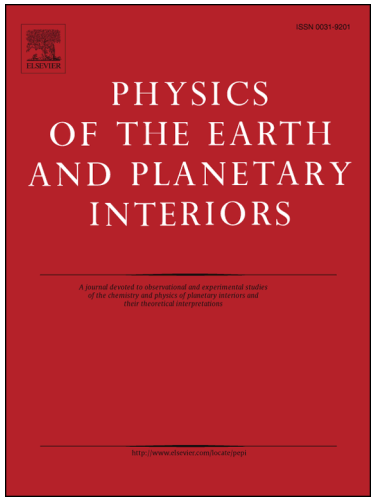

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Iron Valence and Partitioning between Post-Perovskite and Ferropericlase in the Earth's Lowermost Mantle

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Abstract

We use an *ab-initio* based thermodynamic model to study the Fe partitioning ($K_D^{PPv\text{-}Fp}$ = $(Fe/Mg)_{PPv}/(Fe/Mg)_{Fp}$) and Fe^{3+} concentration in the Al-bearing and Al-free post-perovskite - ferropericlase (PPv-Fp) systems, and results are compared to a similar recent model (Xu et al., 2017) for bridgmanite (Bm). Lower mantle (lower oxygen fugacity) and oxidizing experimental conditions (higher oxygen fugacity) are considered. Under lower mantle conditions, we predict that the Fe^{3+} concentration in both Al-free and Al-bearing PPv-Fp systems is very limited, due to the Fe^{3+} and Fe^{0} recombination and Fe^{2+} production ($2Fe^{3+} + Fe^{0} \rightarrow 3Fe^{2+}$). This effect leads to the majority of the total iron in the