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Investigation of Scandium-Based III-V Compounds: A Density Functional Examination of Chemical, Electronic, Elastic, and Structural Bonding Properties

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ABSTRACT

The structural, elastic, electronic, and chemical bonding characteristics of scandium-based III-V compounds across crystal structures of zinc-blende, rock-salt, and cesium chloride are examined in this work using density functional theory. We found bulk moduli, elastic constants, lattice parameters, and electronic band structures using WC-GGA and mBJ-WCGGA potentials. The findings show that bulk moduli and lattice constants are inversely correlated. ScN is a semiconductor, according to electronic band structure analysis, whereas the other compounds, depending on the crystal structure, have semimetallic or metallic characteristics. These compounds also exhibit a combination of covalent and ionic bonding. These discoveries deepen our knowledge of these substances and provide important new information about how they might be used in optoelectronics and other technological domains.

Keywords: Scandium III-V compounds, DFT, Electronic band structure, Elastic properties

INTRODUCTION

III-V compounds based on scandium, namely scandium pnictides, are becoming more and more well-known due to their distinct optoelectronic, structural, and electronic characteristics [1]. These materials exhibit a broad range of crystal structures and electronic behaviors, making them promising candidates for novel applications in optoelectronics and electronics[2]. Applications for them in light-emitting diodes (LEDs) are possible, solar cells, high-density optical memory devices, transparent conductors, and laser diodes. Scandium nitride (ScN), one of these compounds, is distinguished by its direct bandgap between 2.1 and 2.4 eV, which makes it a

semiconductor. Also, in contrast to many other conventional semiconductors, it stabilizes in a unique rock-salt crystal structure. This structure produces innovative electronic configurations that support the production of cutting-edge devices. Moreover, ScN exhibits a minimal lattice mismatch with gallium nitride (GaN) and a high melting point exceeding 1500 °C, providing opportunities for high-performance GaN/ScN heterostructures and alloys.Band gaps of other scandium pnictides, such as ScP, ScAs, ScSb, and ScBi, range from 0 to 4 eV. The creation of novel III-V compounds, superlattices, and alloys with unique properties is made easier by this variability[3]. The crystal structures of these materials mainly stabilise in the forms of zinc-blende (B3), cesium chloride (B2), or rock-salt (B1). Although the compounds have not received enough attention for thorough electronic and elastic characterization, they have promise as wide-bandgap semiconductors. We apply density functional theory (DFT), a flexible technique in computational materials science, to gain a deeper understanding of these compounds[4]. It does this by concentrating on electron density instead of wave functions, which simplifies many-body quantum mechanical calculations. High accuracy band gap predictions are made possible by the generalised gradient approximation (GGA) and the modified Becke-Johnson (mBJ) potential model, lattice constant, and elastic constant are made [5].The structural, elastic, electrical, and chemical bonding characteristics of III-V compounds based on scandium in B1, B2, and B3 crystal phases are investigated in this work. We analyse bulk moduli, lattice parameters, and electronic band structures of the compounds using WC-GGA and mBJ-WCGGA potentials.We provide an understanding of the basic characteristics of these compounds by examining band structures, lattice constants, and bulk modulus relationships. This work lays the groundwork for the development of new electronic and optoelectronic devices and encourages further study into scandium-based III-V compounds[6].

METHODOLOGY

The Schrodinger equation can be solved for more complex systems than just one or two electrons by using several approximations, the first of which is the Born-Oppenheimer approximation. Based on the notion that nuclear mass is so much greater than electron mass that nuclei are

Journal of Techno Trainers
Vol.1, Issue.1, (2024)
https://www.technotrainers.net

essentially "fixed" particles, it divides motion of electrons from that of nuclei. Electrons respond instantly to shifts in the nuclei's positions. This formula can be expressed as

$H\square = E\square$

The wave function and Hamiltonian for an atom or molecule are dependent on the nuclei and electrons. We can identify four terms in the Hamiltonian for an atom.

