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Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Giorgio Visentin

PhD Program: Materials Science and Engineering

Title of Thesis: Accurate ab initio evaluation of the interatomic potentials and long-range coefficients

Supervisor: Professor Alexei Buchachenko

Name of the Reviewer: Robert Moszynski

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 04-10-2021**

The purpose of this report is to obtain an independent review from the members of PhD defense Jury before the thesis defense. The members of PhD defense Jury are asked to submit signed copy of the report at least 30 days prior the thesis defense. The Reviewers are asked to bring a copy of the completed report to the thesis defense and to discuss the contents of each report with each other before the thesis defense.

If the reviewers have any queries about the thesis which they wish to raise in advance, please contact the Chair of the Jury.

Reviewer's Report

Reviewers report should contain the following items:

- Brief evaluation of the thesis quality and overall structure of the dissertation.

The doctoral dissertation of Mr. Giorgio Visentin reports the results of accurate calculations of the interatomic potentials and long-range coefficients for various diatomic dimers. This is a very timely subject given the tremendous advances in many areas of experimental molecular physics, just to quote ultracold molecules or laser resonance spectroscopy. I have a very high opinion of the obtained results and of their presentation.

The thesis consists of the Introduction and Conclusions of one chapter reporting a pretty exhaustive review of the computational methods applied in the thesis, and of four chapters reporting original results, mostly published in highly ranked scientific journals.

- The relevance of the topic of dissertation work to its actual content

In my opinion, there is a one-to-one correspondence between the research tasks that the Author decided to treat and their actual description in the dissertation. It suffices to say that the Author defines his scientific goals in four questions in the Introduction, and all over the thesis he convincingly presents his results showing that he achieved his goals and got the answers to these questions.

- The relevance of the methods used in the dissertation

The Author applied state-of-the-art ab initio methods of quantum chemistry to very difficult problems of interactions between heavy systems, especially he extended the combination rules to the case of homonuclear diatomic molecules composed of open-shell species. Finally, he developed a novel model of the induction (polarization) interaction in systems with heavy cations, and applied it to the mobilities of singly charged lanthanide and actinide cations.

- The scientific significance of the results obtained and their compliance with the international level and current state of the art

The results obtained by the Author for the dimers of alkali earth atoms (including ytterbium) are of significance for high-resolution spectroscopy both in the hot and ultracold regimes. The same is true for the extended combination rules applied to long-range interactions in dimers containing open-shell atoms. In addition, the ab initio results could be nicely used to interpret the experimental mobility of singly charged lanthanide and actinide cations from laser resonance chromatography.

I have a very high esteem of the reported research and find that it is top class at the international level in the field of intermolecular forces. The results obtained in the thesis are state-of-the-art in this field.

- The relevance of the obtained results to applications (if applicable)

The results obtained in the present thesis can be applied in practice to guide some experiments in the area of ultracold molecules and mobility of ions, but do not have direct practical applications.

- The quality of publications

The core part of the thesis consists of four scientific publications published in the top quality international journals in chemical physics and physical chemistry (Journal of Chemical Physics and Frontiers in chemistry).

The summary of issues to be addressed before/during the thesis defense

No issue to be addressed.

Provisional Recommendation

☑ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

☐ *I recommend that the candidate should defend the thesis by means of a formal thesis defense only after appropriate changes would be introduced in candidate's thesis according to the recommendations of the present report*

☐ *The thesis is not acceptable and I recommend that the candidate be exempt from the formal thesis defense*