

Review of: "Dynamic structure factors and equation of state of fluid iron under Earth's core condition"

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Potential competing interests: No potential competing interests to declare.

The present manuscript calculates the static structure factors, ion-ion dynamic structure factors, and EOS of liquid Fe under the Earth's core conditions by ab initio molecular dynamics simulations. Numerical results of the static structure factor and the radial distribution function of liquid Fe are presented, and a discussion is provided. The work presented seems to be interesting and has a real-world application in the recent trend of research. However, still, the present work needs a major revision before coming to a final decision. My comments and suggestions are as follows:

1. The first paragraph of the Introduction should be revised in terms of robust motivation by bearing in mind its aim, objective, and application.
2. Introduction: The last paragraph should be revised by discussing section-wise what is done in the present manuscript.
3. The captions of Figures 2 and 5 should be reduced.
4. How many terms (number of particles) are taken to simulate the numerical results in the context of the present solution should be explained.
5. The computational cost of the numerical results should be discussed.
6. Conclusion: The main concluding remarks should be highlighted by using bullet points. Further, the limitations and the future scope of the research need to be discussed.