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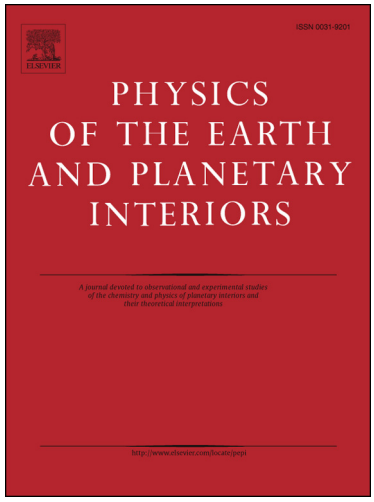

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Structure and elasticity of phlogopite under compression: Geophysical implications

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Abstract:

We investigated the response of the crystal structure, lattice parameters, and unit-cell volume of hydrous layered silicate phlogopite at conditions relevant to subduction zone settings. We have used *first principles* simulation based on density functional theory to calculate the equation of state and full elastic constant tensor. Based on the generalized gradient approximation, the full single crystal elastic constant tensor with monoclinic symmetry shows significant anisotropy with the compressional elastic constants: c_{11} = 181 GPa, c_{22} = 185 GPa, c_{33} = 62 GPa, the shear elastic constants- c_{44} = 14 GPa, c_{55} = 20 GPa, c_{66} = 68

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