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Theoretical investigation of the electronic structure, optical, elastic, hardness and thermodynamics properties of jadeite

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ABSTRACT

A detailed theoretical study of the electronic structure, optical, elastic and thermodynamics properties of jadeite have been performed by means of the first principles based on the state-of-the-art of density functional theory within the generalized gradient approximation. The optimized lattice constants and the atomic positions are in good agreement with experimental data. The total density of states and partial density of states of jadeite have been discussed. The energy gap has been calculated along the Γ direction found to be 5.338 eV, which shows that jadeite has wide direct band gap. The optical properties, such as the dielectric function, refractive index, extinction coefficient, reflectivity coefficient, loss function and absorption coefficient for [100] and [001] directions have been described for the first time in the energy range 0–40 eV. The elastic constants, bulk modulus, Young's modulus, anisotropic factor and Poisson's ratio have been calculated. Furthermore, the Vickers hardness and Debye temperature of jadeite have been predicted. The calculated values of all above parameters are compared with the available experimental values.

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1. Introduction

Jadeite ($NaAlSi_2O_6$) has important gemmological implications for identifying and grading the bowlder in Myanmar jadeitite because jadeite has such excellent physical properties including higher hardness, good luster, etc [1,2]. Since ancient times especially in China, jadeite is particularly interesting because it has often been used as jewelry.

According to earlier investigation, jadeite is generally considered to be a high-pressure mineral. Birch et al. [3–5] reported the albite ($NaAlSi_3O_8$) transforms to jadeite+quartz $NaAlSi_3O_8 = NaAlSi_2O_6 + SiO_2$ near the crust-mantle boundary at 2–3 GPa and 1000 °C. Robertson et al. [6] observed that albite and nepheline ($NaAlSiO_4$) reacted to form jadeite $2NaAlSi_3O_8 + NaAlSiO_4 = 3NaAlSi_2O_6 + SiO_2$ in the temperature range 600–1200 °C and under a pressure of 1–2.5 GPa. Ringwood et al. [7] found that nepheline disproportionated into a mixture of jadeite and α-$NaAlO_2$ at 12–25 GPa and 900 °C. These investigations have revealed the method of formation of jadeite in petrology. However, the above synthetic jadeite cannot be used as jewelry, until the 1980s, jadeite as jewelry was synthesized using different techniques [8–13].

First-principles calculations could provide powerful theoretical evidence for corresponding experimental results. However, the theoretical calculation of the physical properties of jadeite has not been researched deeply. Walker et al. [14] had studied the elastic constants tensors of diopside ($CaMgSi_2O_6$) and jadeite at pressures between 0–20 GPa. Wu et al. [15] investigated the bond length, bond angle and distortion variation, and the equation of state (EOS) of jadeite under extern pressure. To the best of our knowledge,

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for jadeite, the studies have mainly focused on synthesized under high temperature–high pressure. However, systematical studies on the electronic structure, elastic and optical properties, Debye temperature, Vicker hardness are still lacking. In this paper, we present a detailed study of these physical properties of jadeite by using the first-principles.

2. Calculation methods

All the calculations presented in this work have been carried out using the CASTEP code [16], which is an implementation of the ultra-soft pseudo-potential plane-wave (UPPW) method, based on the state-of-the-art of density functional theory (DFT). The electronic exchange–correlation interactions are treated with the Perdew–Burke–Ernzerhof for solid in generalized gradient approximation (GGA-PBEsol). [17] In this study, the cutoff energy of plane-wave is 600 eV in order to ensure convergence of the computed structures and energetics. The O-$2s^2 2p^4$, Na-$2s^2 2p^6 3s^1$, Al-$3s^2 3p^1$ and Si-$3s^2 3p^2$ were treated explicitly as valence electrons. The well-known Broyden–Fletcher–Goldfarb–Shanno (BFGS) [18–21] variable-metric minimization algorithm, which provides a fast way of finding the lowest energy structure, is utilized to seek the ground state or geometry optimization. In the Brillouin zone integrations, $8 \times 8 \times 8$ grid of Monkhorst-Pack points has been employed to ensure well convergence of the computed structures and energies. For the calculation of the elastic and optical properties, which usually requires a dense mesh of uniformly distributed *k*-points, the Brillouin zone integration was performed using a $10 \times 10 \times 18$ and $15 \times 15 \times 25$ grid of Monkhorst-Pack points, respectively.

