

## Jury Member Report – Doctor of Philosophy thesis.


**Name of Candidate:** Iosif Leibin

**PhD Program:** Materials Science and Engineering

**Title of Thesis:** Spectra and mobility of open-shell atoms in rare gas crystals: effects of interaction anisotropy

**Supervisor:** Professor Alexei Buchachenko  
Assistant Professor Dmitry Aksenov

### Name of the Reviewer:

I confirm the absence of any conflict of interest  U	<b>Date: 29-08-2024</b>
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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

The thesis is dedicated to describing the properties of open-shell atoms trapped in rare-gas lattices. The thesis is well-written and well-structured.

The thesis features a broad range of methodologies used. In particular, the thesis derives a pair potential for interaction between atoms which is parameterized from high-level (e.g., CCSD(T)) quantum chemistry calculations. Once the interaction has been obtained, it is used to calculate the vibrational, zero-point energy, diffusion, etc., properties of the system. Electronic properties are also calculated with a diatomics-in-molecule model.

The properties of a number of systems have been calculated and a satisfactory compliance with experimental results have been established. Thanks to the anisotropy of a molecule-lattice interaction that the Iosif accounted for in his work, new insights on these systems have been obtained. As I understand, the Iosif's findings, at least at this stage, are purely scientific (Iosif is welcome to comment on that), nevertheless, the work is no doubt of the highest quality as proved by Iosif's top-level publications.

While examining the thesis, I had the following two questions:

1. In Section 2.4 a time-dependent oxygen in Kr reaction kinetics is described which is said to run fast at temperatures between 20 and 23 K and then stops as the temperature increases until about 30K where it starts again. Did I misunderstand it? It is hard for me to imagine thermally-activated nonmonotone kinetics. Why would the migration slow down as the temperature increases?
2. In Section 3.4.1 I did not find it written, but I presume the pair potentials have been calculated for a pair of atoms in a CCSD(T) simulation cell. Is it expected that the matrix of other atoms contribute little through many- (three-, four-, ...) body interactions?

**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*