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On the sharpness of the perovskite/post-perovskite transition in the Earth's mantle

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The phase transition of pure $MgSiO_3$ perovskite (*Pbnm*) to the post-perovskite (*Cmcm*) structure has been reported recently at pressures corresponding to the Earth's lowermost mantle. We use ab initio calculations to assess whether this transition survives, in the Earth, for more realistic mantle compositions containing significant amounts of Al and Fe. We estimate phase coexistence pressures as functions of minor element concentration, and from this we obtain the effects of Al and Fe on the depth and sharpness of the transition. For a pyrolitic mantle composition, with all of the Al partitioned into $MgSiO_3$, we find that Al preferentially partitions into perovskite, and increases the transition pressure by approximately 5 GPa. The transition takes place over a depth range of width 225 km. Fe competes with Al by lowering the transition pressure, so that post-perovskite is likely to exist in the lower mantle; however, the transition is still smooth, and hence not seismically observable.