# OPINION

to

Assoc. Prof. Dr. Nevena Petrova Ilieva-Litova
regarding the competition for occupation of the academic position "Professor"
in the Institute of Information and Communication Technologies
at the Bulgarian Academy of Sciences
in the higher education area 4. Natural Sciences, Mathematics and Informatics,
professional field 4.5 Mathematics,
scientific specialty "Mathematical Modeling and Application of Mathematics
(Applications to the Computational Physics and Biology)"
announced in State Gazette issue 41/21.05.2019

by

Prof. Dr. Neli Stoyanova Dimitrova
Institute of Mathematics and Informatics at BAS
member of the Scientific Jury constituted by Order No 179/19.07.2019
of the на Director of the Institute of Information and Communication Technologies
at the Bulgarian Academy of Sciences

The only candidate in the announced competition is Assoc. Prof. Dr. Nevena Petrova Ilieva-Litova from the Department of Scientific Computations at the Institute of Information and Communication Technologies (IICT).

All required documents concerning the competition are prepared and submitted in immaculate form.

Nevena Ilieva acquires her PhD degree in 1988 in the United Institute of Nuclear Research in Dubna, Russia, in the scientific specialty "Theoretical and Mathematical Physics". In the period 1988–2015 she occupies the academic positions Chief Assistant and Associate Professor in the Institute for Nuclear Researches and Nuclear Energy (INRNE) at BAS. She gets the academic position "Associate Professor" in 2003 in the specialty "Theoretical and Mathematical Physics" in INRNE. In this period N. Ilieva works in the Institute of Theoretical Physiscs of the Vienna University, Austria, as postdoc and as main contractor in a project within the Austrian Science Fund (FWF), as well as a visiting scientist in the International Erwin Schrödinger Institute for Mathematical Physics, Vienna, Austria. From 2015 until now she is Associate Professor in Department "Scientific Computations" in the IICT at BAS.

Table 1 below summarizes the submitted candidate's report for the fulfillment of the minimum national requirements and of the requirements of the IICT related to the academic position "Professor" in the professional field 4.5 Mathematics.

Table 1

| Data by group of indicators | Number | Credits | Requirements for minimum credits |
|---|---|---|---|
| **C** (publications) | 6 | 204 | 100 |
| **D** (publications) | 16 | 544 | 260 |
| **E** (citations) | 51 | 279 | 140 |
| **F** (PhD students, projects, etc.) | -- | 540 | 150 |

In the recent competition Nevena Ilieva presents 23 scientific papers, published in the period 2009–2019. The papers are not used for occupation of the academic position "Associate Professor", thus the requirements of the Law for Development of the Academic Stuff in Republic of Bulgaria as well as its Regulations, the corresponding Regulations of BAS and IICT are satisfied. There is a *technical error in Table 3 of the Author's Report*, concerning the number of the candidate's publications distributed in the quartiles of the journals with impact factor (IF) according to JournalCitationReports of Web of Science as well as of the journals with impact-rank (SJR of SCOPUS); the correct numbers are given in Table 2 below.

Table 2

| Type of the publication | Number of publications | Credits |
|---|---|---|
| IF, Q1 | 4 | 200 |
| IF, Q2 | 5 | 200 |
| IF, Q3 | 5 | 150 |
| IF, Q4 | 2 | 48 |
| SJR | 6 | 120 |
| none of the above | 1 | 0 |
| **TOTAL:** | **23** | **718** |

This technical error does not change the fact that the applicant's scores repeatedly exceed the required minimum number of credits.

In the Author's Report the candidate has grouped her research activities conditionally in four thematic areas:

*(A) Methods for modeling, investigation and visualization of protein structures and dynamics*

This area is covered by 9 publications from the attached list, among them 3 articles belong to quartile Q1, 3 articles to Q2, 1 article to Q3, 1 article to Q4, and 1 paper with SJR.

Presented are innovative approaches, models and computational techniques related to investigation of protein folding processes, to molecule-dynamics simulations aimed to extract functional data information. Proposed are appropriate visualization techniques for better understanding and interpretation of the experimental results.

The investigations in this field possess a strong potential for biomedical and pharmaceutical applications.

(B) *In silico investigations of immune-active molecules and complexes*

This area is presented in 9 publications from the attached list, among them 2 articles within quartile Q1, 1 article within Q2, 4 articles within Q3, 1 article within Q4, and 2 papers with SJR.

