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Thermodynamic and thermoelastic properties of wurtzite-ZnS by density functional theory

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Abstract

In the present paper, we provide a detailed theoretical investigation on fundamental thermodynamic, thermomechanical, and electronic properties of wurtzite ZnS between 0–20 GPa and 0–2000 K, obtained by ab initio density functional theory and the B3LYP functional. Several properties, such as phonon dispersion relations, elastic and piezoelectric constants, and thermodynamic and thermoelastic behaviors were calculated and reported. The analysis of the data via volume-integrated third-order Birch-Murnaghan fitting resulted in $K_0 = 72.17(4)$ GPa, $K' = 3.87(1)$, and $V_0 = 85.781(1)$ Å^3 at $T = 0$ K. The Born criteria for the mechanical stability of the mineral phase showed that wurtzite is unstable above about 19 GPa in static conditions. We calculated a direct bandgap for wz-ZnS of 4.86 eV at zero compression, which became an indirect one by increasing pressure above 17 GPa. The results are in good agreement with the experimental and theoretical ones reported in the literature, and further extend the knowledge of an important zinc sulfide phase, for both geological and industrial applications.

Keywords: Wurtzite ZnS, thermodynamic properties, elastic properties, electronic properties, density functional theory, quasi-harmonic approximation