$$H_{atom} = T_n+T_e+V_{ne}+V_{ee},$$

The kinetic energy of the nucleus is represented by Tn, the electrons' kinetic energy (represented by Te), their Coulomb attraction to the nucleus (represented by Vne), and their Coulomb repulsion to one another (represented by V ee). Density functional theory allows for the study of all properties related to excited states. Density functional theory (DFT) comes in two flavours: time dependent and time independent. The work of Hohen-berg and Kohn serves as the foundation for the current formulation of density functional theory (DFT).Hohenberg and Kohn's two fundamental theorems laid the groundwork for modern density functional theory.The Hohenberg-Kohn theorem does not provide a way to calculate the ground state density itself, but it does show that the ground state density can be used to compute system properties. The way to this is through the Kohn-Sham. To derive these equations, take into consideration the ground state energy, which is given as a function of the charge density.The exchange correlation energy at a given point in a material with a slowly varying charge density can be thought of as being the same as that of a locally uniform electron gas with the same charge density. This is the basic tenet of the local density approximation (LDA). The Kohn-Sham equations can be solved within the DFT framework with a high degree of accuracy and efficiency by using the FP-LAPW method. Through this process, muffin-tin spheres (MT) are produced, which evenly surround every atomic and interstitial area in the crystal unit cell. By using this technique, the potential and associated charge density of each muffin-tin sphere are expanded into Fourier series in the interstitial regions and radial wave-functions times spherical harmonics.

$$V(r)=\left\{\sum_{lm} V_{lm}(r)Y_{lm}(r)\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(a)\right.$$

Journal of Techno Trainers
Vol.1, Issue.1, (2024)
https://www.technotrainers.net

where Eqs. 1(a) and 1(b) represent the atomic sphere's interior and exterior, respectively. The wave function's maximal value, l, is spherically symmetric and expands to lmax = 10 inside the sphere, but it remains constant outside.

RESULTS

Fig. 1 displays the prototype optimisation curve for the ScN compound. This graph unequivocally demonstrates that unit cell energy falls as unit cell volume rises. At a specific volume, known as the ground state volume, it reaches its minimum value. The system becomes unstable as a result of it rising along with the unit cell's volume.

