

Thesis Changes Log

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: Assistant Professor Dmitri Aksenov

The thesis document includes the following changes in answer to the external review process.

First, I would like to take the opportunity to thank the Jury Members of the Reviewing Committee. I would like to acknowledge and appreciate the time and effort that they have spent on my Thesis and for the constructive comments and suggestions provided for improving it. The responses to the comments and suggestions provided by each Jury Member have been provided below:

Comments from Prof. Alexander Shapeev:

- 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?**

Response: First sentence of the third paragraph in Sec. 2.4 has been changed:

If one would gradually increase the temperature of the A@RG sample, one would notice that there are one or several distinct temperature thresholds for atomic mobility. If we take oxygen in Kr as an example: **the migration-indicating $O + O \rightarrow O_2$ reaction** can be observed at 20 K, proceeds at a rapid pace, and then stops at approximately 23 K, **as reactive oxygen atoms are depleted.**

- 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 contributes little through many- (three-, four-, ...) body interactions?**

Response: Effects of many-body interactions within the rare gas crystal itself (without the guest atom) are partly accounted by the modification of RG—RG diatomic potentials [Ref. & in the Thesis]. CCSD(T) calculations performed by Rościszewski et al. [1] on a pure rare gas crystals point out that in an ideal crystal three-body interactions amount for about 5% of the total energy with four-body amounting for another 1%. Failure to account for this 6% leads to the underestimation of lattice parameters and overestimation of atomization energies. This, in turn, leads to severe overestimation of the migration barriers if unmodified potentials of Aziz et al. are used.

And as for the many-body interactions involving guest atoms, they might have an impact in particularly strained interstitial structures. In order to prove our point before one of our article's reviewers, we have performed a model CCSD(T)/AVDZ calculation of a strained LiAr₆ fragment, cut from the IS(O_h) structure, and it have yielded that the contribution of many-body interactions in this, rather extreme case, does not exceed 5% of total interaction energy. Additionally, since we for the most part are not interested in interaction energies themselves, but rather in differences in interaction energy between different structures, many-body contributions, bearing the same sign, are expected to, at least partially, cancel each other out.

However, we do acknowledge that many-body interactions most certainly influence energies of tight structures (particularly, migration transition states) and migration barriers, and may be one of the reasons for the discrepancies between our theory and the experiment.

Comments from Dr. Alexander Larin:

- 1. Spin-orbit coupling was evaluated as minor effect for O@RG (Fig. 48, Table 13) while this estimate is of higher interest for heavier Ba or Sm atoms.**

Response: In the part of the Sm@RG project that did not make it into the Thesis, we have estimated the SO-coupling for Sm—He and Sm—Ne using the state-interacting SO configuration interaction (SI-SOCI) method [2]. The matrix elements of the Breit-Pauli operator were computed on the MRCI wave functions within the ECP LC (ECP on Sm, 6s4f correlated in MRCI) approximation for the ground and excited states simultaneously. The diagonal part was represented by the counterpoised interaction potentials, with those describing excited states shifted asymptotically (practically, at R = 40 Ang) to the 21857 cm⁻¹. The calculations show that the SO-coupled potentials are indeed slightly, yet notably different than “no-spin” ones.

