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A pyrolitic lower mantle with $(Mg,Fe^{3+})(Si,Al^{3+})O_3$ perovskite

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To better understand the Earth's lower mantle (LM), thermodynamic properties (TDPs) of LM minerals with Fe and Al dopant should be illustrated more clearly. We have so far reported the TDPs of Fe-bearing MgO, $MgSiO_3$ perovskite (Pv) and post perovskite. [1-4] We furthermore study the TDPs of Fe- and Al-bearing Pv, where the internally consistent LSDA+U method and the lattice dynamics method are applied. Two spin states, high (HS) and low spin state, two substitution sites, Mg and Si site, and several possible distribution configurations are considered. In the LM pressure range, HS Fe^{3+} substituted at the Mg site with Al^{3+} at the adjacent Si site (Fe-Al pair) is the most stable configuration and tends to distribute homogeneously in LM. Furthermore, negative frequency cannot be observed in the Fe-Al pair-bearing Pv, and Al contributes to middle frequency while Fe mainly to low part due to its heavy mass. This indicates that the Fe-Al pair is vibrationally stable. Incorporation of the pair for geophysically relevant concentrations can increase volume of Pv a little and has marginal effects on the TDPs of Pv except for thermal expansivity and Gruneisen parameter. Simulated densities, adiabatic bulk moduli ,and bulk sound velocities show that a composition close to pyrolite is accountable for the reference Earth model.

References:
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