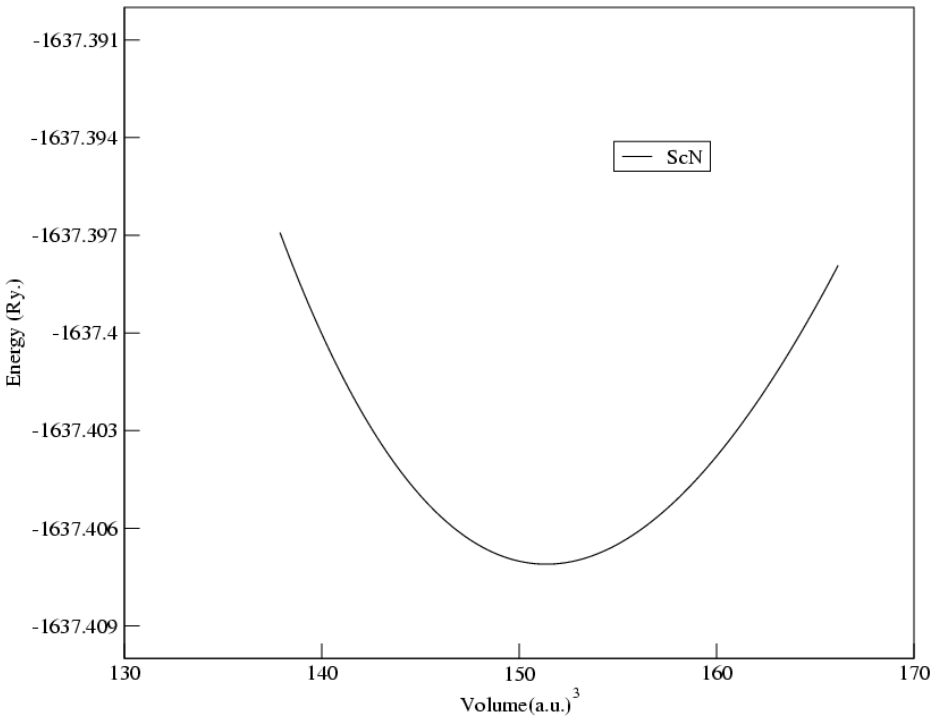

Fig 1. Optimization plot of ScN

Tables 4.4, 4.5, and 4.6 provide the elastic constants for ScB compounds in the B1, B2, and B3 phases, respectively. To the best of our knowledge, no experimental value has been published for the ScB compounds' elastic constants. It can be observed that the unidirectional elastic constant C11 is much larger than C44 when compression is examined along the principal crystallographic directions. This implies that pure shear deformation is less likely to occur in these materials than

Journal of Techno Trainers
Vol.1, Issue.1, (2024)
https://www.technotrainers.net

unidirectional compression. Certain constraints are imposed on the elastic constants when taking into account the need for mechanical stability in a cubic structure. These requirements are satisfied, with the exception of ScSb and ScBi, suggesting that the compounds are elastically stable. Because of its close relationship to the likelihood of microcrack formation in materials, the concept of crystal elastic anisotropy is important in engineering science. With reference to the current elastic constants, we have calculated the anisotropy factor. is equivalent to 1 for an isotropic material; any value between 0 and 1 denotes anisotropy. The amount of elastic anisotropy in a crystal is indicated by how far it deviates from unity. It is evident from the computed anisotropy values that each compound has an anisotropy factor value that differs from unity, indicating a strong anisotropy. For ScB single-crystals, first-principles calculations are used to estimate the elastic constants Cij. It is crucial to evaluate the moduli that correspond to the polycrystalline species, though, because the prepared materials are usually polycrystalline. We have used the Voigt-Reuss-Hill approximation for this. Voigt and Reuss proposed that the arithmetic mean of the two well-known bounds for monocrystals could be used to approximate the true effective modulus for polycrystals. The moduli for the cubic structure are thus defined as follows: $G_V = \frac{1}{5}\left(C_{11} - C_{12} + 3C_{44}\right)$ (2)

$$G_R = \frac{5C_{44}\left(C_{11} - C_{12}\right)}{4C_{44} + 3\left(C_{11} - C_{12}\right)} \quad (3)$$

$$B_V = B_R = \left(C_{11} + 2C_{12}\right)/3 \quad (4)$$

The shear modulus G is given by:

$$G = (G_v + G_R)/2 \quad (5)$$

The following equations also allow us to predict the Young's modulus, E, and Poisson's ratio, v, which are connected to the bulk modulus B and the shear modulus G.

$$E = \frac{9BG}{3B + G} \quad (6)$$

$$v = \frac{3B - 2G}{2\left(3B + G\right)} \quad (7)$$

Journal of Techno Trainers
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https://www.technotrainers.net

Table 2 also includes the computed values of the aforementioned elastic moduli for polycrystalline ScB compounds. The Young's modulus E is a material's stiffness metric. It indicates how stiff a particular material is when it is higher. We can infer from the current E results that these compounds become less stiff as we move from N to Sb in ScB compounds. Out of all the compounds in this family, the nitride compounds are the stiffest. More information about the bonding force characteristic can be found in Poisson's ratio than in any other elastic property. The lower and upper bounds for central force solids are 0.25 and 0.5, respectively. The interatomic forces are central for some compounds and non-central for others because the computed Poisson's ratio falls between these ranges for some compounds but not for others.Poisson's ratio (v), Cauchy pressure (C12–C44), and Pugh's index of ductility (B/G) are three measurements that help determine whether a material is brittle or ductile[7]. A gauge of ductility is Cauchy's pressure, which is the difference between two specific elastic constants (C12−C44). A positive or negative pressure indicates the material's predicted brittleness or ductility. The (B/G) ratio is an additional ductility indicator. Pugh's ratio indicates that either a high (low) or ductile (brittle) B/G ratio correlates with the properties of the materials. The critical number that distinguishes brittle from ductile materials was found to be 1.75. We can also refer to Frantsevich et al., who distinguish between the brittleness and ductility of a material using Poisson's ratio (v). According to the Frantsevich rule, the critical value of a material is 0.26. The material is brittle if the Poisson's ratio is less than 0.26; otherwise, it behaves ductilely. Based on the previously mentioned criteria, every investigated compound is brittle, except for ScAs and ScSb.

