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Review

# Structural and electronic properties of III–V scandium compounds

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**Abstract**

We present calculations of the structural, and electronic properties of the scandium compounds ScX (X = N, P, As and Sb). They are based on the generalized gradient approximation (GGA) within the density functional theory (DFT), employing the first-principles, full potential-linearized augmented plane wave (FPLAPW) method. Bulk properties, including lattice constants, bulk moduli and derivatives, cohesive energies, and band structure are reported in both NaCl (B1) and CsCl (B2) structures. The transition pressure for the NaCl-type to CsCl-type is calculated to be about 364.32, 245.61, 92.40 and 39.78 GPa for ScN, ScP, ScAs and ScSb, respectively. We show that our results are in agreement with the available experimental data and the first-principles theoretical studies.
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**Contents**



## 1. Introduction

The group-III–V have attracted extensive experimental and theoretical interest because of their technological applications. The question arises, how to extend the studies on the Group III–V in order to have a new class of materials with promising properties that remain too interesting in device application? One possible way is to explore new III–V compounds such as ScN, ScP, ScAs and ScSb.

Only a few theoretical papers and little experimental work have been devoted to the study of structural and electronic properties of this series of scandium compounds.

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The structural properties of ScN have been determined by Takeuchi et al. [1,2] and Stampfl et al. [3,4] using the full potential-linearized augmented plane wave (FPLAPW) method. Using the linear muffin-tin orbitals (LMTO) method, the optoelectronic properties have been calculated by Lambrecht et al. [5] for ScN and ScAs. Recent high-pressure experiments from Hayashi et al. [6] studied ScSb up to 45 GaP at room temperature and a first-order phase transition was reported from the B1 to B2 structure in this compound.

We will concentrate in the present work on the bulk structural properties of scandium compounds (ScN, ScP, ScAs and ScSb). We calculate the ground-state total energy in the B1 and B2 structures using the FPLAPW method, which would complete the existing experimental and theoretical works.

The article is organized as follows: in the next section, we give a description of the ab initio theoretical method that we use to study the high pressure phase. In Results and discussion, we present our results and the comparison with the available experimental and theoretical studies. Finally, we present our conclusions.

## 2. Method of calculation

In this work, we have used the self-consistent FPLAPW method [7] within density functional theory [8,9]. This method has been carried out using the WIEN2 K code [10] and for exchange-correlation potential we have chosen to use the generalized gradient approximation (GGA) [11]. In this code, the unit cell is divided into no overlapping muffin-tin spheres of radius $R_{MT}$ and an interstitial region, where the Kohn–Sham wave functions are expressed in spherical harmonics within spheres and in plan waves in the remaining space of the unit cell.

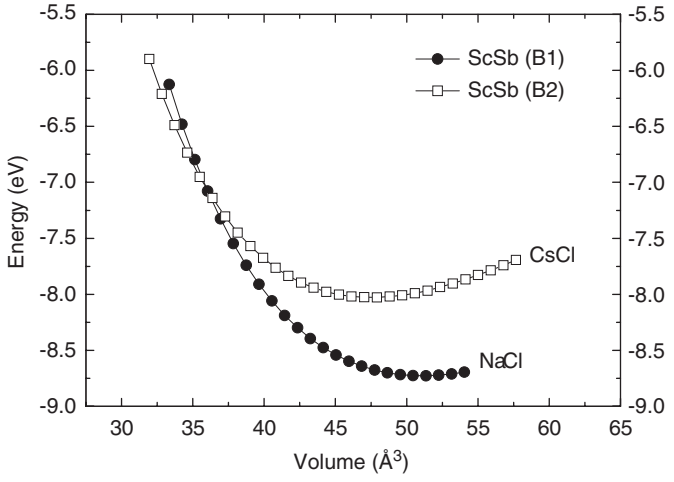


Fig. 1. Energy versus volume curves of the B1 (NaCl) and B2 (CsCl) phases of ScSb.

We use the value 8 for the parameter $R_{MT}K_{max}$ which determines the matrix size, where $K_{max}$ is the PW cut-off and $R_{MT}$ is the muffin-tin radius. Basis functions, charge density, and potential were expanded inside the muffin-tin spheres in spherical harmonic functions with cut-off $l_{max}$, and in Fourier series in the interstitial region. The iteration process was repeated until the calculated total energy of the crystal converged to less than 0.5 mRy/unit cell. A mesh of 30 special $k$-points in NaCl (B1) structure and 35 special $k$-points in CsCl (B2) structure were taken in the irreducible wedge of the Brilloiun zone.

Table 1
Calculated lattice constant $a$, bulk modulus $B$, its pressure derivative $B'$ and cohesive energy $E_{coh}$ at equilibrium volume for NaCl (B1) and CsCl (B2) phases for ScX compounds

| | | Present work | Experiment | Other theoretical works | |
|---|---|---|---|---|---|
| ScN | | | | | |
| B1 | $a$(Å) | 4.520 | | 4.501[a], 4.44[b] | 4.54[d,e], 4.44[d], 4.50[f], 4.42[f] |
| | $B$(GPa) | 201.576 | | 182±40[a] | 201[d,f], 220[d], 218[e], 235[f] |
| | $B'$ | 3.89 | | | 3.31[d] |
| | $E_{coh}$ (eV/cell) | 13.428 | | | 13.69[d],15.14[d] |
| B2 | $a$(Å) | 2.79 | | | 2.81[d] |
| | $B$(GPa) | 178.60 | | | 170[d] |
| | $B'$ | 4.43 | | | 3.47[d] |
| | $E_{coh}$ (eV/cell) | 11.34 | | | 11.58[d] |
| ScP | | | | | |
| B1 | $a$(Å) | 5.323 | | | |
| | $B$ (GPa) | 99.270 | | | |
| | $B'$ | 3.58424 | | | |
| | $E_{coh}$ (eV/cell) | 10.821 | | | |
| B2 | $a$ (Å) | 3.274 | | | |
| | $B$ (GPa) | 101.098 | | | |
| | $B'$ | 3.662 | | | |
| | $E_{coh}$ (eV/cell) | 9.740 | | | |
| ScAs | | | | | |
| B1 | $a$ (Å) | 5.489 | | | |
| | $B$ (GPa) | 91.522 | | | |
| | $B'$ | 3.484 | | | |
| | $E_{coh}$ (eV/cell) | 9.859 | | | |
| B2 | $a$ (Å) | 3.388 | | | |
| | $B$ (GPa) | 87.014 | | | |
| | $B'$ | 4.251 | | | |
| | $E_{coh}$ (eV/cell) | 8.983 | | | |
| ScSb | | | | | |
| B1 | $a$ (Å) | 5.887 | | 5.851[c] | 5.797[g] |
| | $B$ (GPa) | 70.90 | | 58±3[c] | 71.3[g] |
| | $B'$ | 3.47 | | 9.5±0.8[c] | 3.65[g] |
| | $E_{coh}$ (eV/cell) | 8.727 | | | |
| B2 | $a$ (Å) | 3.622 | | 3.36(1)[c] | 3.54[g] |
| | $B$ (GPa) | 69.78 | | | 81[g] |
| | $B'$ | 3.77 | | | 3.70[g] |
| | $E_{coh}$ (eV/cell) | 8.027 | | | |

The results are compared with the experiment and other theoretical works.
[a]Ref. [14].
[b]Ref. [15].
[c]Ref. [6], at room temperature.
[d]Ref. [1], using FPLAPW.
[e]Ref. [13], using FPLAPW.
[f]Ref. [4], using FPLAPW.
[g]Ref. [16], using LDA: PWPP.

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