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FP-LAPW investigation of mechanical and thermodynamic properties of X_2O (X = Na and K) under pressure and temperature effects

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ABSTRACT

In this paper the ground-state structural, elastic and thermodynamic properties of alkali-metal oxides X_2O (X = Na and K) binary compounds at different pressures and temperatures are investigated by using full-potential augmented plane wave plus local orbitals method (FP-LAPW) within density functional theory, using generalized gradient approximation (GGA). The calculated results are in excellent agreement with the available experimental data and other theoretical results. The thermodynamic properties of Na_2O and K_2O are predicted by using the quasi-harmonic Debye model. The pressure–volume–temperature (P–V–T) relationship, the variations of the bulk modulus B, heat capacity C_V and C_p with pressure P and temperature T, thermal expansion coefficient α and Debye temperature are obtained systematically in the ranges of 0–80 GPa and 0–1200 K.

1. Introduction

The alkali metal oxides Na_2O, K_2O, Li_2O and Rb_2O crystallizes in the cubic antifluorite (anti-CaF_2-type) structure [1], which exhibits fast ion conduction, a property useful in solid-state batteries [2,3], gas detectors and fuel cells [4,5]. However, despite the role it plays in geosciences and its potential technological utility. From the experimental point of view, Li_2O, Na_2O, K_2O and Rb_2O crystal have been extensively studied experimentally [6–17]. Various researchers have undertaken several theoretical studies of this crystal family. From theoretical point of view, Dovesi et al. [18] calculated the lattice constants and elastic properties of Li_2O, Na_2O and K_2O at zero pressure have been reported by using Hartree–Fock linear combination of atomic orbital method (LCAO-HF). This method (LCAO) is also applied by Cancarevic et al. [19] to study the stability of the alkali metal oxides under pressure. The electronic band structures of these materials at ambient conditions were discussed by Zhuravlev et al. [20]. and Eithiraj and co-workers [21] using the self consistent pseudopotential method (PP) and tight-binding linear muffin-tin orbitals (TB-LMTO), respectively. The Wannier function based LCAO formalism has been reported by Shukla et al. [22] on Li_2O and Na_2O compounds. Moakafi et al. [23] have performed a detailed investigation of structural, electronic and optical properties of alkali metal oxides at normal and under pressure conditions using FP-APW+lo method. S.M. Alay-e-Abbas et al. [24] applied the first-principles study of structural and electronic properties of alkali metal chalcogenides: M_2Ch [M: Li, Na, K, Rb; Ch: O, S, Se, Te].

To the best of our knowledge, there are no earlier theoretical calculations for the elastic and thermodynamic properties under high pressures and temperature for these compounds. It is therefore timely to investigate these properties of Na_2O and K_2O compounds in order to provide reference data for the experimentalist and to complete exciting theoretical works on this fascinating class of materials, using the full-potential augmented plane-wave plus local orbitals (FP-APW+lo) method. The rest of the paper is arranged as follows. In Section 2 we give a brief description of computational methodology employed in this study. Section 3 deals with the results and their discussion. Whereas, in Section 4 we summarize conclusions drawn from our study.

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0030-4026/

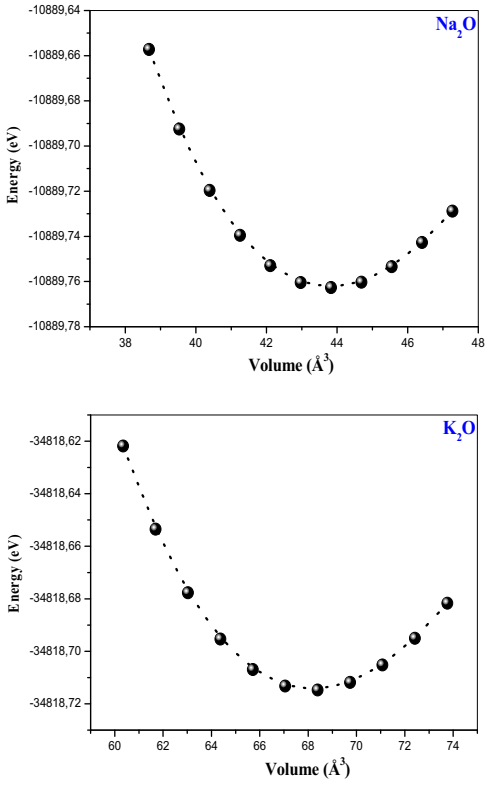

Fig. 1. Total energy as a function of volume for Na_2O and K_2O with GGA calculation.

