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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: Vladimir Feldman

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 14-08-2024**

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 PhD Thesis of Mr. I. Leibin is devoted to detailed theoretical investigation of trapping and dynamics of isolated atoms in noble gas solids. The topic is worth investigating for basic reasons, because it is generally related to the fundamental problems of chemical physics and solid-state physics concerned with accurate description of transport and chemical reactions of impurity species in a wide class of solids. More specifically, this is one of the key points of matrix isolation concept developed and widely used for spectroscopic and chemical investigation of highly reactive (and obviously elusive) species. Numerous experimental studies of matrix isolated atoms were reported for several decades, and attempts were made to provide the theoretical description of their spectroscopic signs and transport behavior. Nevertheless, the agreement between theory and experiment is still not satisfactory (even for H atoms) and adequate theoretical models are virtually lacking for the P-state atoms. The work of Mr. Leibin aims to fill this gap based on a new methodology, which may be considered as a reformulation of the known "Diatomics-in-molecule" (DIM) formalism, with specific attention to the atoms with non-zero angular momentum.

The dissertation is properly structured in five chapters (Introduction, Literature Review, Methodology and Techniques, Results and Discussion and Conclusions) providing comprehensive information on the work performed. The dissertation text is fully relevant to the topic. First of all, I would like to emphasize that the author has really good knowledge of state of the art in the field and he is able to discuss and analyze the available experimental data, even though the main focus of his investigation is theory and computations. Second, it is important that the computations made through this study provide reasonably good agreement with most available experimental data for both spectroscopic and transport (diffusion) properties. Actually, the conclusions made for light atoms in the frame of isotropic model are intuitively understandable. The model provides a clear interpretation of the effects of impurity atom size and matrix nature for these atoms (from H to Be). The simulations for the P-state atoms demonstrate strong effect of interaction anisotropy on both spectroscopic and transport properties of these species in the noble-gas lattices, which may be the guide for future detailed experimental investigations (lacking in many cases). Finally, it should be mentioned that the new approach developed and tested in the work of Mr. Leibin is promising as a relatively economic computational procedure for modeling the properties of complex systems, including large number of lattice atoms, which implies broader significance of this work. The list of references is complete and balanced.

The results are presented in four full papers in the high-ranking international journals, which justify their novelty and compliance to the international level in the field.

One thing that I would like to mention is that the comparison with experiment is mainly based on the data on emission spectra and transport barriers, while some crucial information for verification (particularly, for the anisotropic interactions) could be extracted from the EPR (ESR) data (actually, it is recognized by the author). Unfortunately, no attempts were made to calculate magnetic properties (including g-values and hyperfine coupling constants) based on the proposed model. Nevertheless, in my view it is not a real drawback of the work, but rather a prospect for future development. Also, a few misprints might be corrected.

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*

Professor Vladimir Feldman, Department of Chemistry,
Lomonosov Moscow State University

14 August 2024