We thank the reviewers for their time and their comments. All comments have been addressed below and in the manuscript. If there are further revisions requested, we will be happy to incorporate them.

Reviewer #1: In this paper, Ab initio molecular dynamics (AIMD) simulations were performed to evaluate thermophysical properties of ten compositions of LiF-NaF-KF (FLiNaK) molten salts at 5 temperatures. The calculated values are validated using the experimental data where available. The AIMD data reported for eutectic as well as non-eutectic FLiNaK compositions is of importance to reactor engineers, designers, and other scientific community.

I recommend accepting the manuscript for publication in Journal of Nuclear Materials after minor revisions. For revision, I have following comments:

1. The authors mentioned uncertainties for calculated values of densities in text. It would also be good to show that in Figure 5. Similarly, experimental uncertainties are reported in text, which should also be included in Figure 5.

Figure 5 has been regenerated with error bars included in both Fig5a and Fig5b. Discussion indicating the overlap of error bars and the nature of the errors has been included.

2. In Section 3.3. while discussing heat capacity, authors mentioned "Compared to the reported literature value, this work underpredicts the heat capacity by 13.2%, but is neglecting the electronic contribution to the heat capacity, which, if included, would decrease the discrepancy".  
Can authors add a reference where it is shown that including electronic contribution has resulted in better prediction of heat capacity values?  
  
Heat capacity is a contribution of the phonon and electronic contributions. Inclusion of the electronic heat capacity in the methods outlined will always increase the heat capacity of the system, as it is neglected otherwise. Depending upon the material system and temperature, it may be negligible. A reference and more discussion has been included.

Reviewer #2: This manuscript presents an ab initio molecular dynamics investigation focusing on the thermophysical properties of the LiF-NaF-KF molten salt system. Properties such as density, thermal expansion, bulk modulus, compressibility, heat capacity, and enthalpy of mixing have been predicted, and the results are in good agreement with experiments.  
  
However, given the proposed application of LiF-NaF-KF eutectic salts as coolant salts in Molten Salt Reactors (MSRs), it is crucial to explore additional properties such as viscosity or thermal conductivity, which are particularly relevant for their use as heat transfer medium. These important properties are however not discussed in the present study, which diminishes the manuscript's value to the molten salt community.  
  
In light of these considerations, the reviewer believes that a revision of this paper should be undertaken. Incorporating an investigation into the viscosity or thermal conductivity of the LiF-NaF-KF molten salt system will significantly enhance the impact of the revised manuscript.

We completely agree with the importance of transport properties such as viscosity and thermal conductivity for the implementation of molten salts. However, this manuscript was intended to be a thorough analysis of composition and temperature to obtain the thermophysical properties of FLiNaK salts. Recent work that was just published in JNM (https://doi.org/10.1016/j.jnucmat.2023.154601) has rigorously analyzed how transport properties should be calculated using AIMD methods. The conclusions are that simulations of at least 50 ps, and total time trajectories of up to 300 ps, are required for the appropriate investigation of transport properties. An extension of this work to determine the transport properties would require an additional 3 to 6 months of effort, and we would argue that the effort and data is sufficient to warrant a separate publication, due to the specifics of treating transport properties appropriately. Per discussions with the editor, we believe that this paper is sufficient being restricted to thermophysical properties. If we should adjust the title to appropriately communicate that this investigation only targets thermophysical properties, we will pursue a title change.

A note indicating the importance of transport properties and their difficulty to obtain has been included in the introduction, with appropriate references.