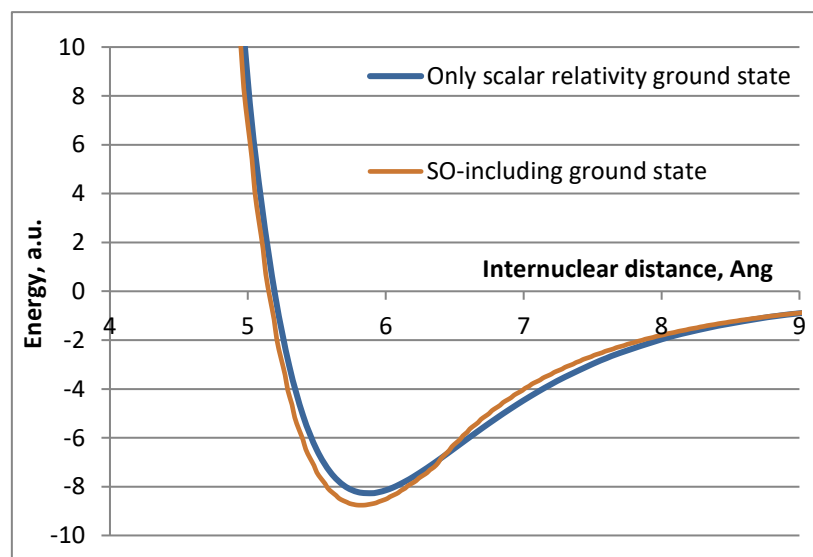


Fig. 1. Sm—Ne ground state calculated within ECP LC approximation, plotted against the same dissociation limit.

Unfortunately, the Sm@RG project is unfinished and it was ultimately decided to not include the SO-coupled Sm—RG potentials.

As for the Ba@RG, in our calculations only the ¹S₀ and ¹P₁ states are relevant, both of which have S = 1, so there is very little room for SO-coupling to affect our properties of interest.

2. **For the last atoms with the larger polarizabilities the test of three-body dispersive terms is more instructive (as a criterion for DIM scheme) because Axilrod-Teller-Muto terms are proportional to atomic polarizabilities. The case of relative importance of the three-atom terms for lattice dynamics of heavier RG was done by Barker et al. [IBM Journal of Research and Development, 20, 222, 1976. doi:10.1147/rd.203.0222].**

Response: As for the many-body interactions involving guest atoms, they might have an impact in strained site structures (e.g. TV site in Ba@Ar or migration transition states), but would be much less pronounced for spacious S6 and S7 sites. Additionally, since we for the most part are not interested in interaction energies themselves, but rather in differences in interaction energy between different structures, many-body contributions, bearing the same sign, are expected to, at least partially, cancel each other out. In summary, we suppose that even for Ba@RG the many-body contributions influence our properties of interest to a small degree.

However, we do acknowledge the fact that many-body interactions most certainly do influence our calculations and the absence of their appropriate treatment may be one of the reasons for the disparity between our calculations and the experimental data.

3. **For vacancies and self-interstitials author realized the evaluations of formation enthalpy, the heights of the barrier for migration and apparent activation energy. The apparent self-diffusion activation energy was underestimated by around 30% for both vacancies and self-interstitials (or less depending on the RG atom for vacancies). No other computational results were given for these RG properties which have more general character (and should occur more frequently in any computations of RG solids) than atomic properties of isolated atomic species. Is it possible to compare activation energy with other calculations and why the agreement is rather poor (Tables 17, 18)?**

Response: Yes, there is a substantial body of theoretical research dedicated to the estimation of vacancy formation and self-diffusion properties in rare gas crystals. The majority of this research was conducted in 1970-2000, with calculations of vacancy formation enthalpy, entropy, migration barrier and self-diffusion apparent activation energy. Most of those calculation employ various two-body potentials, from Morse and Lennard-Jones, to more sophisticated semi-empirical functions, like HFD. In many works, Axilrod-Teller-Muto triple-dipole interaction terms are explicitly included, correcting for the neglect of many-body interaction. To derive enthalpies/free energies of vacancy formation, authors also used approaches of various levels, from simple derivation from cohesion energy to more rigorous statistical thermodynamics' treatment.

The results of such calculations lie in a wide interval around the experimental estimations (see the tables below), which are derived from the equilibrium vacancy concentration measurements. Self-consistent statistical method of Karasevitskii et al. with the PES parametrized by LJ potentials yields a severely overestimated value; simpler calculation with Morse potentials, which included the contribution from matrix relaxation, yields similar results. In fact, nearly all calculations overshoot the experimental estimations of vacancy formation enthalpy, as you can see in the table below:

Source	Vacancy formation enthalpy $\Delta H_v, \text{cm}^{-1}$			Comments
	Ar	Kr	Xe	
Burton et al. [3]	666			Lennard-Jones potential + ZPE
	626			Lennard-Jones potential + ZPE + ATM triple dipole terms
Karasevitskii et al. [4]	823			Self-consistent statistical method
Cotterill et al. [5, 6]		919	1323	Morse potentials
Card et al. [7]	572	782	1084	Monte-Carlo MD (ATM triple-dipole terms included)
Simmons et al. [8, 9], Burton et al. [2] and Refs. within	444 605	619 623 601	739 864	Empirical estimations
Present work	530	841	1238	

