

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A first-principles investigation of hydrous defect and IR frequencies in forsterite: The case for Si vacancies¹ MARC HIRSCHMANN, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, DAVID KOHLSTEDT, ANTHONY WITHERS, University of Minnesota — We investigate charge-balanced hydrous magnesium and silicon defects ($(2\text{H})^X_{Mg}$, $(4\text{H})^X_{Si}$) by first principles. Here we propose two new lowest-energy hydrogen configurations for $(4\text{H})^X_{Si}$. With these new configurations, the distribution of OH-stretching phonon frequencies in Group I ($> 3450 \text{ cm}^{-1}$) are better reproduced. Substitution of silicon with 4 hydrogens gives rise to significant elongation of distances between oxygen ions at the tetrahedron of the silicon vacancy. Our calculations indicate that the correlation between O-O distances and O-H-stretching phonon frequencies, which has been well established for hydrous minerals, does not apply directly to nominally anhydrous minerals and should not be used to determine the identity of the hydrous defects responsible for infrared absorption peaks.

¹This work was supported by NSF under EAR-0757903 and EAR-1019853. The computations were performed at the Minnesota Supercomputing Institute (MSI).

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Date submitted: 19 Nov 2010

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