Elastic and Thermal Properties of Orthorhombic and Tetragonal Phases of $Cu_2ZnSiSe_4$ by First Principles Calculations

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In this paper, based on density functional theory (DFT), the structural, elastic and thermal properties of different structures of the quaternary compound $Cu_2ZnSiSe_4$ were studied theoretically. The structural parameters are found to be in good agreement with experimental results. The independent elastic constants are calculated and analyzed, the results show that the structures have mechanical stability. The bulk modulus, Poisson's ratio, and universal anisotropy index of $Cu_2ZnSiSe_4$ are obtained in detail. In order to accurately describe the thermodynamic properties of $Cu_2ZnSiSe_4$, the parameters of Debye temperature, thermal expansion coefficient, heat capacity C_v and C_p were analyzed under different pressures and temperatures.

Keywords: $Cu_2ZnSiSe_4$, density function theory, elastic, thermal.

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