The old calculations of migration barriers and activation energies quite often do not properly account for the matrix relaxation along the migration path (rigid lattice approximation), which gives wildly inaccurate results. However, more accurate calculations are also present, such as in the work of Glyde et al. and van Vechten et al:

Source	Vacancy migration enthalpy, cm^{-1}			Comments
	Ar	Kr	Xe	
Van Vechten et al. [10]	802	1048	1532	Ballistic model
Glyde et al. [11]	428			LJ potentials, calculation for 60 K. Three results were obtained with different pair potentials
	447			
	469			
Present work	519	744	1074	

Apparent activation energy for self-diffusion, like in our work, is usually calculated by combining the formation enthalpy of single vacancies with its migration enthalpy. The results most usually underestimate experimental values, some even worse than our calculations:

Source	Apparent self-diffusion activation energy Q, cm^{-1}			Comments
	Ar	Kr	Xe	
Burton et al. [3]	1233			Lennard-Jones potential + ZPE
	1157			Lennard-Jones potential + ZPE + triple dipole terms
Glyde et al. [11]	857			LJ potentials, calculation for 60 K. Three different results were obtained with different pair potentials
	894			
	937			
	1450 1330	1680 1815	2590	Experiment
Present work	1037	1571	2301	

As for why there is such large discrepancy between the calculations and the experimental data, there are several points to consider. First, the experimental measurements of vacancy concentration and self-diffusion were taken at higher temperatures, usually near the triple point, while we use the lattice parameter as extrapolated to 0 K. Different lattice parameter (due to the thermal expansion) would, inevitably, produce a discrepancy. One can use more sophisticated models, like the one used in the study of Glyde and Venables [11], which accounts for the temperature dependence of migration

barrier and vacancy formation enthalpy. This model, however, predicts that both vacancy formation and migration enthalpies would decrease upon increase in temperature, and their estimation of Q is even lower than ours.

Second, nearly all calculations consider an ideal monocrystal, while the experimental matrices and even some FSCs are polycrystalline. The existence of grain boundaries and other defects can both facilitate and hamper the self-diffusion. Moreover, while single vacancies contribute the most to self-diffusion, the contribution of other defects may skew the apparent activation energy.

Third, the experimental values themselves vary by a pretty wide margin between different measurements performed by different authors.

In summary, self-diffusion in RG solids is quite a complicated issue, and since it is not the focus of our work, nor our calculations yield remarkable results, it was decided not to do an extensive coverage of this topic.

Changes made: Table 17 was expanded with the data listed above, a short paragraph about comparison with other theoretical calculation of rare gas solids' properties was added.

4. **VTST and CVTST methods of the calculation of rate constant are mentioned but it seems that all the results of the Thesis were considered with STST. If the VTST and CVTST are commented to facilitate the comparison with literature then it could be clearly shown.**

Response: I admit, I have been using the terms TST, CTST, VTST and CVTST rather frivolously. So, in Sec 2.6.5 only three terms are used now: CTST – classical transition state theory; STST – simple transition state theory; and CVTST – classical variational transition state theory, not used within our work and described here only to facilitate comparison with literature data and highlight the fact that choice of the approach used to calculate k_{jump} is largely irrelevant, since the biggest source of discrepancy with the experimental data comes from the inaccuracy in E_a calculation.

In our work CTST was used for O@RG in our 2021 article, while STST was used for all later calculations because the difference these two approaches provide is marginal, especially considering that we failed, for the most part, get within the order of magnitude of experimental values due to the inaccuracy in activation energies. Said inaccuracies in E_a completely overshadow the discrepancy STST provides in comparison to CTST or CVTST.

