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Ab-initio investigation of GdLiF4 structure under pressure

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Abstract

This work is devoted to the ab-initio studies of rare-earth double fluoride GdLiF4 under external hydrostatic pressure. Structural and mechanical properties were considered by means of Vienna Ab-initio Simulation Program (VASP). A good agreement of lattice parameters and bulk modulus with experimental data has been obtained. The seven independent elastic constants of I41/a GdLiF4 structure were calculated from stress-strain method. The provideab-initio studies has revealed the instability of GdLiF 4 crystal structure above 10 GPa in accordance with available experimental findings.

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