INSTYTUT FIZYKI
POLSKIEJ AKADEMII NAUK
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OPINION

on a dissertation

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

in professional direction 4.1 Physical Sciences,

under the defense procedure at the Faculty of Physics of the University of St. Kliment Ohridski

The opinion was prepared by: **Prof. dr. hab. Włodzimierz Jastrzębski** from Institute of Physics Polish Academy of Sciences, in his capacity as a member of the scientific jury according to Order № РД 38-469/23.07.2024 of the Rector of Sofia University.
The dissertation entitled: " **Extrapolation properties of the Morse-Long Range potential at large internuclear distances**"
Author of the dissertation: **Alketa Sinannaj**

The dissertation prepared under supervision of:

Prof. DSc. Asen Pashov and Assoc. prof. Dr. Snejana Iordanova

PhD student data

Ms. Alketa Sinanaj was born in Elbasan, Albania on February 13, 1992 and possesses double, Albanian and Bulgarian citizenship.

She graduated from Faculty of Natural Science, University ”Aleksander Xhuvani” of Elbasan (2011-2014) and then Department of Physics, University of Tirana (2014-2016).

From 2016 to 2024, she is employed as a Asistent Lecturer at the University 'Aleksander Xhuvani', Elbasan.

From 2019 to 2024 she is a PhD student at the Department of Optics and Spectroscopy of the 'St. Kliment Ohridski' University in Sofia. During this time she published two scientific papers in journals on the so-called *Philadelphia List* and related to her doctoral dissertation subjects.

General description of the PhD student scientific achievements.

In general, the subject of the thesis is the description of the electronic states of diatomic molecules by means of various models of potential energy curves (PECs). But of particular interest to the Author is the description of the long-range parts of PECs, for internuclear distances larger then LeRoy radius.

I find the choice of such a topic very appropriate and up-to-date, certainly not fully explored in the literature. And it is very important and of interest not only to spectroscopy. These long-range interactions determine the properties of ultra-cold atomic and molecular species, the possibility of evaporative cooling, sympathetic cooling, production of cold molecules by photassociation and generally determine collisional properties that also lead to decoherence of quantum states which is of particular concern due to applications in future quantum technologies.

The thesis has a classical structure: chapters 1- 3 provide a very good introduction to further considerations. In addition to the rather detailed description of the energy structure of molecules (Chapter 2) I really like the overview of the possibilities and limitations in the experimental determination of PECs (Chapter 3). This is a very mature form of discussion, I read it with pleasure. Here the comparison of different models of PECs is particularly important, beginning with Morse Potential, Lennard-Jones Potential to Morse-Long-Range and Spline point-wise form.

In the next Chapter 4, the Author presents literature examples of determination of the long-range part of the PEC for the ground states of selected molecules: Rb_2, Ca_2, NaRb and some

hydrogen halides (eg. HF, HCl and similar). The papers quoted and discussed in Chapter 4 each used a slightly different strategy for determining long range PECs. This literature review was a prelude to the Author's own numerical experiments for ground state of Ca_2 presented in Chapter 5. The performed simulations allowed her to estimate, among other things, the uncertainties of the fitted parameters depending on the extrapolation distance. And in the current case of Ca_2 they have a reliable criterion for assessing the quality of the potential curve. It is the agreement with the available in this case experimental data. Most often we do not have from the experiment the energies of these highest lying (long-range) oscillation levels, so realizing how large error we make when extrapolating PECs for distant levels is crucial. The conclusions of these numerical experiments will be applicable in the future in situations where we do not have positions of these high lying, long-range oscillatory states and can only extrapolate their energies. And this is the most common case, if only because of the small Frank-Condon factors.

In my opinion, this is the most valuable result obtained by Ms. Sinannaj and I think it will be used in future studies of long-range PECs.

Critical notes

The only slight criticisms and questions I can make are the following:

- why numerical experiments are performed for only one molecule, whereas in Chapter 4, PECs are reported for several molecules,
- whether the presented numerical simulations can be applied to electronic states with hyperfine structure (e.g. when singlet-triplet interactions occur),
- more generally, could such analyses be performed in states where perturbations are observed.

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Other remarks

The language of the thesis is clear. I did not notice any significant linguistic errors, however I am not a native speaker.

I have no other significant criticisms.

It is worth noting that performing the numerical experiments required running several thousand simulations.

Final conclusion

Alketa Sinannaj's dissertation, abstract, and research publications meet the standard requirements for a doctoral dissertation. The candidate satisfies the national ZRAS requirements in the area, as well as the requirements of the Faculty of Physics, and no plagiarism has been found in the dissertation.

I support awarding of the educational and scientific Doctor degree to Ms. Alketa Sinannaj.

Włodzimierz Jastrzębski

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