Linear Combinations of Gaussian Type Orbitals Calculation of the Metallization Pressure for Lithium Fluoride*

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The Linear Combinations of Gaussian Type Orbitals – Fitting Function (LCGTO-FF) method is used to calculate the zero-temperature isotherm of crystalline lithium fluoride (LiF) to pressures greater than 700 Mbar and to determine the metallization pressure of LiF. The calculations are carried out within the local-density (LDA) and generalized-gradient (GGA) approximations to density functional theory (DFT) for two distinct crystal structures, the NaCl structure (observed at ambient conditions) and the CsCl structure (predicted to appear under pressure at elevated temperatures). The results obtained here are compared with previous calculations and experiment.

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