OPINION

by associate professor Dr Ivan Dimov Lirkov
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on documents, submitted for participation in a competition
for the academic position of Professor in professional area 4.5
"Mathematics", scientific specialty "Mathematical Modeling
and Application of Mathematics" (applications in computa-
tional physics and biology) with candidate Nevena Petrova
Ilieva-Litova

1. Short biographical information

   Nevena Ilieva graduated from the Sofia University "St. Kliment Ohridski" in
   1985 with Master's Degree in Physics. In 1988 she defended her thesis on the
   topic "Quantum effects in two-dimensional calibration theories". In 2003 she
   has been elected for the academic position "associate professor" at the Institute
   of Nuclear Research and Nuclear Energy - BAS.

2. General description of the presented materials

   Publications — 23, of which 17 are articles in scientific journals with Impact
   Factor and 5 are articles in series with Impact rank.

3. Impact of the candidate's scientific publications in the literature

   Fifteen from the presented by the applicant candidate publications have been
   cited in 49 scientific papers, referenced and indexed in world famous scientific
   information databases (Scopus and IEEE Xplore).

4. General characteristics of the applicant's activities

   (a) Scientific and applied scientific activity

       Nevena has authored and co-authored more than 100 research publications
       and in the last years has participated in 17 research projects, of which:

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leader of 3 international and 3 national, participant in 7 international and 4 national projects.

(b) Contributions

The applicant's contributions in the presented materials have scientific and applied scientific nature and are undoubted.

- Contributions to the methods of modeling, exploration and visualization of protein structure and dynamics. The following topics are considered:

  - The process of protein folding;
  - Development of advanced methods for extracting functional information from molecular-dynamics data;
  - Development of methods for visualization and structural analysis of proteins.

- Contributions in the field of In silico studies of immunoactive molecules and complexes. The following phenomena are considered:

  - Design of mutated forms of human interferon-gamma with strongly reduced biological activity;
  - Formation and dynamics of MHC class I molecules as well as the influence of emerging point mutations in different parts of the complex on its functionality.

- Contributions to the field of physical process modeling. The following problems are considered:

  - Design and development of a hybrid imaging system that combines Positron Emission Tomography (PET) with Magnetic Resonance Imaging (MRI) in a single device.

- Contributions in the field of high-performance computing. The following tasks are included:

  - Development and analysis of tools and methods for high-performance computing to study the structure and interactions of biomolecules.

I would like to emphasize one particular point in the results of the first group – the development of methods for modeling, investigation and visualization

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of the structure and dynamics of proteins. An original multi-step method for modeling the protein folding process is presented, combining deterministic and stochastic methods and allowing for the description of protein structure with subatomic precision. The method uses elements of the theory of integrable models and topological field theory, in conjunction with high performance computations to simulate the evolution of the system. Using so complex mathematical tools to solve biological problems is a risky approach, which makes the obtained convincing results all the worthier of praise. Such studies confirm the enormous potential of mathematical biology, whose founders in Bulgaria were the biologist Acad. Rumen Tsanev and the mathematician Acad. Blagovest Sendov.

5. **Evaluation of the personal contribution of the applicant**

I have no doubt about the personal contribution of the applicant in the presented publications.

6. **Critical remarks**

I have no critical remarks.

7. **Conclusion**

The presented materials convincingly prove the high professionalism of Assoc. Prof. Dr. Nevena Ilieva, the importance of her scientific achievements and their scientific impact. My personal impressions confirm the conclusions based on these materials.

Given the above, I wish to propose to the Scientific Jury to make a recommendation to the Scientific Council Assoc. Prof. Dr. Nevena Petrova Ilieva-Litova to be elected for the academic position "full professor" in professional area 4.5 "Mathematics", scientific specialty "Mathematical modeling and application of mathematics".

August 25, 2019
Sofia

Member of the scientific jury:

assoc. prof. Dr Ivan Lirkov

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