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.

Seems the author's calculation is carried out by a code following a series of steps. The author should emphasize the novelty that they add to these algorithms.
"The ab initio molecular dynamics calculations are implemented in the plane wave density functional VASP code (Kresse and Furthmüller, 1996; Kresse and Hafner, 1993). In this calculation, projector augmented waves (PAWs) (Blöchl, 1994; Kresse and Joubert, 1999) and the generalized gradient approximation (GGA) in the parameterization of Perdew, Burke, and Ernzerhof (Perdew et al., 1996) are adopted."

"The ion-ion dynamic structure factors were calculated by Eq." missing equation label

In Figure 1, even though the trend looks similar, it shows the results from different conditions: 136 GPa simulation vs. 116.1 GPa experiment. It is hard to estimate the simulation precision in a relative sense". The author should be better to show the results from the exactly same condition.

"Figure 2. The shape of the calculated ion-ion dynamic structure factors was similar to the reported high-pressure inelastic x-ray scattering measurements of liquid Fe (Kuwayama et al., 2020)." The authors claim their simulation matches the inelastic x-ray scattering measurements in (Kuwayama et al., 2020). But it lacks evidence and a quantitative comparison. It is hard to tell.

Figure 5, the plot is not clear. The author should clearly label each line in that plot. It's hard to find which line is from the result of the author vs. the line from experiment data in the literature.

The author only focuses on Fe; I think simulations of more different elements will add to the robustness of the algorithm and make the paper more convincing.