

# A First Principles Study of The Structural and Electronic Properties of Vanadium Selenide

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**Abstract:** The electronic and structural properties of vanadium selenide (VSe) nanostructure have been calculated from first principles using density functional theory (DFT) within the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) as implemented in the Quantum Espresso simulation code. The findings revealed that VSe is a metallic crystal whose conduction properties are influenced by the V(4D) and Se(4P) energy states. This nanostructure has a density of state of 3.13 states/eV and is a promising material for a wide range of engineering applications, such as in linear and nonlinear optics and lasers.

**Keywords:** electronic, density functional theory, metallic, energy states, and density of states.

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## I. INTRODUCTION

Early transition metal complexes [1], [2] made from elements like sulfur, selenium, or tellurium mixed with metals like vanadium are gaining traction across the technological world [3]. This is due to their ability to quickly and reliably switch states and control how light or heat moves through materials. This makes them incredibly valuable for data storage [4], optical systems [5], and energy devices where performance, speed, and efficiency are vital. Chalcogenide materials consist of at least one chalcogen anion (group 16 element), in particular sulfide, selenide, and telluride. The transition metals chalcogenides [6], [7] consist of a transition metal (d-block elements) bonded with a chalcogenide (S, Se, Te). These materials exhibit unique material properties and are highly covalent, exhibiting mostly semiconducting properties [8]. Considering this, the materials of groups II-VI have significant and unique features that may be tuned by modifying the composition of the constituent compounds, resulting in tuned electronic and optical responses [9] that are crucial for photoelectronic devices for commercial purposes and operate over a broad variety of wavelength spectra. The direct and indirect electronic bandgap properties of the II-VI semiconductor materials involving transition metal-doped ZnSe alloys [10] can make them an attractive candidate for various industrial applications in optoelectronic [11], photonic [12], and magnetic sensing devices [13].

Vanadium selenide (VSe) compound belongs to the space group that crystallizes into a cubic structure. So far, this is the first time the structural and electronic properties have been calculated, and there is none, but similar literature to compare the calculated properties with. Aside from this study is an opportunity to explore more of its unexplored properties, like mechanical, optical, and transport properties for industrial applications.

### 1.1 Computational framework

The properties of VSe have been investigated from first principles by applying density functional theory [14], [15] using Quantum Espresso (QE) simulation package [16, 17]. The generalized gradient approximation (GGA-PBE) [18] exchange energy was used. Throughout this study, ultrasoft pseudopotentials (UPP) have been employed, and an energy cut-off of 400 Ry was applied to limit the number of components in the plane wave expansion. A Gaussian smearing technique has been used with a smearing width of  $2.0 \times 10^{-2}$  Ry. A  $14 \times 14 \times 14$   $k$ -points mesh has been produced utilizing the Monkhorst-Pack program for the Brillouin zone integration [19] to generate a uniform  $k$ -points grid along with the  $a$ ,  $b$ , and  $c$  axes in reciprocal space. The BFGS (Broyden-Fletcher-Goldfarb-Shanno) method has been used to optimize the lattice parameters and was fully optimized after relaxing the atomic positions through several volumes till the disparity in total energy is less than  $1.0 \times 10^{-8}$  Ry.

### 1.2 Structural properties

Vanadium selenide (VSe) compound belongs to the space group that crystallizes into a cubic structure [20], [21], and has the atomic coordinates: V (0.33, 0.67, 0.08), Se (0.67, 0.33, 0.25). **Error! Reference source**

**not found.** depicts the crystal structure of VSe. We have relaxed the variable cell to minimize the total energy to attain the equilibrium crystal structure of the studied compound. After relaxing the atomic coordinates, we have used the final atomic coordinates to converge the cut-off energy and k-points to get values that increase independently of the total energy of the system.

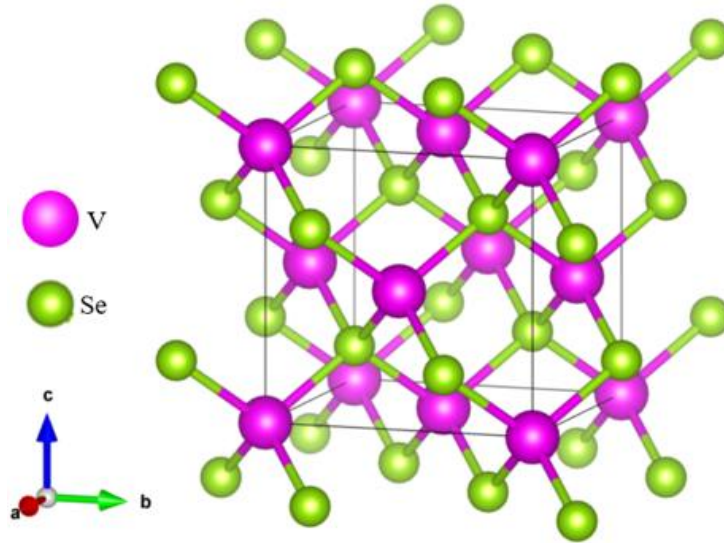


Fig. 1. Crystal structure of VSe (VESTA generated)

The optimized lattice parameters have been computed at an equilibrium state with a minimum correlating ground state energy, and the calculated structural values of the VSe crystal are recorded in **Table 1**. **Figure 2(a)** and **(b)** show the optimized lattice parameter  $a$ , and energy-volume (E-V) curve, which has been fitted to the Birch–Murnaghan’s third order equation of state (EOS)[22], equation **Error! Reference source not found.** The calculated bulk modulus  $B_0$  (GPa), its derivative  $B'_0$  and the minimum ground state energy  $E_0$  have also been calculated at zero pressure. The result shows that VSe has zero bulk modulus in a stable state.

$$E(V) = E_0 - \frac{9}{16} B_0 \left[ (4 - B'_0) \frac{V_0^3}{V^2} - (14 - 3B'_0) \frac{V_0^{7/3}}{V^{4/3}} (16 - 3B'_0) \frac{V_0^{5/3}}{V^{2/3}} \right]$$

1

The crystal-generated structures were analyzed in cubic symmetry. Although there is no literature to compare with, the findings agree with the reported similar literature [23]. All the structural parameters computed are summarized in **Table**. This study shows that the bulk modulus of VSe depicts the toughness of the material, indicating that VSe has a stronger and larger bulk modulus.

