of the topic of candidate‘s Ph.D. thesis, namely the use of quantum-chemical NMR parameters for studying tautomeric and conformational equilibria.

I would characterize the contributions as an enrichment of existing knowledge of the problems the candidate is working on, using theoretical quantum-chemical methods to optimize the properties of known materials and structures, as well as to create new ones. I believe that these studies are important for the practical use of the materials and structures being studied.

CONCLUSION

Dr. Silvia Angelova's comprehensive research activities show that she is a researcher with extensive knowledge and experience in the application of quantum-chemical methods for studying the intermolecular interactions and evaluation of the relative thermodynamic parameters of various chemical and biological objects and reactions at the microscopic level. On the basis of the examination of the competition documents, taking into account the evaluation of the submitted publications and the importance of the scientific contributions, as well as my personal impressions on the applicant's qualities, I express a positive opinion in accordance with Art. 26, para. 3 DASRB and recommend to the honorable members of the Scientific Council of IOMT-BAS to vote Ph.D **Silvia Angelova Emilova to be elected Associate Professor** at IOMT-BAS.

09.09.2019

Statement prepared by:

/Prof. DSc N. Malinowski/