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Theoretical Calculations for Structural, Elastic and Thermodynamic Properties of MgB_2 under High Pressure

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Abstract: We have investigated the structural and elastic properties of MgB_2 under high pressures using the full-potential linearized muffin-tin orbital (FP-LMTO) scheme within the generalized gradient approximation correction (GGA) in the frame of density functional theory. The calculated pressure dependence of the normalized volume is in excellent agreement with the experimental results. At the same time the elastic constants and acoustic anisotropy as a function of applied pressure are presented. Through the quasi-harmonic Debye model, we also investigate the thermodynamic properties of MgB_2.

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Key words: elastic constants, thermodynamic properties, full-potential linearized muffin-tin orbital, MgB_2

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