物理

高温高压下LiD热力学性质的密度泛函理论研究

段涛[1]; 雷洁红[2]; 唐永建[1]

1.西南科技大学极端条件物质特性实验室，四川绵阳621010 2.西华师范大学理论物理研究所，四川南充637002

摘要　采用MS中CASTEP模块中的密度泛函理论方法，计算晶体的能量随体积变化的关系（E-V曲线），运用准谐振子Debye模型研究了压力0~100 GPa、温度0~2 000 K下的晶体LiD的热力学性质，包括热膨胀系数α随温度和压强的变化关系、体弹模量B_0随温度的变化、热容C_v与温度和压强的关系。预测了LiD晶体在高温、高压下的热力学性质。

关键词　密度泛函理论　热力学性质　LiD晶体

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▸本文作者相关文章
· 段涛
· 雷洁红
· 唐永建

Density Function Theory of Thermodynamic Properties for LiD Crystal Under High Temperature and Pressure

DUAN Tao[1]; LEI Jie-hong[2]; TANG Yong-jian[1]

1.Laboratory for Extreme Condition Matter Properties, Southwest University of Science and Technology, Mianyang 621010, China; 2.Institute of Theoretical Physics, West China Normal University, Nanchong 637002, China

Abstract　Density function theory was presented in the CASTEP to calculate the relation between the energy and volume of LiD. The thermodynamic properties of LiD were studied for pressure up to 100 GPa and temperature up to 2 000 K, including the dependences of the thermal expansion coefficient α with pressure and temperature, the variation of the bulk modulus B_0 on temperature, and the dependences of the heat capacity C_v on pressure and temperature. The thermodynamic properties of LiD under high pressure and temperature were predicted.

Key words　density　function　theory　thermodynamic　property　LiD　crystal

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