SCIENTIFIC OPINION

for a procedure for obtaining an academic position "Professor"
in the professional field 4.5 "Mathematics",
specialty "Mathematical Modeling and Application of Mathematics
(Applications in Computational Physics and Biology) ",
published in the State Gazette no. 41 / 21.05.2019 for the needs
of section "Scientific calculations", IICT - BAS,
with the only candidate Assoc. Prof. Dr. Nevena Petrova Ilieva-Litova

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General description of the presented materials

As a member of the Scientific Jury, determined by Order No. 197 / 19.07.2019 of the Director
of IICT-BAS Prof. Dr. Habil Galya Angelova, I received the following documents
electronically:

(1) Curriculum vitae in the European sample
(2) Copy of the diploma for the educational and scientific degree "doctor"
(3) Copy of the diploma for the scientific title "Senior Research Associate II"
(4) Certificate of internship in the specialty
(5) List of scientific publications
(6) List of scientific publications for participation in the competition
(7) List of selected indexed citations (after habilitation in 2002)
(8) Abstracts of the scientific publications for participation in the present procedure
(9) Information on the fulfillment of the minimum national requirements of Academic Staff
Development Act (ASDA) for the academic position of Assistant Professor (from Nat. Centre
for Inf. & Doc. website)
(10) Information on the fulfillment of the minimum national requirements of the ASDA for
the academic position of "professor" drawn up on the basis of the documents submitted for the
competition
(11) Reference to original scientific and applied scientific contributions
(12) Declaration on the absence of plagiarism in scientific works

The candidate's references also contain information about the scientific and pedagogical
activity of Assoc. Prof. Nevena Ilieva, as well as her participation in national and international
relevant projects. The above documents completely exhaust the list of documents required
under the Academic Staff Development Act and the Regulations for its implementation, as
well as according to the specific requirements adopted by the Scientific according to the
specific requirements adopted by the Scientific Council of IICT - BAS for the procedure for
occupying an academic position "professor".

1. General characteristics of the applicant's scientific activity

According to the complete list (5) of publications, Assoc. Prof. Nevena Ilieva is the author
and co-author of 104 scientific publications, 39 of which are in Impact Factor journals and 12
in Impact-rank journals (JCR). She defended her PhD in 1988 and was selected as Associate

Professor in Theoretical and Mathematical Physics in 2002 (Protocol of the Higher Education Commission of 30.04.2003). The number of published works after habilitation is 72; 24 of them with Impact Factor and 12 with JCR, among them are the publications submitted for the present procedure, which are from 2009 - 2019. A list of selected independent citations is presented, reflected in the world scientific databases Scopus, WoS, IEEE Explore, containing 100 citations (after habilitation in 2002), 49 of which have been submitted to the competition for publications from the list (6).

The presented materials provide also some important (in my opinion) information on the applicant's participation in national and international scientific projects since 2008 - a total of 23 projects, of which 11 are national and 12 international. In 10 of them Assoc. Prof. N. Ilieva is Head (or Team Leader), in 3 of them is Assist. Head of the national team, and in the other 10 - a participant. This project activity proves the relevance of the international and national research conducted by the candidate in the present procedure!

The guidance of PhD students is not a mandatory requirement in accordance with ASDA and the ICTI Regulations, but for me the preparing of future researchers is a professional duty of every scientist! I applaud the efforts of Assoc. Prof. N. Ilieva in this direction - joint leadership of two PhD students (defended 2016 and 2019) at a reputable foreign university Beijing Institute of Technology, see Reference 10.a. Since I have several successfully defended PhDs abroad, I can clearly imagine what the effort has been to bring them to a successful PhD degree! I also appreciate the leadership (as well as the counseling, respectively) of two projects on the career development program of young scientists at BAS, as well as lectures for young scientists and doctoral students at IEMPAM - BAS.

