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Earth's outer core composition constrained by ab initio thermoelasticites of liquid Fe alloys

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The density deficit of the Earth's outer core indicates substantial amounts of light elements (O, Si, S, C, and H) incorporated in the outer core (Birch, 1952; 1964). The chemistry and amount of the light elements have been strongly debated for over 60 years. Ab initio molecular dynamics (AIMD) simulations have been widely applied to investigate several properties of liquid Fe and Fe alloys (e.g., Alfe et al., 2002; 2007; Badro et al, 2014; Ichikawa et al, 2014). Badro et al. (2014) recently reported a likely compositional model being consistent with seismological data. However with applying empirical pressure corrections, the model suggests smaller amount of light elements to reproduce the ICB density jump. In our study, adopting the Ichikawa et al. (2014) technique we determined the equations of state (EoS) of the liquid Fe alloys by means of the AIMD method in the P, T condition widely covering the entire outer core condition without any pressure corrections. From the EoS, densities, adiabatic bulk moduli, and finally P-wave velocities were calculated and compared with the seismological data (PREM) (Dziewonski and Anderson, 1981). After examining alloy systems from binary to quaternary, we could find some optimized compositional models. However, these have almost comparable reproducibility to PREM, suggesting that other observables are required to make further constraints on the outer core composition. If considering the observed large ICB density jump additionally, Fe-Ni-Si-O and Fe-Ni-S-O compositions appear the most likely.

Keywords: Earth's outer core compositional models, Ab initio molecular dynamics simulations, Equation of state of liquid Fe alloys