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Bonding and dynamics of Mg in pyrope: a theoretical investigation

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ABSTRACT

The bonding and dynamics of Mg in pyrope are investigated using density functional theory calculations. The potential which the Mg experiences is highly anisotropic and in one direction is strongly anharmonic. Frequencies corresponding to displacements of a Mg atom along various directions have been obtained from frozen phonon calculations. From the shape of the computed potential, it follows that there is no subsite dodecahedral ordering of the Mg around the 24c site in pyrope.