

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Christian Tantardini

PhD Program: Materials Science and Engineering


Title of Thesis: A study of chemical bonding through quantum chemical topology

Supervisor: Prof. Artem Oganov

Chair of PhD defense Jury: Prof. Xavier Gonze

Date of Thesis Defense: 31 January 2020

Name of the Reviewer: Alexander Shapeev

I confirm the absence of any conflict of interest	Signature:  Date: 30-12-2019
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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 of Christian Tantardini compiles a six of his works united under the umbrella of understanding of chemical bonding. In his work, the chemical bonding is studied from a number of different angles by a common technique: analyzing the corresponding DFT electronic structure.

The thesis is structured as a collage of six publications, ordered from more methodological to more applied, with a preceding section laying the theoretical foundation for the work. The high variance in the topics of those publications makes it challenging to put all the work into a single continuous story, which could not probably be helped with.

Out of the six publications, three are published in Q1 journals, which confirms the high quality of the work.

The quality of the English is sufficient to understand the results of the thesis, although it could be improved. For example, the first sentence of the Introduction,

The PhD thesis is mainly devoted to **studies** of fundamental **insight of** chemical bonding **in** the field of Quantum Chemical Topology using first-principles simulations **on** different **state** of matter with both local basis set and plane wave basis set calculations.

Should be corrected to read

The PhD thesis is mainly devoted to **the study** of fundamental **insights on/into** chemical bonding **within** the field of Quantum Chemical Topology using first-principles simulations **of** different **states** of matter with both local basis set and plane wave basis set calculations.

While reading the thesis I had the following questions left unanswered:

1. The last section "CONCLUSION AND FUTURE PROSPECTIVES" is missing future perspectives as well as a discussion of the relevance of the obtained results to applications. Can the PhD candidate comment on that?
2. In the first work "A new equation of state for real gases..." could the new equations be validated against experimental data? (for such gases as H₂ or He or H₂O it should be known experimentally?) Also, how large would zero-point energy effects be compared to the corrections made by the author?

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