Changes to Sec. 2.6.5: "... k_{jump} is the jump frequency, which can be derived either from the classical TST (hereinafter CTST): [Eq. 36] or simple TST (STST): [Eq. 37] ... "

Changes made to Sec. 3.6.2: From the beginning: "Here, Eq. 35 for diffusion coefficient was used without alterations. To approximate the jump frequency k_{jump} standard classical transition state theory (CTST) approach was employed for O@RG, while STST was used for all the other A@RG systems. CVTST was not employed, but was described in Literature Review to facilitate the comparison with other theoretical works in Sec. 4.9. Regarding CTST, due to the nature of our system, only vibrational partition functions are to be included in the expression: [Eq 70], where ... " ... Conversely, in STST a simplified expression is used: [Eq 71]"

Changes made to Sec. 4.9: First paragraph, a reference to Literature Review is added: "... They have employed a version of the classical variational transition state theory (CVTST, see Sec. 2.6.5) based on the Markov walk/damped trajectory method ..."

5. The author mentioned part 2.6.4 before Table 14 at page 110 as a source of the data commenting two sets of parameters for RG-RG potentials. However, in this part of Review no exact data on the parameters is given because of numerous potentials described there. It is reasonable to give a direct ref. to modified Aziz's data or else. Similarly, the "gas-phase" term used in Tables 17, 18 sounds ambiguously and could be replaced by a footnote as I proposed for the Table 14 above.

Response: The “gas-phase” label is, indeed, misleading, so it has been changed throughout the Thesis to the direct reference to Aziz et al.

Additional changes to section 3.3.1: “Two sets of energy curves are used: semi-empirical potentials of Aziz and co-workers (HFD form, see Sec 2.6.4, parameters are taken from Refs 115–117) and their empirical modification [119] constructed to reproduce the measured lattice parameters and cohesive energies. Goal and nature of this modification were already described in Section 2.6.1”

6. The basic assumptions of DIM method are given in Part 2.6.3 but with clear assignment neither to DIM, nor to exact publication where they come from (possibly, from Ellison [129]). It creates some inconvenience because different authors used the "DIM" name for different approaches adopted for particular objects. The features of current NR DIM version (including the ones from the basic DIM involved) can be given somewhere together using some additional comments.

Response: References to Ellison’s works have been added to the beginning of section 2.6.3. I admit, there may be a confusion related to the use of “NR DIM” label. In section 2.6.3 original DIM method, written in a basis of three P state functions (related to three possible projections of the orbital momentum of the central atom) is referred to as “NR DIM”. It has the same features and drawbacks as the original DIM. The “NR” prefix was added mainly to contrast with the spin-orbit-coupling-including version, described right after. Yet, from the section 3.3.2 onward, after we describe our modification of the “DIM in the basis of P state functions”, we label the modified version as “NR DIM”.

To alleviate the confusion, I have removed the denomination NR DIM from the Literature Review entirely (now it denotes exclusively the approach we used) and expanded the description of NR DIM features in the section 3.3.2.

7. Misprints are not too numerous but are presented even in Conclusions. Some examples are at:
- Page 55, lines 15, 16 from the bottom.
 - Page 86, line 6 from the top.
 - Page 125, line 8 from the bottom.
 - Page 141, line 3 from the top. Diffusion coefficient D is not used herein.
 - Page 151, lines 9, 11 from the bottom.
 - Page 152, line 10 from the top.
 - Page 152, lines 9, 12 from the bottom.
 - The ref. [33] is wrongly given in Figures 40-42 instead of ref. [15].

Response: All mentioned misprints have been corrected.

Comments from Dr. Ricardo Lambo:

- 1. The introduction claims that the thesis is dedicated to the study of atoms in RG (RG = Ne, Ar, Kr and Xe) matrices (p. 21). While there was work presented on the Sm-Ne interaction potential, there was none on modeling Ne matrices. Since Ne is commonly used in matrix isolation spectroscopy it is probably worth mentioning why it was generally excluded and whether the methodology applied classical matrices (RG = Ar, Kr, Xe) would work for it.**

Response: There was no fundamental reason to exclude Ne matrices from our study, since our methodology can be (and was) applied to them and there is a vast amount of experimental data regarding atomic and molecular spectroscopy in Ne matrices (Refs. [12-14], at the very least). The actual reason is that our calculations of atoms in Ne matrices have been sporadic and incomplete – we have composed the stability diagrams for the ground state (and only the ground state) Sm and C atoms isolated in Ne, but no significant progress was made beyond that. Neither diffusion barriers, nor spectroscopic properties were explored and the projects those calculations were the part of still remain unfinished. After some consideration, it was decided not to include those results in the Thesis, but it is possible that they will be a part of a future study.

