Here are the answers to the referee's report. We thank the referee for their comments.

Please find enclosed the revised version of our manuscript, modified by the comments. All the points have their respective answers. Our methodology is the following: paragraph in yellow corresponds to the comments, in green our answers, and in blue the corrected text.

Comments from Reviewer 2
Manuscript ID: molecules-1863819-peer-review-v1.pdf
Title: Molecular Dynamics study of structural and transport properties of silver iodide using effective charges.
The current form's presentation of methods and scientific results is satisfactory for publication in the Molecules journal. The minor and significant drawbacks to be addressed can be specified as follows:

1. Abstract. "The total number of temporal (…)". This sentence should be removed. Too much detail about the calculations.

The abstract has been rewritten:

> The superionic conductor, solid state, and body-centered cubic structure, silver iodide at room temperature, has been studied by molecular dynamics simulations. The calculated results using a pairwise Coulomb-Buckingham potential, zero pressure on the sample, a semi-rigid model system of 1000 Ag and 1000 I ions, (NVE) as a statistical ensemble, and an effective charge of Z = 0.63 for the pairs Ag−Ag and I−I, we found to be consistent with experimental data and one study using Z = 0.60, different potential, and simulation software. For the pair Ag−I there is a discrepancy due to the high iodide ion diffusion. The dynamic transport properties (velocity autocorrelation function) results indicated a typical behavior reported by other authors, using different potentials in their DM simulations for iodine and silver ions.

(pag. 1, lines 1−9.)

2. Fig. 1. (i) Panel (a) Repeated "(a)". (ii) "Ag" is bolded in contrary to "I". Why?

The pair of errors in Fig 1 were corrected:

(i) Panel(a) label "(a)" was deleted.

(ii) The curves were corrected. When plotted, the data of the respective curves of the Ag-I, Ag-Ag, and II pairs were not in the same order.

(pag. 4, first figures.)

3. Fig. 1, figure captions. For Z = |0.60| or |0.63| ---> For Z = |0.63|.

The caption was corrected to Z = |0.63|.

(pag. 4, first figures.)

4. Fig. 1. A strange sequence of curves- panel (a) Ag-Ag, Ag-I, and I-I, but panel (b) Ag-Ag, I-I, and Ag-I. Why?

The strange sequence is mainly due to the fact that the data table for the Ag-I, Ag-Ag, and I-I pairs did not have the same sequence. For example, for Figure 1a, the sequence was Ag-I,Ag-Ag, and I-I; for Figure 1b it was Ag-I, Ag-Ag, and I-I.

(pag. 4, first figures.)

5. Why do the authors analyze such close values of Z, i.e. |0.60| or |0.63|? Why not, for example, |0.53|?

The choice of 0.63 is due to a reported work in $RbAg_4I_5$ where the best value for Z was 0.63, which fit very well with the reported experimental data. However, it can be done with the suggested value.

6. Fig. 3, figure captions. Please add the information that the red and black lines coincide.

To clarify the PDF description a paragraph has been written

In the schematic illustration of PDF, the line broadens due to thermal vibrations, showing the "liquid-like" motion of Ag and I ions in AgI [33]: PDF value oscillates about 1 until gradually approaching 1 [34,35] [see dotted line in Figure 2(a)]. The magnitude of the oscillations shows that this system has a lower density due to the diffusion of silver ions. This behavior is consistent for $Z_{Ag,Ag}$ = |0.60| and $Z_{Ag,Ag}$ = |0.63|. However, for $Z_{Ag,Ag}$ = |1.00|, the PDF does not tend to be one, or the AgI density has a higher density. In other words, there is no diffusion of silver ions. The coordination number $N_{ij}(r)$ (proportional to the PDF integral) is the area under the corresponding curve, therefore, for $Z_{Ag,Ag}$ = |0.60|, $N_{Ag–Ag}$ = 7; $Z_{Ag,Ag}$ = |0.63|, $N_{Ag–Ag}$ = 7 and $Z_{Ag,Ag}$ = |1.00|, $N_{Ag–Ag}$ = 7. Figure 2(b) shows the respective results.

(pag. 4, lines 124−133)

The information required has been written

The blue line shows the similar behavior of PDF for the Ag–Ag pair, i.e., the I-ion does not diffuse. Ions with values Z = 1.00, 0.63, and 0.60 occupy the same volume to calculate $g(r)$ [36], the coincidence of the black and red lines is due to the slight difference in Z, of about 5% between 0.63 and 0.60.

(pag. 5, lines 142−146.)

7. Tabs. 3 and 4. The obtained results are confusing. I-I and Ag-Ag: high agreement compared to [1] as opposed to [16] and [21]. Ag-I: low agreement compared to [1] as opposed to [16]!!!

Table 3 has a mistake for the value of the Ag-Ag pair in our work. There are two values instead of one. This error was corrected. Tables 2, 3, and 4 are discussed in a new paragraph to avoid confusion.

Comparing Tables 2, 3, and 4, our results for the pairs Ag-Ag and I-I are according to the experimental data [1] and are similar to Ref. [16]. For the pair Ag-I there is a discrepancy; the reason is the high iodide ion diffusion.

(pag. 6, line 160−162.)

Additional references

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