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Skolkovo Institute of Science and Technology

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

Date of Thesis Defense: 31 January 2020

Name of the Reviewer: Carlo Gatti

I confirm the absence of any conflict of interest	**Signature:** **Date: 23-12-2019**

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

The report prepared by Christian Tantardini to summarize the results obtained during his PhD and as a prerequisite to his PhD defense consists of a very brief introduction, followed by a chapter dedicated to the theoretical tools which have been mostly used during the PhD period and of three chapters related to 6 of the 11 papers which the candidate has authored or co-authored during the thesis and which have been specifically selected for the PhD defense. The last chapter deals with a recently started project on the evolution of the properties of elements, in particular of their electronegativity, upon an external pressure. This one is the only chapter for which publications have not yet been reported. Conclusions and perspectives are presented in a one-page ending paragraph.

The introduction is very succinct and not particularly informative, while the chapter related to the theoretical background is complete enough, but it is in general rather imprecise, not particularly well written and with some errors. Hints for corrections will be soon forwarded to the candidate.

The chapters illustrating the published results include each an introductory paragraph, the text of the published paper and the data related to supplementary information. The introductory paragraphs do not generally contain more information than the one recoverable from the introduction and conclusion sections of the corresponding papers. The introductory paragraph of Chapter II is instead of much better quality.

The numbers of papers published by the candidate is impressive and far beyond the standard for a PhD student. They were presented on international journals with good or very good impact factor. This is clearly a quite positive aspect.

However, the quality and the scientific impact of the six presented papers is quite heterogeneous. I personally found that three of them, namely those presented in Chapter II and related to the study of non-covalent interactions within Oxicams, are of excellent quality. They address an important and well defined problem, they report on a work competently conducted and using the most appropriate tools. Clear and scientifically sound conclusions are reported, which are of relevance for applications. Finally, these three papers are also very accurate and well written.

The two papers on developments of Quantum Theory of Atoms in Molecules (QTAIM) and related to the proposal of a new equation of state for real gases and of a way to neatly distinguish H-bonds from van der Waals (vdW) interactions, are, at first sight, undoubtedly more innovative, but also contain several critical issues that will be matter of discussion during the defense. The writing style and clarity of exposition should have been also largely improved.

The paper on Dess-Martin periodinane affords an interesting problem and uses some pertinent tools to provide useful insights. An NBO analysis should have been useful to clarify the partial contradiction between charge density topology, Source Function and Domain Averaged Fermi Hole (DAFH) analyses. At present, I think that no sufficient elements have been presented to clearly distinguish between the strength and lability of the four I...O interactions. However, this issue may also be a subject of discussion during the PhD defense.

The ongoing work on pressure effects presented in the last chapter is very interesting and I'm looking forward to hearing about its recent progresses. Again, it could have been illustrated with a better style.

Overall, despite the various criticisms I've illustrated above, the report and the work performed during the PhD correspond on average to the international standards to obtain a Ph.D.
I therefore recommend the report for defense.

Provisional Recommendation
x☐ *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*