Claim regarding Ne matrices was removed from the Introduction.

- 2. A minor point is that the second sentence of conclusion 3 in Chapter 5 is somewhat ambiguous (p. 152). My understanding is that anisotropy generally reduces the migration barrier in the case of B-type anisotropy only. For C-type anisotropy one may observe both increases and decreases in the migration barrier depending on the atom. It is not clear which type of anisotropy is being referred to in the beginning of that paragraph.**

Response: Changes have been made the paragraph 3 of Sec. 5: Interaction anisotropy of both B- and C-types stabilizes this transition state, reducing the migration barrier and facilitating mobility in the former case and having either positive or negative effect in the latter. Non-adiabatic transitions, represented by sudden rotations of the atomic p-orbitals, are needed to maintain the system in its ground electronic state and add shoulder-like features to the energy profiles. After the point of critical phenomenon, IS*(D2h) becomes a stable IS(D2h) site and, consequently, symmetric double-barrier migration energy profiles are produced.

- 3. I have highlighted some issues of grammar, phrasing and spelling in an annotated PDF of the dissertation which I can provide to the candidate.**

Response: All highlighted issues have been corrected. I would like to express my sincere gratitude to the Jury Member for the questions, comments and annotations.

Comments from Prof. Amar Vutha:

Minor points:

- 1. The use of hyperlinks within the document (using the LaTeX package hyperref, for example) would greatly help readers to navigate back and forth between different sections of the thesis and/or the references.**
- 2. There are a number of minor typos in the document. While they do not affect any of the scientific content, they should be easy to fix using a spellchecker. I recommend that the document should be carefully proofread before final submission.**

Response: Hyperlinks were added to the PDF file. The Thesis was proof-read using a spell-checker and a number of spelling and grammatical errors were fixed.

Major points.

- 1. Atoms vs molecules. The last paragraph of Section 4.3.3 mentions that the physics of matrix-isolated P-state atoms is likely to be similar to that of diatomic molecules in matrices. It should be clarified whether this comment refers to homonuclear diatomic molecules (e.g., Mn₂), where the electron density does resemble that of P states in atoms, or whether it is also applicable to polar diatomic molecules (e.g., BaF) where the electron density is quite asymmetrically distributed.**

Response: The comment mentioned was referring to homonuclear molecules. The clarification was added to the last sentence of the last paragraph of Sec. 4.3.3:

“... In a sense, electron density distribution on the (¹P₁)Ba outer p-orbital is similar to the electron density distribution in a **homonuclear** diatomic molecule and as such, many similarities between P state atoms’ and such diatomic molecules’ trapping and diffusion can be expected. It is possible that any of the aforementioned sites, stable for P state atoms might be found for matrix-isolated **homonuclear** diatomic molecules. ...”

Albeit it is, in principle, possible to rewrite our model for P-state atom – RG atom interaction to be applicable to the description of heteronuclear molecules, it would require three potential curves to be calculated beforehand (one for interaction in the plane perpendicular to the interatomic axis, two for interaction along this axis), and I have neither tried to derive such a description from the more rigorous approaches, nor can I say anything about its possible accuracy.

- 2. References and details. I recommend the addition of references in a few places, and slightly clearer explanations of symbols. For example:**
 - a. Paragraph following equation (1) on page 44: it is unclear which of these is related to alpha, and which one to beta, and how. A reference to further details, or a more detailed explanation, would be useful.**

Response: The following changes were implemented:

“[after Eq. 1] ... where R is the interatomic distance, V is the potential energy and α , β are the two parameters, **determined by the two reference calculations: 1) lattice parameter optimization and 2) cohesion energy calculation (E_{coh} and the procedure used to calculate it are defined by the Eq. 42 in Sec. 3.1). Because the dependence on β parameter is nonlinear, this parameter was first determined using an iterative procedure with $\alpha = 1.0$. Then α was then calculated from the ratio of the experimental and calculated E_{coh} values.” This forces the crystal model to reproduce the lattice**

parameters, cohesive energies and relative stabilities of hcp and fcc modifications. [More details on the modified potentials and their influence can be found in Refs. 14, 119.](#)

