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.

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?  
  
  
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.