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Pressure-induced ferroelastic phase transition in LuLiF₄ compound

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Abstract

© 2015 Taylor & Francis. The behavior of LuLiF₄ sheelite (I41/a, Z = 4) under hydrostatic pressure was investigated by means of first principles calculations. The ferroelastic phase transition from the tetragonal structure of LuLiF₄ to the fergusonite structure (C12/c1, Z = 4) has been found at 10.5 GPa. It has been determined that this is the second-order phase transition.

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Keywords

ab initio calculations, fluorides, high pressure, phase transitions