

OPINION

of a Ph. D. Thesis

for the acquisition of the educational and scientific degree "doctor"

in professional direction 4.1 Physical sciences, physics of atoms and molecules,

by defense procedure at the Faculty of Physics (FzF)

of Sofia University "St. Kliment Ohridski" (SU)

The review was prepared by: Associate Professor Peicho Stoev Petkov, PhD - SU "St. Kliment Ohridski", Faculty of Physics, in his capacity as a member of the scientific jury according to Order No. ПД-38-469/23.07.2024 of the Rector of Sofia University.

Ph. D. Thesis topic: "Extrapolation properties of the Morse-Long Range potential at large internuclear distances"

Author of the dissertation: Alketa Ali Sinanaj

I. General description of the presented materials

1. Data on the submitted documents

The candidate Alketa Sinanaj has submitted a dissertation in English and two extended abstracts in Bulgarian and English, as well as the mandatory tables for the Faculty of Physics at Sofia University from the Regulations on the Terms and Conditions for Acquiring Scientific Degrees and Holding Academic Positions at SU "St. Kliment Ohridski". 5 other documents (in the form of official notes, declarations and other appropriate evidence) supporting the applicant's achievements are also presented.

The documents submitted by the candidate for the defense correspond to the requirements of the LAW ON THE DEVELOPMENT OF THE ACADEMIC STAFF IN THE REPUBLIC OF BULGARIA, REGULATIONS FOR IMPLEMENTING THE LAW ON THE DEVELOPMENT OF THE ACADEMIC STAFF IN THE REPUBLIC OF BULGARIA and the Regulations for the terms and conditions for acquiring scientific degrees and occupying academic positions at SU "St. Kliment Ohridski".

2. Applicant data

Alketa worked as an assistant Lecturer from 2016 to 2024 at the Alexander Giovanni University in Elbasan, where her responsibilities included organizing seminars, laboratory exercises

and courses in various physics disciplines. She also worked as a physics teacher in several schools in Elbasan.

Alketa graduated from Dhaskal Todri General High School in Elbasan and earned a BA in Mathematics and Physics from Alexander Gjuvani University. She continued her studies in physics at the University of Tirana, and then began doctoral studies in optics and spectroscopy at the University of St. Kliment Ohridski" in Sofia, Bulgaria.

Alketa speaks English (IELTS B2), Italian (C1), German, Macedonian and Bulgarian. Her technical skills include working with Microsoft Office, Origin, Qti-Plot and Python.

She attended 4 summer schools. She participated in 10 international conferences.

Alketa conducts research on topics including element concentration in environmental samples and potential energy curves for diatomic molecules, with results published in journals such as the Journal of Molecular Spectroscopy, Acta Physica Polonica and RAD Conference Proceedings.

Alketa's CV highlights her experience teaching physics, active research in spectroscopy, and constant engagement with the scientific community.

3. General description of the candidate's scientific achievements

The scientific achievements of Ms. Alketa Sinanaj can be summarized based on the thesis she submitted, in which the extrapolation properties of the Morse-Long Range (MLR) potential at large internuclear distances are investigated. Specifically, the candidate's work is focused on analyzing the potential energy curves (PEC) of diatomic molecules, with the aim of achieving accurate extrapolation at large internuclear distances and limited experimental data.

The research included in the thesis was published in two impact factor publications and one with SJR. The main results are published in the articles A. Sinanaj and A. Pashov, Extrapolation properties of the Morse-Long Range potential at large internuclear Distances, J. Mol. Spectrosc. 396, 111811 (2023), Q3, IF 1.4. and A. Pashov and A. Sinanaj, "Extrapolation properties of the Chebyshev-Polynomial-Expansion potential", Acta Phys. Pol. A, vol. 146, no. 3, p. 259, Sep. 2024, doi: 10.12693/AphysPolA.146.259., Q4, IF 0.5. The research was reported at the 11th International Conference of the Balkan Physical Union and posters were presented at three international conferences. The scientific publications included in the dissertation meet and even exceed the minimum national requirements and the additional requirements of SU "St. Kliment Ohridski" for the acquisition of the educational and scientific degree "doctor" in the professional field of physical sciences;

According to the submitted declaration of authorship, the study and the scientific results presented in the thesis are original and have not been used in other procedures for awarding the scientific and educational degree "doctor".

The presented protocol and opinion from the procedure for checking for plagiarism prove that such was not detected.

4. Characterization and assessment of the candidate's teaching activity (if required)

There are no such requirements for the candidate. There are no quantitative data in the submitted documents.