- b. **Section 2.6.1: for a non-expert like me, it was not easy to understand terms such as «GGA functionals». An explanation of such new terms, wherever they are introduced in the text, would make the thesis useful to readers who are new to the field. Internal references would also help. For example, the discussion in Section 4.1.1 where the «TT model» is referred to could use an internal reference back to Equation (34), where this model is described in more detail.**

Response: The following changes were implemented:

“... results of the Tang-Toennies (TT) model ([see Sec. 2.6.4, Eq. 34](#)). Hyperlinks were added.

“... [More advanced DFT with functionals based on generalized gradient approximations](#) yield anything from weak binding to strong repulsion depending on the functional chosen. ...”

- c. **There are some discussions where the details are hard to follow. For example, on page 119 in last paragraph of Section 4.5.4, we have the sentence «reaffirming the original authors’ interpretation». Original authors of which paper? What was their interpretation? To make the thesis easier to follow and understand, internal references to sections of the thesis where these ideas were first introduced — or external references to the original papers — to should be included for such paragraphs. Again, hyperlinks in the document would be very useful in such situations.**

Response: The Section 4.5 is indeed a bit confusing. The summary of the experimental spectra and the original interpretation, provided by the authors of the experimental papers, was given in the third paragraph at the beginning of Section 4.5. So, the following changes were implemented:

1. New subsections were created – 4.5.1. “Experimental spectra” and 4.5.2 “Vertical transition energies”
2. “Experimental spectra” subsection was moved to the beginning, now it goes right after the first paragraph of the Section 4.5. “Vertical transition energies” follows right after.
3. References and hyperlinks to the section 4.5.1 were added to the section 4.5.3-4.5.5.

3. **«Convex hull». On page 44 paragraph 1, it is indicated that the convex hull method would be described in greater detail in Section 3. (Should that be Chapter 3? Section 3.1? Again, an internal hyperlink would be helpful here). However, the paragraph after Equation (43) in Section 3.1 has just one single line regarding the stability diagram and the convex hull.**

It is possible that the term «convex hull» is used with a particular meaning in theoretical quantum chemistry. But to someone who is not an expert in this field — but quite familiar with the concept of a convex hull from geometry — the use of this term in the thesis is a bit confusing. As this notion of convex hull is repeatedly mentioned in the thesis, it will be useful to readers if the following basic ideas are clearly laid out: a. Exactly what distribution of points in a 2D plane is this convex hull being calculated for? b. Why is the convex hull a useful concept? Instead of just using the plot of $\Delta E(N_{\text{del}})$ versus N_{del} , why bother with the convex hull?

Response: The convex hull concept is used in our work in the same meaning as it is used when discussing Frost diagrams and it is calculated for the $\Delta E(N_{\text{del}})$ versus N_{del} plot. I will provide a brief explanation just below and then list the changes to the Thesis I implemented to clarify the use of the convex hull concept.

The main advantage of $\Delta E(N_{\text{del}})$ is that we can use it to compare different site structures in terms of their tendency to transform into other possible site structures. For that, we assume that a kind of disproportionation process is possible – that 2 sites with the same N_{del} have a way of transforming into a site with $N_{\text{del}}' = (N_{\text{del}} - 1)$ and $N_{\text{del}}'' = (N_{\text{del}} + 1)$, conserving the total numbers of atoms in the system. Then, in the state of thermodynamic equilibrium, only the sites, for which the following is true:

$$2\Delta E(N_{\text{del}}) < \Delta E(N_{\text{del}} + 1) + \Delta E(N_{\text{del}} - 1)$$

will constitute the overwhelming majority of trapping sites within the crystal. Applying this criterion of stability is identical to the procedure of drawing a convex hull on the $\Delta E(N_{\text{del}})$ versus N_{del} plot – all sites for which $\Delta E(N_{\text{del}})$ lies on this plot below the line connecting $\Delta E(N_{\text{del}} + 1)$ and $\Delta E(N_{\text{del}} - 1)$ would satisfy the aforementioned stability criterion. This concept is useful because it gives us the stable trapping sites in the thermodynamic limit, which usually are the most populated sites, observed in the experiments.

