



STATEMENT REPORT

under the procedure for acquisition of the educational and scientific degree "Doctor"
by candidate Rossen Mikhov Mikhov,

of the PhD Thesis entitled: "Monte Carlo approach for optimization of bimetallic
nanostructures ",

In the Scientific field: 4. Natural Sciences, Mathematics and Informatics /

Professional field: 4.6. Informatics and Computer Sciences,

Doctoral program "Informatics", Department „Information processes and decision-making
systems",

Institute of Information and Communication Technologies, Bulgarian Academy of
Sciences,

The statement report has been prepared by: prof. Dr. Zlatinka Svetoslavova Kovacheva, Institute
of Mathematics and Informatics, BAS, as a member of the scientific jury for the defense of this
PhD thesis according to Order № 303 / 28.11.2025 of the Director of IICT, BAS.

1. General characteristics of the dissertation thesis and the presented materials

The presented dissertation contains 124 pages and consists of an abstract, 6 chapters, conclusion,
7 tables, 34 figures, 149 titles in the provided bibliography, a list of abbreviations and notations,
a list of publications on the dissertation, and a list of discovered citations of the publications.

2. Short CV and personal impressions of the candidate

Rossen Mikhov received his master's degree from Kyoto University, Japan, Master's Faculty of
Natural and Mathematical Sciences, major in Mathematics and Mathematical Analysis, area of
Theory of Programming Languages. From 2009 to 2013, he worked as a research assistant and
teaching assistant at Kyoto University, Japan. Since 2017, he has been working as a programmer
and assistant at the Institute of Information and Communication Technologies, Bulgarian
Academy of Sciences.

According to the presented documents, Rosen Mikhov was enrolled in doctoral studies for
independent preparation on 01.01.2025 for a two-year term. He has completed his individual plan
for one year, taking all his exams with excellent grades.

I do not know the candidate personally and my impressions of his work are based only on the
documents presented.

3. Content analysis of the scientific and applied achievements of the candidate, contained in the presented PhD thesis and the publications to it, included in the procedure

Based on the analysis of the methods for modeling and numerical optimization of the atomic configurations of metallic and bimetallic nanostructures, the aim of the dissertation is to develop a Monte Carlo approach with simulated annealing, using the tight-building potential, for the optimization of various types of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms.

A significant and useful work has been carried out. The following principal scientific and scientific-applied contributions of the dissertation work can be pointed out:

- A two-stage lattice Monte Carlo method is proposed for optimization of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms. The first stage is simulated annealing on a wide lattice and the second stage is simulated diffusion. The method allows the optimization of nanostructures from several hundred to several thousand atoms on a standard personal computer.
- Experimentally is established an effective strategy for distributing computational resources between the two stages of the method.
- The influence of the initial temperature on the performance of the wide-lattice Monte Carlo algorithm is investigated for different lattices and chemical elements.
- An adaptation of the two-stage method is made for nanocages. It is used for studying the atomic ordering and the processes of surface segregation in gold–silver nanocages with 3000 atoms. A comparative analysis of the results for three compositions and two lattices has been presented.
- A software architecture is proposed for the implementation of the two-stage method, which allows a high degree of optimization for performance of the computations, flexibility for concurrent execution and combination of the constituent algorithms in different conditions, and good compatibility with external applications for analysis and visualization of the results.

4. Approbation of the results

The results are presented in 4 publications, indexed in Scopus. Three of them are with SJR and fall into Q4. They bring the candidate 108 points on the fourth scientometric indicator with a minimum required score of 30 points.

Rossen Mikhov's dissertation includes results obtained while working on two research projects:

- Information and communication technologies for a single digital market in science, education and security (2018-2021) under the national scientific program of the Ministry of Education and Science;

- Mathematical models, methods and algorithms for solving difficult optimization problems to achieve high security in communications and better economic sustainability (2021-2025) of the National Science Fund.

The internationally recognized significance of the results is striking. A total of 7 citations were noted for 2 of the articles.

It is clearly stated that:

- The presented materials meet the minimum national requirements (under Art. 2b, para. 2 and 3 of ADASRB) and respectively to the additional requirements of IICT, BAS for acquiring the educational and scientific degree "Doctor" in the scientific field and professional field of the procedure;
- The results presented by the candidate in the dissertation work and scientific works to it do not repeat such from previous procedures for acquiring a scientific title and academic position;
- The submitted Similarity Report shows that there is no plagiarism proven in accordance with the statutory procedure in the submitted dissertation work.

5. Qualities of the abstract

The presented abstract in Bulgarian (47 pages) and in English (44 pages) fully meets all the requirements for its preparation and presents the results and content of the dissertation work comprehensively and correctly.

6. Critical notes and recommendations

I have no questions or critical remarks to the candidate. I recommend to continue the development of the proposed two-stage method with experimentation with similar particles with explicit confidence level data.

7. Conclusion

Having become acquainted with the PhD thesis presented in the procedure and the accompanying scientific papers and on the basis of the analysis of their importance and the scientific and applied contributions contained therein, **I confirm** that the presented PhD thesis and the scientific publications to it, as well as the quality and originality of the results and achievements presented in them, meet the requirements of the Act on Development of the Academic Staff in the Republic of Bulgaria, the Rules for its Implementation and the corresponding Rules of the IICT, BAS for acquisition by the candidate of educational and scientific degree "Doctor" in the Professional field 4.6. Informatics and Computer Sciences. In particular, the candidate meets the minimal national requirements in the professional field and no plagiarism has been detected in the scientific papers submitted for the competition.

Based on the above, **I strongly recommend** the scientific jury to award **Rossen Mikhov Mikhov**, the educational and scientific degree "Doctor" in the Professional field 4.6. Informatics and Computer Sciences.

Date: 06.01.2026

Sign:

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