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Ab initio calculation of the pleochroism of fayalite

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ABSTRACT

Optical properties of fayalite, Fe_2SiO_4, have been obtained from ab initio calculations on the basis of the self-consistent energy band structure. The semi-relativistic, extended linear-augmented plane wave method (ELAPW) was used. Comparison of the calculated polarized optical spectra with experimental absorbance spectra shows satisfactory agreement. This observation allows a semiquantitative interpretation of the origins of the observed d-d transitions. Energy level diagrams for Fe^{2+} ions in the M1 and M2 sites have been constructed using the $X\alpha$-scattered waves cluster method. These calculations quantitatively justify the use of the relationship $\Delta E \propto 1/R^5$, which is often used for the derivation of crystal-field stabilization energies at high pressures.