Journal of Techno Trainers
Vol.1, Issue.1, (2024)
https://www.technotrainers.net

Table

Elastic constants Cij (in GPa) for ScB compounds in B1, phase.

Compounds	Present work						
	C_{11}	C_{12}	C_{44}	**E(B1)**	**G(B1)**	**A(B1)**	**B/G(B1)**
ScN	384.55	94.1	156.07	368.6	151.7	1.07	1.42
ScP	225.76	37.36	40.84	156.9	62.18	0.43	1.76
ScAs	207.06	19.66	18.14	124	48.4	0.19	1.94
ScSb	162.08	7.32	-20.31	51.7	18.77	-0.26	3.74
ScBi	230.1	-14.44	-7.74	107.5	44.26	-0.06	1.42

Table 4.5

Elastic constants Cij (in GPa) for ScB compounds in B2phases.

Compounds	Present work						
	C_{11}	C_{12}	C_{44}	**E(B2)**	**G(B2)**	**A(B2)**	**B/G(B2)**
ScN	550.27	23.39	-128.78	80.48	28.1	-0.48	6.98
ScP	142.63	89.02	-54.15	-69.4	-21.7	-2.01	-5.04
ScAs	125.05	77.37	-69.8	-109	-32.3	-2.93	-2.92
ScSb	-23.59	117.72	-74.39	-322	-72.9	1.05	-1.03

ScBi	81.24	54.67	-72	-142	-37.9	-5.42	-1.65

Table 4.6

Elastic constants Cij (in GPa) for ScB compounds in B3phases.

Compounds	Present work						
	C_{11}	C_{12}	C_{44}	**E(B1)**	**G(B1)**	**A(B1)**	**B/G(B1)**
ScN	166.54	142.35	108.69	181.7	70.1	8.98	2.14
ScP	62.81	69.3	53.66	80.56	30.89	-16.54	2.22
ScAs	78.86	53.48	52.42	91	36.53	4.13	1.63
ScSb	43.99	46.54	29.06	45.07	16.93	-22.8	2.62
ScBi	-515.85	320.66	-239.7	876.1	-311	0.64	-0.12

The electronic properties of ScB (B=N, P, As, Sb, and Bi) compounds are described in terms of their electron density, density of states (DOS), and band structure.

