ELECTRONIC AND MAGNETIC STRUCTURE OF ORTHOFERROSILITE: ELECTRONIC STRUCTURE CALCULATIONS

Zherebetskyy, Danylo[1] Amthauer, Georg[1] Grodzicki, Michael[1]
[1]Fachbereich Materialforschung und Physik, Universität Salzburg, Austria

The electronic and magnetic structure of orthoferrosilite $FeSiO_3$ has been investigated by cluster molecular orbital calculations in local spin density approximation. Under ambient conditions orthoferrosilite crystallizes in the orthorhombic space group *Pbca* with orthorhombic unit-cell parameters a=18.418 Å, b=9.078 Å, c=5.237 Å at room temperature (RT). M1 and M2 octahedra have been earlier described as having an approximate symmetry of D_{4h} and C_{2v} respectively, Sueno et al. (1976). The calculated spin-allowed d-d transitions for Fe^{2+} at the M1 site are 9591 cm^{-1}, 11422 cm^{-1} and 1581 cm^{-1}, 5074 cm^{-1}, 13615 cm^{-1} for Fe^{2+} at the M2 site, compared with the measured absorption peaks of 2350 cm^{-1}, 5400 cm^{-1}, 8500 cm^{-1}, 11000 cm^{-1} and13000 cm^{-1}, Goldman and Rossman (1977, 1979). The quadrupole splittings for Fe^{2+} at the M1 and M2 sites are 3.12 and 2.01 mm/s, respectively, in quantitative agreement with the experimental values of 3.131 and 2.047 mm/s, Lin et al. (1993). A detailed analysis of the theoretical results shows that the M1 and M2 octahedra cannot, even approximately, be described by D_{4h} and C_{2v} symmetry. The difference in the spectroscopic properties between the two iron sites can be correlated with differences in the geometrical structure of the first coordination spheres. The spin structure is derived and explained on the basis of different superexchange intrachain and interchain pathways via edges of the silicon tetrahedra.

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