Here, the methods of the molecular dynamics and computer modeling (*in silico* investigations) are skillfully combined with various approximation techniques on the basis of high performance computations, and further applied to:

- studying the activity of the human interferon-gamma (hIFN-γ). Model structures of some specific mutated forms of hIFN-γ are elaborated and experimentally investigated for the first time.
- simulation of large molecules of the immune system (major histocompatibility complex class 1, presented epitope, T-cell receptor, CD8 coreceptor);
- simulation and monitoring of MHC α-helices, forming the antigen binding cleft in immunological reactions.

These investigations suggest strong social impact, since they could improve the therapy of many autoimmune diseases and contribute to better risk assessment of transplanted organs rejection.

(C) *Modeling of physical processes*

This area is covered by 2 articles, 1 article in quartile Q2 and 1 article with SJR.
The investigations are focused on the development of a hybrid system for image diagnostics. The latter combines the positron-emission tomography (PET) and nuclear magnetic resonance imaging (MRI). To optimize the detector design specific simulations are carried out using the software package GEANT4. The PET–MRI system could be successfully used for early diagnostics in oncology, neuro-radiology, cardiology etc.

*(D) Tools and techniques for high-performance computations*

This area is presented by
– one publication in journal with SJR, related to installing the software package GEANT4 in the supercomputer Avitohol@BAS;
– one publication in electronic edition, representing a best practice guide for working with the co-processor *Intel Xeon Phi.*
Although the latter results seem not to be of major priority, they strongly contribute to solving specific and with large amount of data problems in the field of computational physics and biology.

To my opinion the large variety of techniques, methods and models used in studying different phenomena in biosciences is highly impressive. This fact explains the large number of articles co-authored with other scientists, which is natural in the interdisciplinary research. The unifying point in all studies is the use of advanced innovative high performance computations and visualization techniques.

The scientific papers of Nevena Ilieva have national and international recognition. This is confirmed by the presented 100 selected citations in indexed journals only from year 2002 to date.

Assoc. Prof. Nevena Ilieva is:

- Co-mentor of 2 successfully defended doctoral students (in 2016 and 2019) from the Beijing Institute of Technology in China;
- Mentor in two projects within the Programme of the Bulgarian Academy of Sciences for supporting young scientists and doctoral students (in 2016 and 2017).

It is worth to mention the active participation of N. Ilieva in at least 23 international and national projects from 2008 to date as a member of the research team, principle investigator, coordinator or coordinator from Bulgaria.

The active contacts of N. Ilieva with scholars from renowned European universities and research institutions, her participation in national and international projects, the large number of citations of her papers in indexed journals clearly demonstrate that the candidate's research results in the field of computational physics and biology are well known to the scientific community abroad and in Bulgaria.

I know Nevena Ilieva from her participation in the seminars of Department "Biomathematics and Scientific Computing" at the Union of Bulgarian Mathematicians as well as in the international conferences BIOMATH. From October 2018 N. Ilieva has been appointed in the Department of Mathematical Modelling and Numerical Analysis at IMI. My personal impressions of her are excellent. She is extremely communicative, responsive and correct in her relationships with colleagues.

## CONCLUSION

From everything said so far, it is clear that the candidate Assoc. Prof. Nevena Ilieva-Litova has enough in quantity and quality scientific and practically applicable results in the field of computational physics and biology.

Assoc. Prof. Nevena Ilieva-Litova satisfies and significantly exceeds the requirements of the Law for Development of the Academic Stuff in Republic of Bulgaria as well as its Regulations, the corresponding Regulations of BAS and IICT related to the academic position "Professor" in the professional field 4.5 Mathematics.

The assessment I give for the research activities of Assoc. Prof. Nevena Ilieva-Litova is highly *POSITIVE*.

My proposal to the Scientific Jury is to propose unanimously to the Scientific Council of the Institute of Information and Communication Technologies

*to grant Assoc. Prof. Nevena Petrova Ilieva-Litova the academic position "Professor"* in the higher education area 4. Natural Sciences, Mathematics and Informatics, professional field 4.5 Mathematics, scientific specialty "Mathematical Modeling and Application of Mathematics (Applications to the Computational Physics and Biology)"

September 4, 2019
София

Signature: ...