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Transition phase and electronic structure of SrS under pressure from first-principles calculations

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Abstract

The transition phase and the electronic properties of SrS in the NaCl structure (B1) and the CsCl structure (B2) are investigated by *ab initio* plane-wave pseudopotential density functional theory method. The transition pressure obtained is in good agreement with the experimental data and other theoretical results. The pressure and temperature dependences of the band gaps of SrS in the B1 structure are presented. It is found that the effect of pressure on energy gaps is contrary to that of temperature. For SrS in the B2 structure, the pressure dependence of the band gaps is also plotted. The calculated metallization pressure is 63.3 GPa, well consistent with experimental and other theoretical data.

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Keywords: Electronic structure; Generalized gradient approximation; High pressure; SrS

1. Introduction

As one of the alkaline earth chalcogenides, SrS forms an important closed shell ionic compound crystallizing in NaCl structure (B1) at room condition, and is proposed as host materials for device applications, such as multicolor thin-film electroluminescent and magneto-optical devices. It is actively investigated experimentally [1] and theoretically [2–5].

X-ray diffraction experiment [1] showed that, SrS were found to undergo first-order phase transition from NaCl structure to CsCl structure (B2) at 18 GPa and the equations of state (EOS) was obtained up to 35 GPa. Later, Ching et al. [2] theoretically investigated the linear and nonlinear optical responses, band structure, and frequency-dependent dielectric functions. Cortona et al. [3] reported the results for the electronic property and found the transition pressure 23 GPa. Khenata et al. [4] found the pressure structural phase transformation occurred at 18 GPa. More recently, Rached et al. [5] investigated the elastic properties and the volume dependence of energy gap in B1 structure.

The aim of this work is to give a comparative and complementary study of the structural phase transition and electronic properties of SrS from B1 structure to B2

Table 1
Lattice constants (Å), bulk modulus (GPa) and its pressure derivative of SrS in the B1 and B2 structures at zero pressure

		a	B_0	B_0'
B1 structure	Present results	6.024	53.9	4.66
	Exp. [1]	6.024	58.0	
	Others	6.076[a], 5.774[b]	47.0[a], 62.0[b]	4.19[a]
B2 structure	Present results	3.646	50.6	4.50
	Exp. [1]	3.61		
	Others	3.68[a], 3.481[b]	50.0[a], 67.3[b]	3.88[a]

[a]Ref. [4].
[b]Ref. [12].

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Table 2
The calculated pressure (GPa) coefficients of Gibbs free energy (Hartree) for SrS in the B1 and B2 structures, where $G(P) = a + bP + cP^2$

T (K)	Structure	a	b	$c(10^{-5})$
0	B1	−41.31337	0.01179	−4.26455
	B2	−41.29128	0.01048	−3.84938
300	B1	−41.31651	0.01185	−4.33033
	B2	−41.29513	0.01054	−3.91709
600	B1	−41.32536	0.01196	−4.43523
	B2	−41.30505	0.01065	−4.01765
900	B1	−41.33724	0.01208	−4.54927
	B2	−41.31803	0.01076	−4.12692
1200	B1	−41.35118	0.0122	−4.67332
	B2	−41.33306	0.01088	−4.24613

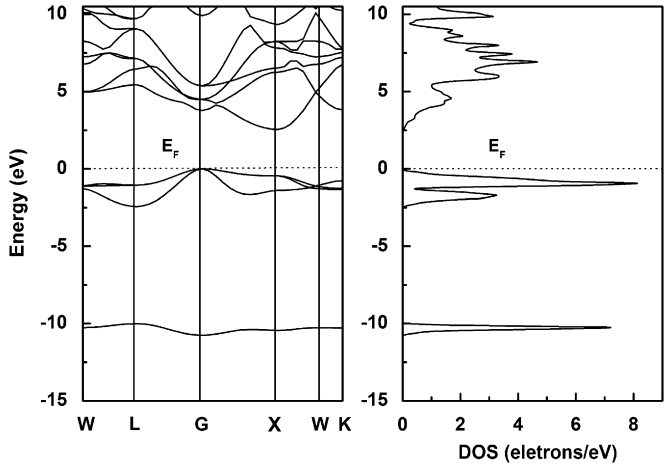

Fig. 1. Band structure and total density of states for the B1 structure SrS at 0 K and 0 GPa.

