

STATEMENT

by Prof. Dr. Emanouil Atanassov, ICT-BAS

on the materials submitted for the competition
for occupation of the academic position of "Associate Professor"
at the Institute of Information and Communication Technologies - BAS
in the professional field 4.5. Mathematics

Reason for this statement: By order No. 131/13.05.2022 of the Director of ICT-BAS I was appointed as a member of the scientific jury of the competition for the occupation of the academic position "Associate Professor" in the professional field 4.5 Mathematics, announced in the State Gazette, no. 21/15.03.2022.

Only one candidate has applied for participation in this competition: Dr. Elena Lilkova from the Department "Scientific Computations with Laboratory on 3D Digitization and Microstructure Analysis", ICT-BAS.

1. Short CV of the candidate.

Dr. Lilkova obtained her Master's degree in medical physics from Sofia University "St. Kliment Ohridski". Her PhD thesis was also in the field of "Physics of Atoms and Molecules" in Sofia University. From 2015 until now she works at ICT, initially as an assistant professor and then chief assistant professor from 2017.

2. General presentation of the submitted materials

The candidate Dr. Elena Lilkova presented all the necessary documents in accordance with the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Rules for the implementation of this law, the Rules for the Acquisition of Academic Degrees and Occupation of Academic Positions at BAS, and the specific rules of ICT-BAS.

- 21 full-text scientific publications were presented for the competition by the candidate, out of these 2 are accepted for publication. All of the publications are of the type publication in a scientific journal or series, 14 are visible in the world scientific databases – SCOPUS and Web of Science. There are other 5 publications, that are published in PRACE Whitepapers, which is not in Scopus or Web of Science, but still has a rigorous referring process. All of these publications were not used in the doctoral thesis and were not submitted so far in NACID. 14 publications have SJR, and at least 4 have IF. The total number of publications is 37.
- For the competition Dr. Lilkova has submitted a list of 26 citations, all of the citing publications being visible in either Scopus or WoS or both. The author's h-index in SCOPUS (without auto citations) is 3.
- The candidate lead 2 research projects for young scientists and participated in a series of projects. Below is a table with the minimal value of indicators for the academic

position "Associate Professor" in the professional field 4.5. Mathematics at ICT-BAS and the values of the indicators, achieved by Dr. Lilkova.

Table. Minimal value of indicators for the academic position "Associate Professor" in the professional field 4.5 in ICT-BAS, and indicators value of Dr. Elena Lilkova.

Group of indicators	Content	Required indicators for "Associate Professor"	Indicators of Dr. Lilkova
A	Indicator 1 (PhD dissertation)	50	50
B	Indicators 3 and 4	100	110
C	Indicators 5-10	260	300
D	Indicators 11	70	156
E	Indicators 12-18	20	143
		Total: 500	759

3. General characteristics of Dr. Lilkova scientific and applied activities and contributions in the submitted for review materials

Dr. Lilkova's scientific and applied activity is in the field of the competition. The main scientific and applied scientific results are in the applications of mathematics in physics and biology, mainly in the modelling of biological macromolecules and complexes. This is a highly competitive scientific area, which requires multidisciplinary approach and team work. Dr. Lilkova works mainly in the field of "in silico" modelling using HPC. The scientific and applied scientific achievements of the candidate can be summarized in 3 main groups:

- **Molecular modelling of human interferon gamma** (B.1, B.2, B.3, B.4, Г.1, Г.2, Г.4, Г.9, Г.10, Г.11) - investigation of the structure and the conformational changes in the molecule of the cytokine, as well as its interactions with other molecules. The Energies of dilution of different representative conformations of the cytokine molecule were estimated. A detailed explanation was achieved at microscopic level of the expertimental finding of two orders of magnitude (100 times) smaller activity of the marked proteins and the inability to remove the marker by proteins, expressed in insect cells.
- **Modelling of antimicrobe peptides (AMP)**– Г5, Г6, Г7, Г8, Г12 – investigation of the structure, attributes and mechanisms of AMP. It has been shown how, in a solvent, before attacking the target membrane, the native peptid and its mutant take mainly the conformation of spiral – inflection – spiral, and not the expected pure spiral one. The secondary structure of some peptides with antimicrobial properties from some species

of snails has also been studied. Through "in silico" methods it was demonstrated that the AMPs fulfil their function not individually, but after forming of cluters.

- **Development, analysis and/or testing of scientific software – Г14,Г15,Г16,Г17.** Tests and analysys were carried out of existing software as well as newly developed software by the candidate as member of the development team. New modules were integrated to popular free-software packages. The tests were carried out on Avitohol supercomputer as well as other HPC systems.

Many of these scientific achievements have also applied scientific value.

4. Citations

The total number of independent citations, presented by the candidate, is 26, where 23 of the citing publications are in both WoS and Scopus, 2 in Scopus only and 1 in WoS only. A check in scopus shows H-index of 3 without auto-citations, which is a good achievement in the field.

5. Personal contribution of the candidate

All of the publications submitted for the competition are co-authored, but it is natural to work in teams in this multi-disciplinary area. The applicant's personal contribution is clear to me and beyond doubt.

6. Critical remarks and recommendations

It would be better if the personal contribution of the candidate was more clearly marked, although it is clear to me from my personal knowledge of the candidate and the context of the publications. It would be beneficial if possible to split out some definite parts of such common works and do a more elaborate study on the problems as an individual paper, when this is appropriate.

CONCLUSION

The documents and materials presented by Dr. Elena Lilkova fully meet all the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Rules for the implementation of this law, the Regulations of BAS and the corresponding regulations of IICT-BAS. The results achieved by Dr. Lilkova are in full compliance, and by many indicators exceed the specific requirements of IICT-BAS for the academic position of "Associate Professor". There has been no established plagiarism in the works of the candidate or other irregularity.

After acquaintance with the materials and scientific works presented in the competition and analysis of their importance and their contributions, I am convinced of my **positive assessment** and I **strongly recommend** to the Scientific Jury to submit a recommendation to the Scientific Council of IICT-BAS for the selection of Dr. Elena Lilkova in the academic position of "Associate Professor" at IICT-BAS in the professional field 4.5 Mathematics.

7. 07.2022

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