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Fe distribution between (post-)perovskite and ferropericlase

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Thermochemical properties in the Earth's deep mantle is still not completely understood. Fe distribution in major lower mantle phases of (post-)perovskite and ferropericlase is of particular importance, because Fe has several substantial effects on density, elasticity, electric and thermal conductivity. Many high-pressure experiments have tackled this issue to date, but the results at the moment seem less converged both experimentally and theoretically. This is originated mostly in multiple complexities related to the valence state, spin state, and incorporation mechanism of Fe. These lead to pressure-induced charge disproportionation reaction and high-to-low spin transition of Fe, all of which need to be considered for understanding the behavior of Fe comprehensively. In this study, we conducted ab initio density functional computations of the Fe distribution in several complex, more realistic situations including multiple phase and also Al-bearing cases. Although we will report details in the presentation, the calculations so far indicate strong effects of the disproportionation of Fe in Pv and spin transition in Fp. They are more remarkable than expected and have opposite contributions. We anticipate that the predicted behaviors should be observed experimentally.

Keywords: lower mantle, Fe distribution, charge disproportionation, spin transition