Skoltech
Skolkovo Institute of Science and Technology

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:

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	 **Date: 13-09-2021**

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 relevance of the topic of dissertation work to its actual content
- The relevance of the methods used in the dissertation
- The scientific significance of the results obtained and their compliance with the international level and current state of the art
- The relevance of the obtained results to applications (if applicable)
- The quality of publications

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

The thesis under review addresses the problem of accurate computation of interatomic interaction of different atoms with quantum-chemistry methods. The properties including polarizability, coefficients of expansion of Van-der-Waals forces on distance, relativistic corrections were studied.

The thesis starts with Introduction followed by a Methodology section describing the quantum-chemistry methods used, followed by the description of four papers published by the defendant. The structure of the thesis is appropriate; the defendant's attempt to summarize and detail the methods used in his four works was quite successful in my opinion – even I, as a non-chemist, managed to learn something from it. Also the methodology section contains some interesting analogies between interatomic interaction and interaction between people, without giving a reference – if this is an original defendant's finding then I applaud to the defendant.

The four core chapters nicely build up on the exposition of the methodology chapter. The thesis ends with Conclusions that summarize the work and, to my satisfaction, argue about the significance and potential use of the results of obtained.

The defendant published as the first author four papers in top journals, which by far exceeds the requirement on the number and quality of publications.

I do not see any significant weakness of the thesis as viewed as a fundamental work in physics or materials science. I, however, find that presentation may be slightly improved, namely,

- I would suggest to better illustrate some of the aspects of the work. For instance, Chapter 4 talks about a global potential for Yb, quoting the difficulty of merging the atomic (asymptotic expansion at large distances) and molecular (as I understood, direct computation of the interaction). As the interaction energy is a one-dimensional function, I believe this can be nicely illustrated on a graph: I expected to see expansion of the interaction in R^{-6} and R^{-8} and graphically see how these functions diverge faster as R decreases than molecular calculations become sufficiently accurate.

Some minor issues / questions are:

- Brackets missing in the expression for \hat{H}'(t) after (2.16) and in (2.17)
- Section 2.7.2: is "Effective Core Potential" same as the concept of "Pseudopotentials" as used in the plane-wave basis codes?

A more general question:

- Can the defendant explain to a non-specialist in spectroscopy/ultracold physics, what is the practical (scientific) value of the work?

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*