5. Content analysis of the applicant's scientific and scientific-applied achievements contained in the submitted materials

The thesis presents a comprehensive scientific contribution to spectroscopy and molecular physics, focusing on the extrapolation properties of the Morse-Long Range (MLR) potential at large internuclear distances. The candidate's work mainly involves developing new methods and improving existing models for potential energy curves (PECs) of diatomic molecules, increasing the precision of predictions regarding molecular interactions and spectral properties.

Alketa Sinanai's thesis is well structured and well illustrated. A thorough introduction to models for describing diatomic molecules is given. The studies are described exhaustively, and this also applies to the mathematical apparatus used.

The candidate's contributions include the development of new models and methods, in particular a model based on the MLR potential with long-range extrapolation properties. This meets the need for accurate long-range PECs and represents an improvement in theoretical approaches in the field of molecular spectroscopy, allowing the construction of more accurate PECs for internuclear distances where known literature models are deficient, especially in the absence of accurate experimental data. The work advances knowledge in the field of molecular spectroscopy by providing deeper insight into long-range molecular interactions, extending existing theories through models with improved extrapolation properties.

The candidate's contributions have both a scientific and an applied nature. Alketa Sinannai's work introduces advanced PEC modeling technique that is directly applicable. An approach has been developed for motivated limitation of the parametric space when approximating experimental data with different accuracy. More specifically, the “MLR potentials can be classified according to the values of the introduced four parameters r_{ref} , p , q and N ” as a result of the research, recommendations are given for choosing their values and a procedure for fitting all the MLR parameters. The results have practical applications as such methods are useful for calculating photoassociation rates, scattering lengths, and other essential molecular properties. Thus, the candidate's research offers valuable tools for both experimental and theoretical developments.

The research described in Alketa Sinanai's thesis is mainly published in two papers (Q3 and Q4) with a single co-author her supervisor, the candidate's individual contribution is clearly stated in both the publications and the dissertation and is focused on the development and application of the MLR model, especially when applying the parameterization procedure to achieve accurate modeling of the potential energy curves.

Overall, the dissertation demonstrates a balanced combination of theoretical research and practical applications in the field molecular physics and spectroscopy. This combination emphasizes the scientific and practical value of the candidate's achievements, which forms a good basis for further development.

6. Critical notes and recommendations

I have no critical comments on the content and structure of the dissertation and both extended abstracts, but typographical errors are noticeable. In addition, the thesis would benefit from an even more in-depth analysis of systematic and model uncertainties.

I have the following questions for the candidate:

1. One of the research results is that "The MLR potentials can be divided into classes with different values of r_{ref} , p , q and N ". You specify that " p and q should be some small integers and $p + 6$ should be no smaller than 10 (6 being the power of the leading dispersion coefficient C_6 , 10 – the power of the last coefficient, C_{10})" as this was determined for Ca_2 . For which diatomic molecules are these values applicable?

2. The concluding part of the thesis states "In the present case of Ca_2 , allowing for a 5% uncertainty in the theoretical C_6 will automatically reduce the uncertainty in D_e from $\pm 2 \text{ cm}^{-1}$ to about $\pm 1 \text{ cm}^{-1}$ for $v''_{max} = 30$." and also, as it is well explained in the thesis these parameters are quite correlated. Have you investigated whether any relationships between the data quality, the theoretical uncertainty of C_6 and the accuracy with which D_e can be determined? If such a dependency cannot be inferred, then what is the reason?

7. Personal impressions of the candidate

8. Conclusion

After having familiarized myself with the presented Ph. D. Thesis, the Abstracts and other materials, and based on the analysis of their significance and the scientific and scientific-applied contributions contained in them, I **confirm** that the scientific achievements meet the requirements of LAW ON THE DEVELOPMENT OF THE ACADEMIC STAFF IN THE REPUBLIC OF BULGARIA and the Regulations for its application and the relevant Regulations of the SU "St. Kliment Ohridski" for **acquiring the educational and scientific degree "doctor"**. In particular,

the candidate satisfies the minimum national requirements in the professional direction and no plagiarism has been found in the dissertation, extended abstract and scientific works submitted for the competition.

I give my **positive** assessment of the dissertation.

II. General Conclusion

Based on the above, I **recommend** to the Scientific Jury that awarded the **educational and scientific degree "doctor"** in professional direction 4.1 Physical sciences (physics of atoms and molecules) to Alketa Sinanaj

Date: 05.11.2024

Prepared the review:

(Assoc. Prof. Peicho Petkov, PhD)