We thank the reviewers for their time and their feedback. We believe that all comments have been fully addressed below and are incorporated into the manuscript.

Reviewer #1: The minimum system size and simulation time for computational prediction of molten salts is a topic of debate. The authors have concluded from AIMD simulations that 100 atoms sampled for 300 ps are sufficient to calculate transport properties.  
However, the data suggests that diffusion coefficients differ from experiments, and viscosities start to differ for more complex molten salts.  
  
-I find the conclusions too strongly formulated. A more systematic comparison of system size dependency of heterogeneity of the salts would be needed  
After weakening the conclusion - which could lead others astray thinking that 100 atoms is the newly accepted norm - the article could be accepted.  
If the authors want to sustain the claims, I would prefer to see the results for additional, more complex molten salts, to be included.

The stated conclusions have been altered to soften the claims and reduce the chance of confusion about 100 atoms being a newly accepted norm. The text at the beginning of the conclusions now reads: “This work has shown that a system with 100 atoms has comparable results for the transport properties when compared with a 200 atom system, for these specific salt systems. This work also shows that a minimum time increment of 50 ps should be used for the calculations of transport properties and a total simulation time of 300 ps has reasonable agreement with the literature.”

-In addition, I would suggest the authors make the AIMD trajectories available through SIMTK or some other means.  
It is impossible to assess the quality of the analysis without the information provided. Others would also benefit from access to the trajectories as training sets for alternative forcefield developments.

Our policy has typically been to maintain input files required for regeneration of all data and maintain local storage of certain trajectories and associated outputs. Thus, our data is available upon request. However, we understand the importance of these trajectories and have generated a new project on the open science framework which will link to the DOI of this manuscript, once accepted. Selected trajectories will be made available there, improving data access.   
  
Reviewer #2: Authors investigate the diffusion coefficient, viscosity, and heat capacity of chloride molten salts including KCl, LiCl, KCl-LiCl eutectic, NaCl, MgCl2 and NaCl-MgCl2. AIMD is used to predict these properties directly. Overall the paper is well written, and the research is of interest to the molten salt community. The methods are well explained. The convergence work is especially important and well outlined and takes a long time to do. Therefore, the authors are given credit for taking the effort to do this study.  
  
Results:  
- The authors discuss the need for >50 ps simulations for studying diffusivity. In the past, Bengston used block averaging to average out variations for relatively small/short AIMD trajectory. This should be discussed, as it is slightly different then just taking a long simulation trajectory, or running shorter parallel simulations.

A more in-depth comparison between the methods used by Bengston and our study was added to the discussion. “Another difference is the method used to calculate the diffusion coefficient. In this work, the msd trajectory is used to calculate the diffusion coefficient via Eq. \ref{eq:Einstein} for 6 unique trajectories and then averaged for the final value with the error shown as the standard deviation of those 6 simulations. In Bengston's study, they used a slightly different method to calculate the msd. Their method allowed the shifting of the time origin point. They broke their ~12 ps simulation into 4 blocks where each block had a calculated diffusion coefficient with the number of time origins equaling half the block size \cite{Bengston2014}. They note that the selection of time origins is to ensure equal-length trajectories. Following the calculation of the diffusion coefficient of each block they would then average that for their final diffusion coefficient. We utilized a single time origin and a significantly longer simulation time to ensure that any time-dependent behaviors were captured. The method of Bengston would only capture behaviors which occur on a roughly 4 ps timescale.”

- The authors state that for parallel simulations, the simulations are allowed to evolve differently? Why are there differences in the different simulations, if the parameters are all the same? Do you mean that the positions are initialized differently? Or what is causing the stochasticity?

This is clarified in the text by adding “with unique initial velocity distributions”. Thus, the same positions files with different initial velocities generate unique trajectories.

- It is interesting that your plots are under-predicting the KCl diffusion coefficients, especially compared to bengtsons in Fig. 5. This is attributed to differnces in simulation size, time, and dispersion functionals. According to your work, the approximations you made should lead to more accurate results, but somehow Bengtson's work seems to agree better with experiments. Is this a fluke of error cancellation in DFT approximations?

This question has also been addressed within the manuscript by adding “It is unknown what the exact sources of discrepancy with experiment are. We strongly believe that the methods utilized here are more robust and thorough than those of Bengston, and thus should provide more accurate results. Thus, we would argue that Bengston’s methods overpredicted what the actual DFT-predicted diffusion coefficients are, which led to their results being “more accurate” compared to experiment. “

- The use of the Stokes-Einstein-Sutherland for viscosity is a bit concerning, as there are various assumptions of this model. For example, I don't believe that it works well for highly correlated solvents, which would include molten salts. Therefore, the autocorrelation of the stress tensor is the more common approach. Granted, this is not practical with AIMD, but the limitations of the viscosity calculation method should be discussed. This is maybe why it maybe works okay for KCl but not as well for LiCl.

We agree that the SES model may not hold for molten salts, and we hope to be able to provide an answer to this very question in the coming years. The introduction now includes the assumptions made with this model for viscosity: “This method holds a few assumptions in this case. First, the particles move independently from each other, second that the particles have the same mean kinetic energy as gas molecules at the same temperature. This holds true for both dissolved molecules and particles of greater dimension \cite{Miller1924}. The last assumption made is that the spherical particles are moving in the medium that contains proportionately small molecules \cite{Miller1924}.”

In the results for LiCl viscosity, it was addressed that is highly correlated in nature, contradicting some of the assumptions that could lead to observed discrepancies: “Another point to consider is that the method used for the calculation of the viscosity has underlining assumptions and one of the reasons that the viscosity could differ more with LiCl is that this is a highly correlated solvent which means that some of the assumptions discussed in Section 1 won't be as applicable. This could be a cause for the discrepancy observed for LiCl.”

- For the outlook, you mainly say that "AIMD can be used to calculate valid transport properties". Certainly, this is valuable, but it also seems there are other meaningful points that can be made. For example, the convergence tests I think are quite a bit more extensive than most studies and sheds some light on what is necessary to use AIMD consistently. My recommendation is to highlight some of these key learnings/guidelines that would be impactful for the community to highlight the impact of the paper.

This has been addressed by adding a statement addressing the convergence testing in the Outlook section. “This work has conducted extensive convergence testing to determine the minimum simulation size of 100 atoms and simulation length of 50 ps increments is needed for the reliable calculation of the molten salt transport properties”