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Total energy and linear response computations for perovskite and post-perovskite phases in the $MgSiO_3$-$FeSiO_3$-Al_2O_3 system RAZVAN CARACAS, RONALD COHEN, Geophysical Laboratory, Carnegie Institution of Washington — We perform first-principles calculations for the perovskite (pv) and post-perovskite (ppv) phases in the (Mg,Fe,Al)(Si,Al) O_3 system, the dominant chemical system of the Earths lower mantle. We consider different chemical compositions in this system for which we analyze the structural, electronic, elastic and lattice dynamical properties. We use total energy and linear response techniques within LDA and GGA, as implemented in the code ABINIT. We perform calculations in the 0-180 GPa pressure range, in 30GPa increments, to characterize the behavior of these materials over the whole Earths mantle pressure range (up to 137 GPa). We find that the addition of Al in $MgSiO_3$ increases the pv-ppv transition pressure, while the addition of Fe largely decreases this pressure. The pv phase of $FeSiO_3$ is unstable with respect to ppv at all pressures. Fe reduces the electronic gap in both pv and ppv, the Fe-end-member being high-spin and metallic. The pv phase of $FeSiO_3$ is ferromagnetic while the ppv phase is ferromagnetic at low pressures and antiferromagnetic at high pressures. This research is supported by the NSF grant EAR-0310139 and the Carnegie Institution of Washington.

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