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Density functional investigation of the thermo-physical and thermo-chemical properties of $2M_1$ muscovite

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Abstract

In the present study, we computed the thermo-chemical and thermo-physical properties of the $2M_1$ polytype of muscovite in the 0–10 GPa and 0–900 K ranges, using the hybrid DFT/B3LYP-D* density functional, corrected to take into account dispersive forces, and by using the quasi-harmonic approximation. The bulk modulus K_{T0} of muscovite, its first derivative K', and the unit-cell volume at zero pressure V_0 at 298.15 K, calculated using a third-order Birch-Murnaghan equation of state, were $K_{T0} = 59.93$ GPa, $K' = 7.84$, and $V_0 = 940.6$ Å^3. Our theoretical data are in good agreement with previous experimental results obtained by X-ray diffraction. Thermal bulk moduli, K_T, thermal expansion coefficients, α_T, and heat capacity at different *P-T* conditions are given, which could be useful in both geophysical and technological applications. The results of this kind of analysis can be used in the study of the thermodynamic properties of solid phases at physical conditions that are difficult to obtain during experimental procedures, especially under controlled high pressures and temperatures.

Keywords: DFT, quasi-harmonic approximation, muscovite, phonons, thermal equation of state, thermochemistry