structure by the plane-wave pseudopotential density functional theory method using the Cambridge Serial Total Energy Package (CASTEP) program [6,7] and the quasi-harmonic Debye model [8]. After a brief description of calculation details, we give a calculation of the ground state properties. The band structures for both B1 and B2 structures are given and compared with those of the available theoretical results.

2. Theoretical methods

In the electronic structure calculations, the ultrasoft pseudopotentials introduced by Vanderbilt [9] have been employed for all the ion–electron interaction, the generalized gradient approximation (GGA) exchange-correlation function [10] is represented by Perdew–Wang (PW) formula. A plane-wave basis set with energy cut-off 600 eV is applied. Pseudo atomic calculations are performed for S $3s^2 3p^4$ and Sr $4s^2 4p^6 5s^2$. For the Brillouin-zone sampling, in calculation of ground state properties, we use the $8 \times 8 \times 8$ Monkhorst–Pack mesh. The $12 \times 12 \times 12$ Monkhorst–Pack mesh is used in the band structure calculation. The self-consistent convergence of the total energy is 10^{-6} eV/atom.

3. Results and discussion

For both the B1 and the B2 structures of SrS, a series of different lattice constant a are set to calculate the total energy E and the corresponding volumes V, then the calculated $E-V$ data are fitted to the natural strain EOS

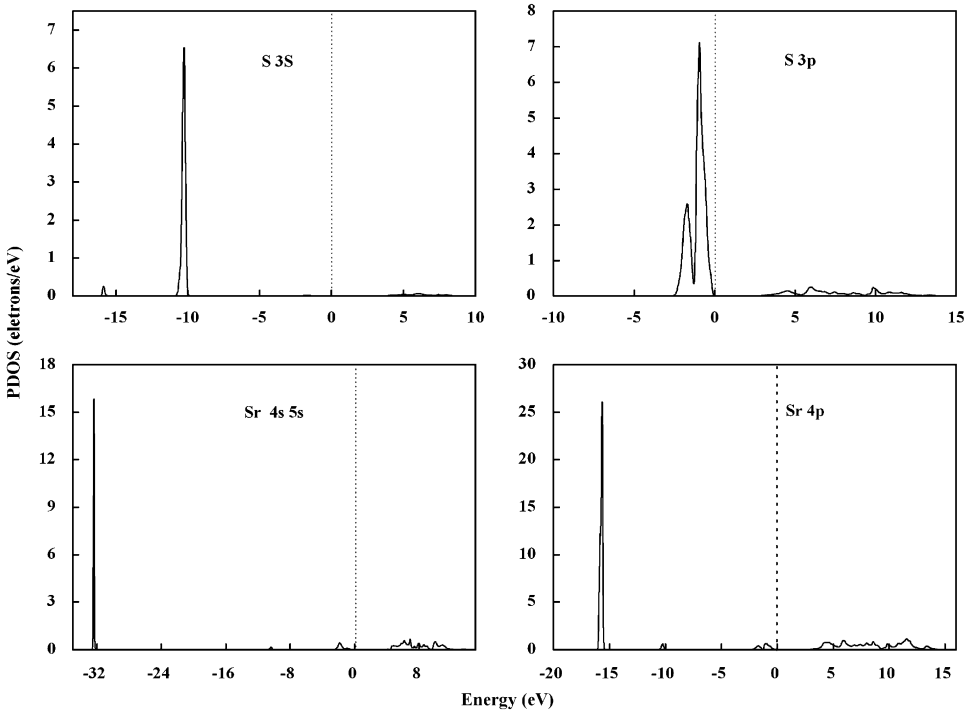

Fig. 2. Partial density of states for the B1 structure SrS at 0 K and 0 GPa.