Journal of Techno Trainers
Vol.1, Issue.1, (2024)
https://www.technotrainers.net

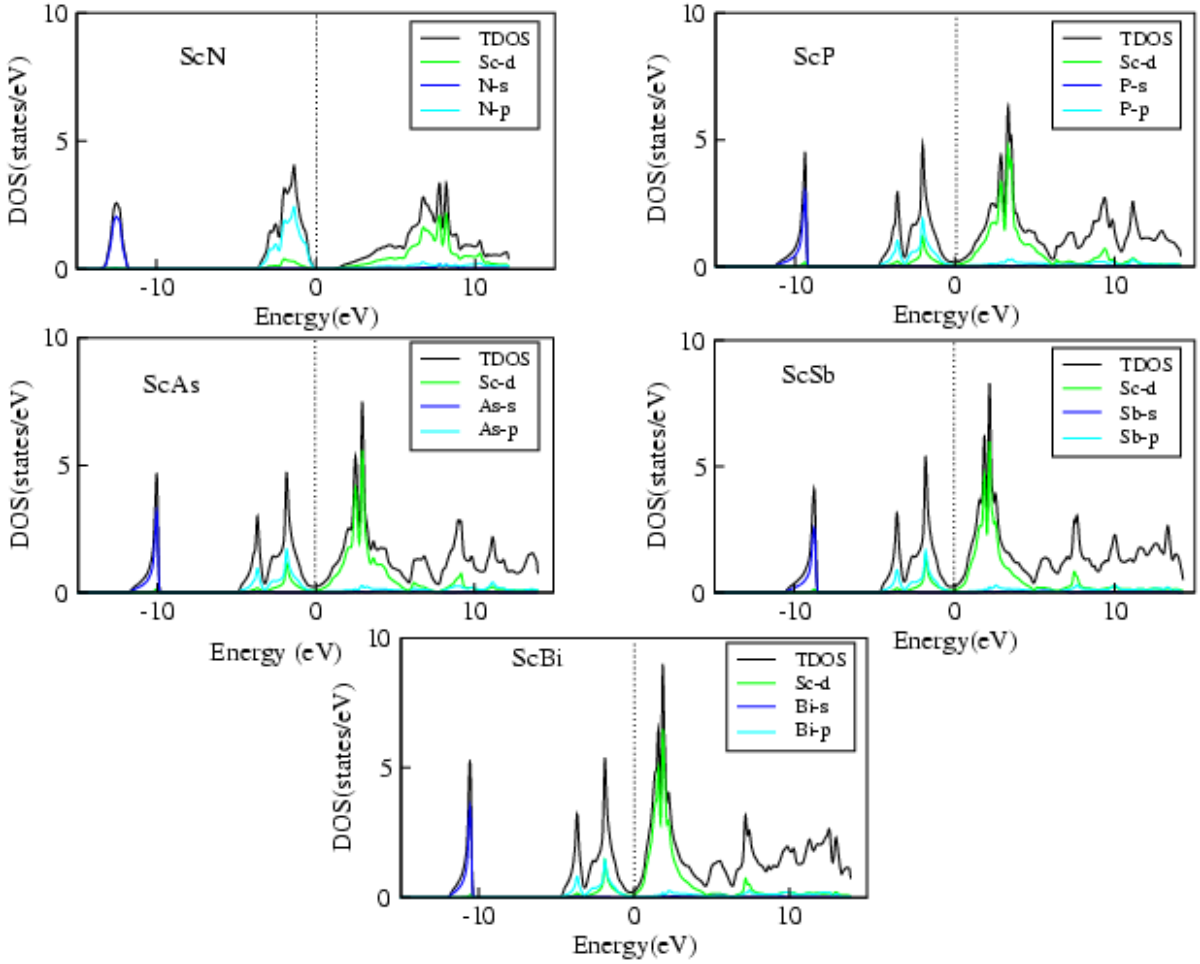

Fig 2: Density of states of ScB (B=N, P, As, Sb, As)

Journal of Techno Trainers
Vol.1, Issue.1, (2024)
https://www.technotrainers.net

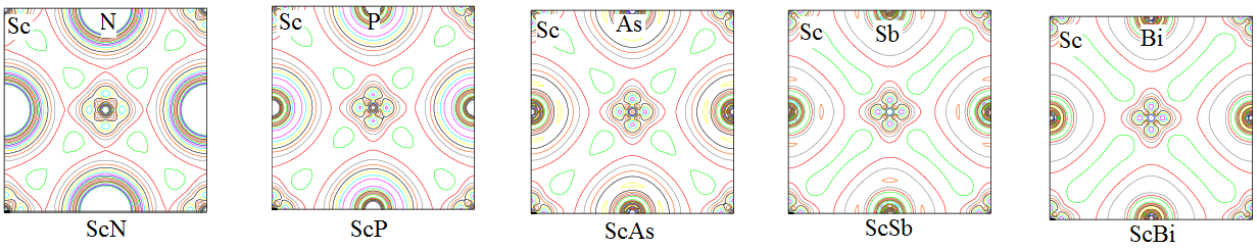

Fig 3. Electron density plots in (100) plane.

Conclusion

Complicated materials are elastically stable but brittle. mBJ predicts bandgap values more accurately than GGA potential. All compounds show a semi-metallic nature, with the exception of ScN..

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