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Coupled (Li^+, Al^{3+}) substitutions in hydrous forsterite

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Abstract

Atomistic computer simulations methods are used to examine the influence of Li and Al impurities on the uptake of hydrogen in forsterite. We find that Li'_{Mg}+$OH^{\bullet}_{O}$ is more stable at the Mg1 site than at the Mg2 site and that Li^+ increases the ability of forsterite to incorporate hydrogen associated with magnesium sites. When both Al and Li are present, then a complex comprising a bound $Al^{\bullet}_{Mg2}$–Li'_{Mg1} defect is highly stable. When all three impurity components are mixed together, then hydrogen will strongly partition to Si vacancies forming the hydrogarnet defect. Thus the ability of forsterite to incorporate water is likely to be intimately linked to the nuances of defect chemistry, and to concentrations of impurity elements such as Li^+ and Al^{3+}.

Keywords: Aluminum, lithium, forsterite, hydrogen, the Earth's upper mantle