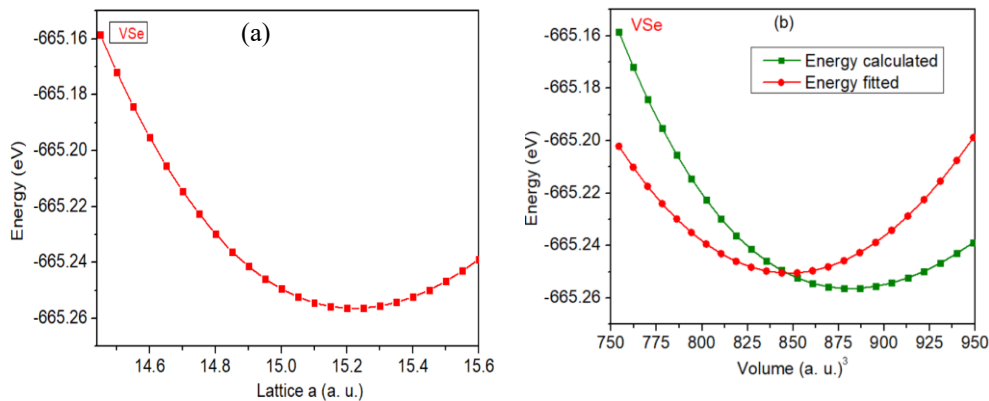


Fig. 2. (a) optimized lattice parameter and (b) fitted energy-volume curve

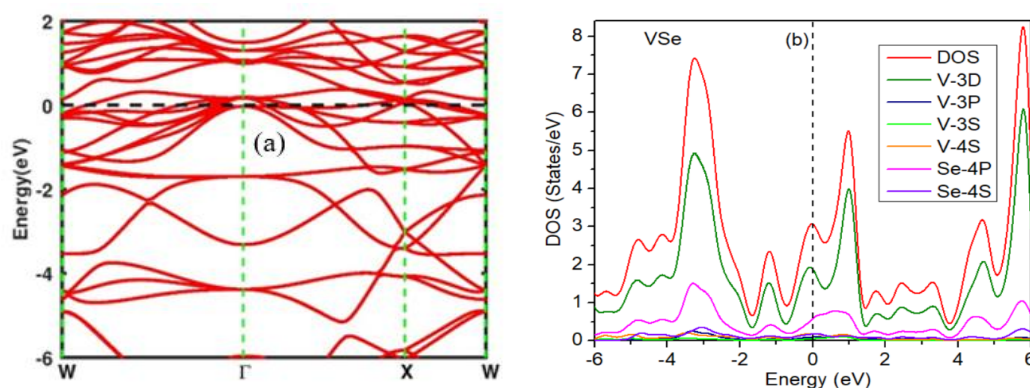
**Table 1. Calculated structural properties of VSe**

Phase	a (Å)	c (Å)	V(Å) <sup>3</sup>	B <sub>0</sub> (GPa)	B' <sub>0</sub> (GPa)	Reference
VSe	8.053		448.6	0	0.16	This work
CdSe	4.229	7.015				[23]
CdS	4.137	6.716				[23]

### 1.3 Electronic properties

The electronic bands and density of states (DOS), respectively, of VSe have been calculated along high symmetry in the first Brillouin zone within the energy range of -6 eV to +6 eV from Fig. 3 (a) and (b), respectively. While plot in Figure 3 (a) depicts the energy bands structure, Figure 3 (b) displays a plot of the total density of states (DOS) and the projected density of states (PDOS) of the elemental orbital contributions. The calculated DOS of the studied material at the  $E_F$  shown in Figure 3b is 3.13 states/eV/cell. The study range of the bands and density of states (DOS) was investigated deeply to clearly understand the electronic behaviours of Vse at the Fermi level.

All the noticeable peaks are due to the hybridization or overlapping of the energy states at the Fermi level and elsewhere within the energy range of -6 to 6 eV. In the first stage (-6eV to -2 eV), the contributions to the total peak in the DOS comes from the V-3D and Se-4P as major contributors; the second region between -2 eV in the valence band to +1.5 eV in the conduction band shows the studied material is metallic and contributions to the total density of state DOS of 3.13 states/eV/cell is coming principally from the V-3D as major contributor and a reasonable contribution from Se-4P. The third region is enshrined in the conduction band and all the elemental orbitals a seen as contributors to the peaks in the DOS within the zone.


**Fig. 3. (a) Electronic energy bands, (b) Density of states of VSe**

## II. CONCLUSION

In this study, we have investigated the VSe crystal by utilizing the GGA-PBE exchange correlation energy from first principles within the DFT. Results show that the VSe compound is metallic in nature due to the bands that significantly impact the electronic density of states at the Fermi level. This shows VSe is a device that can be used in the electronic realm, especially for innovative density of state utilizable devices.

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