

## **Incorporation of Fe<sup>3+</sup> into forsterite and wadsleyite**

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### **ABSTRACT**

An atomistic computer simulation study has been undertaken to determine the energies associated with different mechanisms of Fe<sup>3+</sup> incorporation into forsterite and wadsleyite, and to determine why Fe<sup>3+</sup> substitutions into some mantle minerals (such as forsterite) are less favorable than in others. We have also compared our results to previous results obtained for perovskite. In all three phases, the most favorable substitution mechanism is Fe<sup>3+</sup> entering both the Mg and Si sites. In forsterite, the energy of incorporation is 2 eV less favorable than the same mechanism in perovskite and 1 eV less favorable than in wadsleyite. These differences are due to significantly different energies for the substitution of Fe<sup>3+</sup> into the Si site in each of these silicates. This substitution was most favorable in perovskite (octahedral site), less favorable in wadsleyite (tetrahedral site) and least favorable in forsterite (also tetrahedral). The energy difference between forsterite and wadsleyite was found to be the result of structural effects. The linked tetrahedra in wadsleyite are able to distort more easily to accommodate Fe<sup>3+</sup> than the isolated SiO<sub>4</sub> tetrahedra in forsterite.