OPINION
by Professor Ivan Petkov Bangov
(Professor, first name, last name, last name)
on the dissertation work
FOR OBTAINING THE EDUCATIONAL AND SCIENTIFIC DEGREE
"DOCTOR"
Field of higher education: 4. Natural sciences, mathematics and
Informatics. Professional field 4.2. Chemical sciences
Doctoral program Theoretical chemistry
Scientific supervisor: Assoc. Prof. Dr. Nikolay Kochev
Author: Gergana Ilieva Tancheva
Topic: APPLICATION OF CHEMICAL INFORMATICS METHODS
TO MULTICOMPONENT SUBSTANCES AND NANOMATERIALS.

1. General presentation of the procedure and of the dissertation candidate

The dissertation work of Gergana Tancheva was discussed and directed for reporting at a meeting of the extended department council of the Department of Analytical Chemistry and Computational Chemistry of the Faculty of Chemistry at Plovdiv University "Paisii Hilendarski", held on 14.10.2024.

2. Actuality of the topic.

This dissertation is in a new topic, at least within our country. As the dissertation candidate notes, while the application of chemoinformatics to molecular systems is a well-developed topic over the last 40 years, a new challenge is to develop approaches and methods for applying chemical informatics methods for processing and storing information for multicomponent substances, nano-materials and new materials, as well as discovering prospects for effective information processing through a semantic FAIR data model and its application in scientific experiments and modelling of nano-materials and mixtures of chemical substances.

3. Knowledge of the problem

The dissertation is divided into 4 sections, the first section being the literature review. I would like to note that this section is written quite intelligently and shows a good knowledge of the literature on the given issue. The main emphasis is given to the presentation of nano-materials, both in terms of their properties and their toxicity. It is noted that the safety of nano-materials has been a major topic in several framework programs of the European Commission in the last decades. The different definitions of a single chemical substance or element and mixture or UVCB substances according to the different regulations, UIPAC, the US Chemical Substance Control Act (TSCA), the EU REACH regulation, the British regulation, as well as the ISO regulation, etc.. are presented. Materials with new or improved functionalities AdMa (Advanced Materials) are examined. The different classifications of chemical substances by origin, by structural composition, by number of dimensions, by porosity, by toxicity are examined. The properties of nano-materials and synthesis approaches are considered. The dissertation candidate has become familiar with the classical methods of chemical informatics for representing chemical objects and the corresponding QSAR/QSPR methods for their processing with the theory of molecular descriptors, etc.. The dissertation candidate has become familiar with chemical databases and electronic notebooks, with data models for chemical substances and nano-materials. The acquired knowledge is a good basis for both the further development of the dissertation work and determines the educational part of the dissertation work.

4. **Research methodology.**

The research in the dissertation work is organized into 16 tasks. Here we will highlight the most important of them. Own research is subject to FAIR (Findable, Accessible, Interoperable, Reusable) principles in data management. The Ambit/eNanoMapper data model is chosen to represent information on multicomponent substances and nano-materials. It is planned to use JSON to convert EXCEL files with experimental data on nano-materialness, as well as to study the issue of nano-material safety. ecotoxicity and environmental pollution. Development of the AmbitSLN library, as well as electronic notebooks for connection to the RDkit and CACTUS software libraries. Creation of an Orange3-ToxFAIRy module for the Orange analytical platform, which can be used as a user interface to the ToxFAIRy software library.

5. **Characteristics and assessment of the dissertation work and contributions.**

As can be seen in this dissertation, various tasks are set that require enormous work and good knowledge of the material for the implementation of this dissertation work.

6. **Assessment of the publications and personal contribution of the dissertation candidate.**

The doctoral student has published 3 publications in a team, one of which is a chapter of a monograph, which was of great interest to me. The first work has collected 16 citations, and the second 1 citation. Participated in 9 scientific events with posters and 3 - with reports, on-line. The doctoral student has participated in 5 international scientific projects.

7. **Abstract**

The abstract is well structured and provides good information about the work done on the dissertation.

8. **Recommendations for future use of the dissertation contributions and results.**

The dissertation outlines guidelines for future development, which include the development of software tools for calculating descriptors and indices, as well as the ambitious task of applying new modern algorithms based on artificial intelligence for modelling QSPR/QSAR analysis. I would recommend that, after creating new descriptors, the descriptor fingerprinting method, developed by me and Professor Doychinova for searching databases, be used.

9.**Conclusion**

Based on the documentation presented to me of the scientific achievements and scientific activity of the doctoral student Gergana Ilieva Tancheva, my opinion is that, following the requirements of the REGULATIONS FOR THE IMPLEMENTATION OF THE LAW ON THE DEVELOPMENT OF THE ACADEMIC STAFF IN THE REPUBLIC OF BULGARIA, she fully deserves to receive the educational and scientific degree of DOCTOR.

20. 12. 2024   **Made the Opinion**

Professor Doctor Chem. Sci. Ivan Petkov Bangov