Following changes were implemented: the description of the relationship between the $\Delta E(N_{\text{del}})$ convex hull and the search for thermodynamically stable sites, similar to the paragraph above, was added after the 4th paragraph of Sec. 3.1. “Stability diagram” added to the List of Symbols, Abbreviations.

Comment from Prof. Vladimir Feldman:

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.

Response: Yes, it is indeed possible to calculate shifts in HFC constants and the g-tensor components using the trapping site structures calculated using our methodology, and there are numerous experimental works that ESR spectra simulations calculations may supplement, but this indeed was beyond the scope of the present work.

The text was additionally proof-read and numerous misprints have been corrected.

References

1. Krzysztof Rościszewski, Beate Paulus, Peter Fulde, and Hermann Stoll. Ab initio calculation of ground-state properties of rare-gas crystals. Phys. Rev. B 60, 7905, 1999.
<https://link.aps.org/doi/10.1103/PhysRevB.60.7905>
2. A. Berning, M. Schweizer, H.-J. Werner, P. J. Knowles, and P. Palmieri, Mol. Phys. 98, 1823 (2000).
<https://www.tandfonline.com/doi/abs/10.1080/00268970009483386>
3. J. J. Burton. Many-Body Contribution to Self-Diffusion in Rare-Gas Solids. Phys. Rev. 182, 885, 1969.
<https://journals.aps.org/pr/abstract/10.1103/PhysRev.182.885>

4. A. I. Karasevskii and V. V. Lubashenko. Thermodynamics and microstructure of vacancies in rare gas crystals at high temperature. *Low Temp. Phys.* **33**, 578, 2007.
[doi: 10.1063/1.2755184](https://doi.org/10.1063/1.2755184)
5. R.M.J. Cotterill, M. Doyama. Formation energies of vacancies and interstitials in solid krypton. *Phys. Lett. A*, **25**, 35-36, 1967.
<https://www.sciencedirect.com/science/article/abs/pii/0375960167903246>
6. M. Doyama, R. M. J. Cotterill. Formation Energies of a Vacancy and an Interstitial in Solid Xenon. *Phys. Rev. B* **1**, 832, 1970.
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.1.832>
7. D.N. Card, P.W.M. Jacobs. Monte Carlo calculations on rare-gas crystals, *Mol. Phys.* **34**:1, 1-19, 1977.
<https://www.tandfonline.com/doi/abs/10.1080/00268977700101491>
8. P. R. Granfors, A. T. Macrander, R. O. Simmons. Crystalline xenon: Lattice parameters, thermal expansion, thermal vacancies, and equation of state. *Phys. Rev. B* **24**, 4753, 1981.
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.24.4753>
9. R. O. Simmons Defects in noble gas crystals. *Materials Chemistry and Physics.* **50**, 124-132, 1997.
<https://www.sciencedirect.com/science/article/abs/pii/S0254058497802490>
10. J. A. Van Vechten. Simple ballistic model for vacancy migration. *Phys. Rev. B*, **12**, 1247-1251, 1975.
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.12.1247>
11. H.R. Glyde, J.A. Venables. The vacancy concentration and diffusion in rare gas solids. *J. Phys. Chem. Solids.* **29**, 1093-1098, 1968.
<https://www.sciencedirect.com/science/article/abs/pii/0022369768902011>
12. Yu. A. Dmitriev and N. P. Benetis. Trapping mechanism and sites of H and D atoms in solid Ne. *Low Temperature Physics*, **45**(6):663–675, 2019.
13. Stefano Ossicini, Frank Forstmann. Matrix trapping site for H atoms in solid Ne and Ar. *Chemical Physics*, **66**, 333-337, 1982.
14. R. Lambo, C.-Y. Xu, S. T. Pratt, H. Xu, J. C. Zappala, K. G. Bailey, Z.-T. Lu, P. Mueller, T. P. O'Connor, B. B. Kamorzin, D. S. Bezrukov, Y.-Q. Xie, A. A. Buchachenko, J. T. Singh. High-resolution spectroscopy of neutral Yb atoms in a solid Ne matrix. *Phys. Rev. A* **104**, 062809, 2021