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# Ab initio computation on the Fe *L*-edge X-ray emission spectroscopy of Fe-bearing $MgSiO_3$ perovskite

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## Abstract

We systematically investigated the *L*-edge X-ray emission spectroscopy (XES), a 3*d*-to-2*p* transition, of $Fe^{2+}$- and $Fe^{3+}$-bearing $MgSiO_3$ perovskite under high pressure based on the internally consistent LSDA+*U* technique combined with the Slater-transition method. The Fe *L*-edge XES spectra can be used to directly interpolate the distribution of Fe-3*d* electrons including the spin states and coordination environments of iron. Our results show that the spin transition from the high-spin state to low-spin state of $Fe^{2+}$ and $Fe^{3+}$ can be identified easily by the *L*-edge XES technique. The valence state of Fe (2+ or 3+) can be verified by this, since a shift of the first main peak of $Fe^{2+}$ across the spin transition of 2 eV, in good agreement with the experimental value (~1.6 eV), is significantly smaller than that of $Fe^{3+}$ of 4 eV. The width of the *L*-edge XES of $Fe^{3+}$ also depends strongly on the substitution sites (Mg or Si), meaning that its coordination environments might also be distinguishable based on the Fe *L*-edge XES spectra. These strong sensitivities to the Fe's states suggest that the high-resolution Fe *L*-edge XES would be a useful experimental technique to investigate Fe-bearing silicate minerals.

**Keywords:** First-principles method, *L*-edge XES, Fe-bearing $MgSiO_3$ perovskite, high pressures