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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: Professor Nikolay A. Gippius

I confirm the absence of any conflict of interest	*[signature]* **Date: 17-09-2021**

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 by Giorgio Visentin focuses on evaluation of the interatomic potentials and long-range coefficients. The thesis incorporates six chapters: Chapter 1 is a brief and nice introduction into the historical context of intermolecular forces, Chapter 2 describes theoretical background of the thesis and broad set of computational methods, including Hartree-Fock and cluster approaches. Chapter 3 is devoted to the modeling of dispersion interaction within the complete basis set CCSD limit, Chapter 4 describes the global interaction potential for dispersion-bound systems. In last two chapters the dispersion interaction in open-shell systems and induction interaction in heavy cations are discussed.

The title of the thesis is coherent with the content of the thesis and its structure. The methods used in the thesis are well presented in Chapter 2 and allow good understanding of the basics of all the techniques used.

Overall, the thesis covers several important aspects of the calculation of the interatomic potentials and long-range coefficients. The results of the thesis resulted in three papers published in J. Chem. Phys and one in Front. Chem. The publications included in the thesis are of high quality and are visible on the international level.

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*