REVIEW

by **Acad. Ivan P. Popchev** – BAS

of dissertation work for acquiring the educational and scientific degree

"Doctor"

In professional field 4.6 "Informatics and Computer Science"

Doctoral program "Informatics"

Titled "Monte Carlo approach for optimization of bimetallic nanostructures"

by **Rossen Mikhov Mikhov**

By order No. 303/28.11.2025 of the Director of IICT–BAS, corresponding member S. Margenov, in accordance with Art. 4, para. 2 of the Act of Development of the Academic Staff of the Republic of Bulgaria (ADASRB) and with the decision of the Academic Council of IICT (rec. of proceedings No. 9/26.11.2025) under the procedure for obtaining of educational and scientific degree "doctor" in professional field 4.6 "Informatics and Computer Science", doctoral program "Informatics" by Rossen Mikhov Mikhov with dissertation work titled "Monte Carlo approach for optimization of bimetallic nanostructures" I have been appointed as a member of the Scientific Panel.

When assessing the dissertation work, applicable are the terms of ADASRB, RAADASRB (Decree No. 26 of 13 February 2019) and the Rules for specific requirements of IICT–BAS for the application of the law, and therefore will be accurately delivered:

1. According to Art. 27 (1) of RAADASRB "the dissertation work shall contain scientific or scientific-applied results that represent an original contribution to science. The dissertation shall show that the candidate has in-depth theoretical knowledge in the respective subject, as well as abilities for independent research".
2. According to Art. 27 (2) of RAADASRB "the dissertation work should be presented in a form and volume corresponding to the specific requirements of the primary unit. The dissertation work should contain: title page; table of contents; introduction; exposition; conclusion – summary of the obtained results, accompanied by a declaration of originality; bibliography".

The scientific supervisor of the dissertation is **Prof. Leoneed Kirilov, PhD**.

The aim of the dissertation is formulated on page 25 and it is "to develop a Monte Carlo approach with simulated annealing (SA), using the tight-binding (TB) potential, for the optimization of different types of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms".

The **following six tasks** are defined:

1. To propose a method for optimization of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms.
2. To investigate the effectiveness of the proposed method.
3. To propose an appropriate approach for choosing and adjusting the parameters of the method.
4. To determine which of the following factors most significantly affect the optimal choice of initial temperature for simulated annealing: chemical element, nanoparticle size, lattice type, lattice size.
5. To propose a software architecture and to develop a software system implementing the new method that allows a high degree of optimizability for performance of the computations, flexibility for varying the algorithms and their parameters and good compatibility with external applications for analysis and visualization of the results.
6. To conduct an investigation applying the proposed method to the study of a specific class of gold–silver nanocages with 3000 atoms, which are of interest for many applications, in order to establish how the differences in the Au:Ag ratio and the symmetry of the lattice affect the atomic ordering and the processes of surface segregation.

The dissertation consists of 124 pages, 34 figures, 7 tables, 149 references and it includes:

- Acknowledgements (5);
- Introduction (6–8);
- List of abbreviations and symbols (9–10);
- Analysis of methods for modeling and numerical optimization of atomic configurations of metallic and bimetallic nanostructures (**Chapter 1**, 11–26);
- Two-stage Monte Carlo approach for optimization of bimetallic nanostructures (**Chapter 2**, 27–40);
- Numerical testing of the two-stage method for optimization of bimetallic nanostructures (**Chapter 3**, 41–50);

- Influence of the initial temperature on the wide-lattice simulated annealing algorithm (**Chapter 4**, 51–66);
- Application of the method to the optimization of gold–silver nanocages (**Chapter 5**, 67–85);
- Software architecture and system for the implementation of the two-stage method for optimization of bimetallic nanostructures (**Chapter 6**, 86–101);
- Conclusion – summary of the results (102–104);
- Contributions (105-106);
- List of publications on the dissertation (107);
- List of discovered citations of the publications (108–109);
- Participation in research projects (110);
- Declaration of originality of the results (111);
- Bibliography (112–124).

4 publications on the dissertation are presented.

The analysis of these publications shows the following:

- 3 publications are in **Scopus with SJR Q4** (No. 2, 3 и 4);
- publication is in IEEE Xplore (No. 1);
- all publications are with **coauthors** in English.

7 citations are known, as follows:

- 3 citations of publication No. 1;
- 4 citations of publication No. 3.

Participation in two national research projects.

The dissertation (pp. 105–106) lists "**Contributions**" summarized into **6 main results**, for which there is no evaluation according to Art. 27 (1) of RAADASRB that they "**represent an original contribution to science**".

In brief the obtained results in the dissertation can by systematized as follows:

1. A lattice Monte Carlo method in five steps for optimization of bimetallic nanostructures, with first stage simulated annealing on a wide lattice and second stage simulated diffusion.

2. The two-stage method is adapted to work with nanocages and is used for studying the atomic ordering and the processes of surface segregation in gold–silver nanocages with 3000 atoms.
3. The two-stage method is implemented in a software system with architecture consisting of three components: computational core, template for the master plan of the experiment, supplementary functionalities for analysis of the results, testing and visualization. The system works with Linux and Windows and uses the XYZ format for input and output data.

The minimum requirements of the RAADASRB and specific requirements of IICT–BAS are fulfilled.

Critical notes

1. In "contributions" (pp. 105–106) it is not specified whether they are scientific or scientific-applied results according to Art. 27 (1) of RAADASRB.
2. On p. 25 a task is given "to investigate the effectiveness of the proposed method", but there is no information of such an investigation and for the criteria used for investigation the effectiveness.
3. It would be appropriate to include under "future development of the research" (p. 104) that "in the future, kinetic Monte Carlo on the lattice or MD sampling with machine-learned potentials could be integrated" (p. 84).

Questions on the dissertation

1. Specifically for which main results it can be proven that they **represent an original contribution to science**? What are the **criteria** for an original scientific contribution?
2. By which method was the computational core optimized for speed of the computations (p. 101)?
3. In the section on future development, it is not specified how the two-stage method will "reproduce important aspects of their configurations" (p. 104)?
4. The dissertation as a part of a broader study carried out by a multidisciplinary team, can it answer the question of the ultimate goal of this research in time?

A generalized "**scientific-metric profile**" of the doctoral student Rossen Mikhov can be built on data taken from the world scientific databases:

- Scopus: 13 documents by author, 26 citations, h-index 3;
- Web of Science: 3 publications, 1 citations;
- MathSciNet: 2 publications;
- zbMATH Open: 2 publications, 1;
- IEEE Xplore: 1 publications;
- Scholar.google: 14 publications;
- Researchgate: 14 publications.

The generalized "scientific-metric profile" deserves to be a subject of a careful and critical **self-analysis**, to form future research and to present sufficient grounds for independent publishing activity in publications with IF/SJR.

The Abstracts are in Bulgarian and English, respectively including 47 and 44 pages and present the dissertation.

CONCLUSION

The dissertation work fulfills the requirements of ADASRB, RAADASRB and the specific requirements of IICT–BAS.

I give a **positive conclusion** for acquiring the educational and scientific degree "**Doctor**" by **Rossen Mikhov Mikhov**.

I propose to the Scientific Panel to unanimously vote for awarding Rossen Mikhov Mikhov the educational and scientific degree "Doctor" in 4.6. "Informatics and Computer Science", doctoral program "Informatics".

8.12.2025

Sofia

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