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

Chuntong Li[1]

1 Shanghai Jiaotong University

Potential competing interests: No potential competing interests to declare.

The paper presents interesting work and can be considered for publication.

The equations of state and ion-ion dynamic structural factors of pure iron in the Earth’s outer core are computed by ab initio molecular dynamics. The isentropic profiles of iron in the Earth’s outer core have a 10% higher density, a 7% lower sound velocity, and a nearly identical adiabatic bulk modulus compared to the Preliminary Referent Earth Model.

The manuscript is presenting a new dataset to study liquid iron under Earth's core conditions developed by ab initio calculations. It presents a multivariate polynomial method for accurate equations of state and the direct calculation of pressure- and temperature-dependent thermoelasticity. Compared with the traditional expression for the equation of state, this method has higher transportability and applicability. The two methods for the calculation of sound velocity are verified to be equivalent, and the equation of state method is more appropriate.

However, there is still a need for more improvement in this paper.

1. The authors discuss the light elements in the Earth's outer core but only cite one article on hydrogen. They could improve the comparison of their calculations with previously published simulations with Si, S, C, H, and other elements doping Fe.

2. Clarify the geotherm conditions in section 3.3.

3. More calculation details were needed in section 2.3, including the electronic convergence criteria and the K-point grid. Explain why cells of 128 atoms and 20 ps are used for the factor structure calculations, and only 64 atoms and 6 ps for EoS.

4. There is some missing information in the article that needs to be further supplemented; for example, in eq. (1), please denote the parameter “g” when firstly used.

5. Some of the references are old. It is recommended to use up-to-date references (i.e., from the last five years).

6. Some references should be updated in newly submitted versions, citing references from the past ten years whenever possible.