2. General characteristics of the publications submitted for the present procedure

23 publications were submitted for participation in the present procedure, 17 in Impact-Factor Journals, 5 in Impact-Rank Journals and one is an electronic edition with a guide / manual character. The publications in the Author Reference are grouped (formally) into four thematic cycles:

(A) Methods for modeling, studies and visualization of the structure and dynamics of proteins (9 articles), of which I would like to mark **P12** and **P13**, according to the candidate list. This area of the candidate's research is the closest one to my field of research and it perfectly illustrates the direction of the present procedure: applying mathematical methods to deep physical and biological models. In doing so, starting with the most elementary calculations of the analytical geometry and topology, applied to the individual atoms and molecules (angles, tangents, 3D-torsions, vector fields) to arrive at heavy calculations related to the study of the energy minimum of different structures associated with the names of Gibbs, Schrodinger, Landau; soliton techniques, etc. Of course, the models are non-stationary, that is, all of them are in development over the time, with studies based on a number of natural hypotheses for equilibrium. In this connection, I cannot fail to mention the close to my understanding of the role of visualization, a publication from the same group **P22**, dedicated to a new method for 3D visualization of proteins using deeper properties of mathematical - physical models.
(B) In silico studies of immuno-active molecules and complexes (10 articles);
(C) Modeling of physical processes (2 articles);
(D) Tools and techniques for high performance calculations (2 articles).
The present procedure is announced in the specialty "Mathematical modeling and application

of mathematics (applications in computational physics and biology)". Both the applicant's overall scientific activity and the publications submitted for the procedure correspond to the profile of the procedure. I would like to make explicit the wide range of methods and techniques used - from purely analytical through modeling to computer simulations involving high-performance (supercomputer) calculations. I specifically tried to mention some of them above, of course, not at the right depth.

3. Main scientific and applied contributions of the applicant

The candidate's report presents a synthesized presentation of the original contributions to the works submitted for the competition, as well as their place in contemporary research based on their scientific and social significance and their development prospects. I will not elaborate on the individual contributions, but I will note that they can be characterized (mainly) as contributions in the field of mathematical biology. This relatively young scientific discipline is linked to the hopes of solving fundamental open problems in modern biology with the powerful apparatus of mathematics and mathematical physics, beginning with the problem of protein folding.

I would like to point out in particular:
• the successful use of an extremely abstract construction (soliton solutions to a generalized discrete nonlinear Schrödinger equation) for the analysis of specific proteins with important biological functions - monomeric Myc oncoprotein and glycoprotein from the HIV envelope;
• development of original methods for analysis and extraction of dynamic information from molecular dynamic data - method of interval-selective "lagged RMSD" analysis and method of space-time consensus multistage MCC-clustering;

• the significance (in the long term) of the solutions to the problems under study: development of innovative treatment of autoimmune diseases, including multiple sclerosis, the search for therapeutic alternatives against resistant bacterial strains, imaging diagnostic modality with increased accuracy and significantly reduced radiation.

Let mention finally, that not only the use of experimental data is impressive, but the collaborative research with experimental teams from different scientific groups and countries.

4. Personal contribution of the applicant

Essential in these studies is their inherent multi-disciplinarily, respectively - teamwork, due to the necessary expertise in areas such as mathematics, physics, molecular biology, microbiology, pharmacology, chemistry, biotechnology, high-performance calculations, both theoretical and experimental. In the areas of work in groups (C) and (D) - 4 articles - an alphabetical arrangement of the co-authors was adopted, but in the works of groups (A) and (B) - 19 articles - the role of the candidate was emphasized according to relevant traditions : first, last or correspondent author (14 cases), i.e. a leading / significant contribution recognized by the author team.

5. Critical notes and Personal opinion

I have no critical remarks (which is a little be strange for me), but it is still an Scientific Opinion. I have known the candidate Assoc. Prof. Nevena Ilieva for many years and I have always seen in her person a well-established professional and well-meaning colleague, which in my opinion is especially important in today's difficult time!

6. Conclusion

The presented materials prove the professional expertise of Assoc. Prof. Dr. Nevena Ilieva, the importance of her scientific achievements and their approval by the scientific community. My personal impressions of discussions and reports at international and national conferences and workshops confirm this conclusion.

The requirements laid down in the Law for the Development of Academic Staff to the candidates for occupying the academic position of "Professor" Academic Staff Development Act and the Regulations for its implementation, as well as according to the specific requirements for this position adopted by the Scientific Council of IICT - BAS, have been met by the applicant with great reserve.

With all this in mind, I propose that the Scientific Jury give a positive opinion on the application of Assoc. Prof. Dr. Nevena Petrova Ilieva - Litova and with a proposal to the highly respected Scientific Council to select her as a "Professor" in the professional field 4.5 "Mathematics", scientific specialty „Mathematical Modeling and Application of Mathematics (Applications in Computational Physics and Biology)".

Date:

/ Prof. Dr. Habil Nedyu Popivanov /