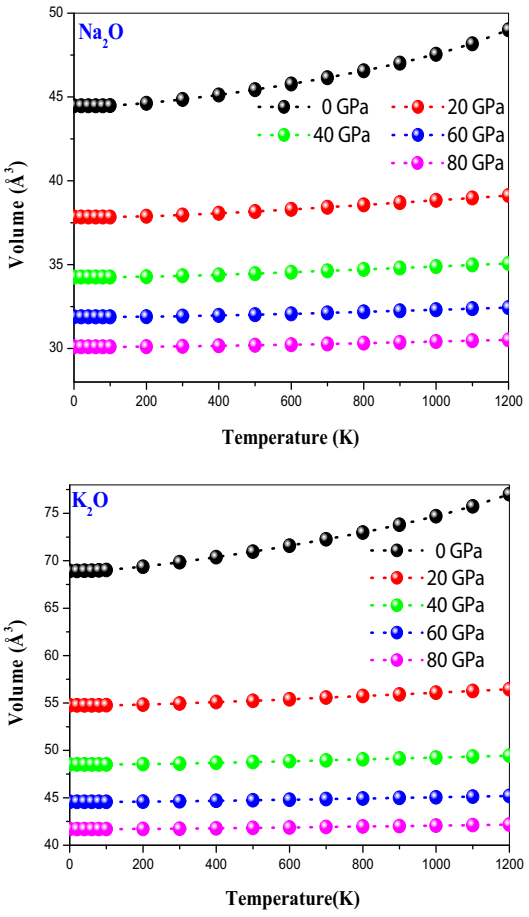

Fig. 2. The variation of the primitive cell volume as a function of temperature at different pressures for Na_2O and K_2O.

2. Computational methods

We have employed the first principles full potential linear augmented plane wave (FP-LAPW) method [25] as implemented in the WIEN2k code [26]. The exchange and correlation effects are described in the framework of the density functional theory [27,28] with the parameterization of Perdew et al. [29]. The unit cell is divided into non overlapping muffin-tin spheres of radius RMTS and an interstitial region, the Kohn-Sham wave functions being expressed in spherical harmonics within spheres and in plane waves in the interstitial regions. To ensure the correctness of our calculations, we have taken $l_{max} = 10$, The R_{MT} values for Na, K and O were chosen to be 2.1, 2.7 and 1.7 atomic units (a.u.). The number of the irreducible Brillouin zone special K-points in the calculations is 35 K-points.

Table 1
Calculated lattice constant a_0 (Å), bulk modulus B_0 (GPa), its first pressure derivatives B'_0 for Na_2O and K_2O, compared to the experimental data and previous theoretical calculations.

	Parameters	Present work	Other calculations	Experimental
Na_2O	a_0	5.595	5.536[b] 5.465[c] 5.45[d] 5.47[d] 5.481[f] 5.484[g] 5.497[h] 5.393[h] 5.559[h] 5.408[m] 5.592[m] 5.398[n] 5.583[n]	5.560[a]
	B_0	45.06	47.10[b] 59.00[c] 62.18[d] 58.63[d] 61.10[f] 57.50[g] 59.1[g] 57.79[m] 47.11[m] 72[q] 69.4[r] 87[s]	–
	B'_0	4.268	4.20[m] 4.71[m]	–
K_2O	a_0	6.484	6.463[b] 6.362[c] 6.430[d] 6.420[d] 6.466[g] 6.466[i] 6.168[i] 6.414[i] 6.195[m] 6.485[m]	6.449[a]
	B_0	26.56	25.4219[d] 33.46[c] 40.74[d] 38.69[d] 34.60[g] 33.4[g] 38.92[m] 26.29[m] 42[q] 68.5[r] 83.5[s]	–
	B'_0	4.335	4.85[m] 4.84[m]	–

[a] Ref. [1].
[b] Ref. [24].
[c] Ref. [21].
[d] Ref. [19].
[f] Ref. [22].
[g] Ref. [18].
[h] Ref. [13].
[i] Ref. [12].
[m] Ref. [23].
[n] Ref. [44].
[q] Ref. [45].
[r] Ref. [46].
[s] Ref. [47].