We thank the reviewers…

*Reviewer #1: The experimental work included in this report is insufficiently detailed and has neglected to accurately represent the uncertainties in the method. I would recommend divorcing the experimental work from the computational work which is exemplary. When comparing the computational work to literature data it is essential to include the published uncertainties of those literature values, which may improve the perceived performance of your models. Detailed comments are included in an attached PDF as edits to the text and comments.*

Primary comments, and the subsequent response, have been summarized below.

*How is standard error calculated for a simulation that does not depend on experimental values? Is this analogous to a convergence coefficient of some kind?*

*Were any of the materials cleaned before use to remove oxide layers which might dissolve into the molten salt, altering the composition? Furthermore, how was the salt composition measured and confirmed?*

*This equation (Eq. 7) neglects the effect of surface tension which has an appreciable effect of the measured density due to the wire transversing the salt surface. If you are going to neglect this effect you should at least state that, so that you can note that any values you measure are likely lower than reality. Ideally, you would measure the surface tension and correct for it.*

*Was only one weight measurement made? Or did you make a series of measurements over time to ensure the system was at equilibrium without volatilization or other thermally induced motion in the system.*

*Using a figure (fig 4) to compare to one data point from literature seems questionable. It would seem more useful to compare the model data to the literature data at the pressure at which it was measured and give a % difference value for each model method.*

*It seems important to note what the uncertainty is in the literature data (fig 5) to which you are comparing. If the uncertainty is larger than your deviation from it, your models may be better than previously thought. Show uncertainty for Janz data.*

*For Fig 7, why linear fits? the data clearly is not linear in many of the temperatures.*

*For KCl at 1000 K: Do you mean you assumed for the sake of the model that it was a liquid, because in actuality it would clearly be a solid. The statement here seems to suggest that you determined (aka measured?) that it was still a liquid below its freezing point. If that is the case, you need to provide evidence.*

*For Table 1: Was there no analysis of fit with these equations? Uncertainty analysis is crucial to any experimental effort.*

*Notably absent is any independent measure of concentration of these salt mixtures, discussion of salt preparation procedures, and trace impurity analysis. How can you be sure you are measuring what you think you are measuring if you don't verify your salt compositions.*

*Reviewer #2: This paper reports a combined experimental and theoretical study of the thermophysical properties of LiCl-KCl molten salt system. The authors have performed ab initio molecular dynamics simulations with different methods to incorporate van der Waals interactions, and the results compare favorably with their new experimental measurements. I recommend this paper for publication in Journal of Nuclear Materials after some minor revisions, see comments below:  
  
1) In Fig. 1, the partial radial distribution function plot for K-K pair exhibits multiple maxima. It is not clear if they are all physical or due to the small size of the computational cell used in AIMD simulations.  
  
2) In Fig. 4, AIMD simulations using SCAN functional suggest that the pressure of liquid KCl is almost independent of density, which is clearly unphysical. Such discussions of the origin of this anomaly will be useful.  
  
3) The definition of Cp in Eq. 3 is incorrect. Since Cp is the first derivative of enthalpy with respect to temperature, it is a generally temperature-dependent property. The limit of Cp as temperature tends to zero Kelvin will be different from Cp values at high temperatures.*