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Calculated role of aluminum in the incorporation of ferric iron into magnesium silicate perovskite

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ABSTRACT

An atomistic computer simulation study was undertaken to address the role of Al in the substitution of ferric iron into magnesium silicate perovskite, $MgSiO_3$. Calculated substitution and vacancy energies at 0 K were used to consider two different substitution mechanisms: (a) Fe^{3+} and Al independently charge balanced by vacancies or by a similar cation in another site, or (b) Fe^{3+} and Al charge balancing each other. Our results show that it is preferential by 1 to 2 eV for Fe^{3+} to substitute into an Mg site charge balanced by an Al substitution into an Si site. This is increasingly favorable if the Fe^{3+} and Al substitute into adjacent sites. The coupled substitution occurs because it is energetically unfavorable for Al to enter the dodecahedral site.