3. Results and discussions

3.1. Structure properties

Jadeite (space group *C2/c*) is composed of parallel sheets of octahedrally coordinated aluminum and eight coordinated sodium polyhedra connected by silicate SiO_4 tetrahedral chains running parallel to the *c*-axis. The crystal structure characteristics of jadeite are shown in Fig. 1. The calculated lattice parameters and atomic positions of jadeite are summarized in Table 1, together with the available experimental data by other scholar for comparison. Compared with the experimental data, our calculated values for lattice constants are $a=9.48016$ Å, $b=8.60274$ Å, $c=5.24955$ Å, respectively. They are in good agreement with the experimental data by other scholar, and the deviations are 0.59%, 0.43% and 0.49%, respectively. The reasons why there is a difference between theoretical values and experimental data as follow: theoretical values have been obtained by GGA method are often higher than experimental data. The result shows and confirms that the method used in this study is reliable thereby the optimized lattice constants can be used for future calculations of other parameters.

3.2. Electronic properties

Fig. 2 shows the calculated band structures along the high symmetry directions in the first Brillouin zone (BZ) of jadeite. The Fermi level (E_f) is chosen to locate at 0 eV and

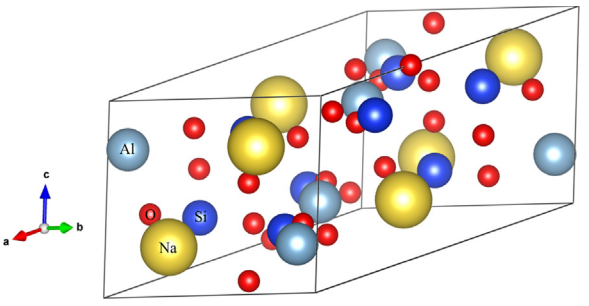

Fig. 1. Crystal structure of jadeite.

Table 1
Lattice parameters and atomic positions of jadeite.

atom	Wyckoff positions	Cal.	Ref. [22]
Na	4*e*	(0,0.3001,0.25)	(0,0.3006,0.25)
Al	4*e*	(0,0.9062,0.25)	(0,0.9061,0.25)
Si	8*f*	(0.2903,0.0937,0.2267)	(0.2906,0.0933,0.2279)
O	8*f*	(0.1099,0.0764,0.1286)	(0.1093,0.0759,0.1280)
O	8*f*	(0.3609,0.2635,0.2926)	(0.3611,0.2634,0.2929)
O	8*f*	(0.3533,0.0067,0.0058)	(0.3537,0.0071,0.0057)
β		107.673°	107.578°
a (Å)		9.48016	9.4242
b (Å)		8.60274	8.5657
c (Å)		5.24955	5.2242

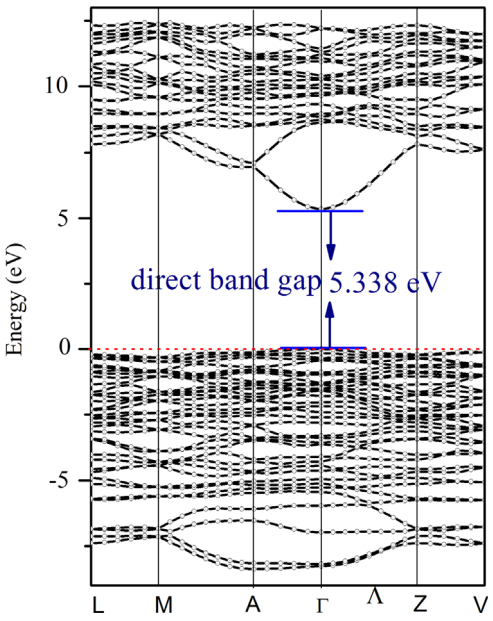

Fig. 2. Band structure of jadeite.

coincides with the top of the valence band. Our calculations show the conduction band minimum (CBM) is located at Γ point. The valence band maximum (VBM) occurs at Γ point, resulting in direct (Γ–Γ) band gap for jadeite. The calculated value of the band gap is found to be equal to 5.338 eV.

In order to get some insight into the bonding nature of jadeite, the density of states (DOS) and partial density of

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