Skoltech
Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Christian Tantardini

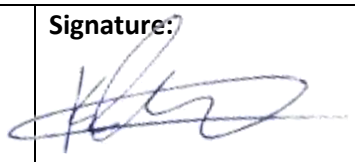
PhD Program: Materials Science and Engineering

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: Dmitry Kvashnin

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Signature:**  **Date: 19-12-2019**

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

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

PhD thesis of Christian is mainly devoted to studies of fundamental insight and understanding of nature of chemical bonding and its relationship with reactivity, atomic hybridization, etc. The main results of the dissertation were published in 11 papers in high ranking scientific journals. Dissertation consists of

Abstract and Introduction parts. Highlighted separately section of “Theoretical background” in which the details of already developed methods and techniques presented. Results of dissertation are presented within 4 chapters logically connected with each other. The Chapter 1 is devoted to the development of a new equation of state for describing real gases which based on the conception of the substitution of van der Waals dumping parameters. New equations found their application within the development of Quantum Chemical Topology Theory, which was described in the Chapter 2. Validation of proposed equation was carried out on a series of gas (monoatomic, diatomic, and triatomic). Within the collaboration with experimental group from Novosibirsk State University crystal structure of meloxicam co-crystal was decrypted. Utilization of the developed theory was performed in the description of chemical bonding in catalysis and at high-pressure in Chapter 3 and 4.

Nowadays there are number of approaches which was developed long time ago. Modern material science at this time needs new fundamental approaches to enable a deeper and more detailed description of physical effect connected with nature of chemical bonding. In the dissertation the fundamental understanding of non-covalent interactions was obtained. One of important question about the correlation between the intramolecular interactions and the solubility of crystals was also highlighted, which presented significantly promising results in the fields of medicine and biochemistry.

The most part of presented PhD thesis relates to the understanding of fundamental insight of van der Waals interaction like the physical limits and borders together with explanation of various properties of molecules. Dissertation contain significant scientific results satisfied to 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*