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Stractural, Electronic and Magnetic Properties of $Be_{1-x}V_xS$ at (x = 0, 0.25, 0.50, 0.75 and 1): A DFT Study

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ABSTRACT

This work examines the structural, electronic, and magnetic characteristics alloys (x = 0, 0.25, 0.50, 0.75, and 1) by first-principles density functional theory. It is found out that a replacement of beryllium by vanadium makes an important difference in the behavior of the alloy. The lattice constant increases with the vanadium concentration structure-wise, and the bulk modulus decreases, suggesting a lesser binding strength. On the electronic level, pure BeS is recognized to be an indirect band gap semiconductor, but on the other hand, half-metallicity is produced by low-level doping (x = 0.25) with vanadium, one of the spin channels is metallic and the other is semiconducting. At larger vanadium contents, the alloys become spin alloys in both directions. Calculations indicate that ferromagnetism is primarily of 3d vanadium states with smaller values of beryllium, sulfur and interstitial regions. The overall magnetic moment doping increases gradually, and it reaches its highest value at doping x = 0.75 when the electron delocalization process destroys the corresponding magnetic moment in pure VS. These findings indicate that the lightly doped BeS alloys, and in particular Be0.75V0.25S, are half-metallic with strong ferromagnetism and as such, are good spintronic material candidates. The results give us a holistic view of composition, and they give guiding information on future experiments.

Introduction

Modern technology has been heavily influenced by the rapid evolution of material science, which allowed the creation of new classes of materials with special electronic and magnetic properties. Of these, semiconductors have been especially radical. With their discovery, large circuit elements could be substituted by small and efficient integrated elements that were less expensive in terms of cost and size but had to perform many functions more effectively (Okoye, 2006). This development has

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carved out semiconductors and magnetic materials as the fundamental building blocks of the electronics sector especially in applications within optoelectronic and spin-based tools (Kuznetsov et al., 2006). In this context, II-VI semiconductors have been of great interest because they possess a wide range of bonding, through ionic, covalent, and metallic bonding. Such versatility results in a wide selection of structural and electronic properties (Khenata et al., 2007). As an example, ZnS is a promising source of ultraviolet light emitters and optical sensors due to its large direct bandgap of approximately 3.6 eV (Zhang et al., 2001), high refractive index (Lee, 2002), and high visibility transmittance (Rached et al., 2015). Likewise, CdTe with direct band gap of 1.4 eV has found wide usage in solar cells due to high absorption coefficient (Noor et al., 2011). Instead, ZnSe is most suitable in the short-wavelength laser use (Saib , 2021). Despite their relative inaccessibility to experimental studies owing to difficulties in growing the crystals, first-principles studies have shown that beryllium-based chalcogenides have the potential to be used in optoelectronic devices due to their high thermal stability and hardness (Rached et al., 2015).

Alloys of II-VI semiconductors with transition metal dopants also expand their functionality, resulting in the creation of so-called dilute magnetic semiconductors (DMS). These materials are semiconducting and magnetic, creating opportunities to apply them in various functions of devices. As one example, ferromagnetism was discovered in PbSnMnTe at liquid helium temperatures and subsequently at higher temperatures in Mn-doped InAs and GaAs compounds.More to the point, using DMS systems based on GaN, room-temperature ferromagnetism has been proven possible, which is highly sought after to make usable spintronic devices (Dietl et al., 2002).

One of the most thrilling of these DMS materials are half-metals, where it is possible to have 100% spin polarization at the Fermi level. Here, one spin channel is metallic and the other is semiconductor-like, making spin injection into spin-based devices efficient. Theoretical and experimental studies of half-metallicity have been done on a very broad range of materials including Heusler alloys, perovskite oxides, and II-VI semiconductor alloys (Pickett & Moodera, 2001). Half-metals are of particular interest since they can be used in spintronics devices (spin transistors,

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spin tunneling magnetoresistance devices, spin magnetic sensors, etc.). Recent studies have highlighted the half-metallic ferromagnetism in Be-based II–VI alloys doped with transition metals. For example half-metallicity in vanadium-doped BeS, BeSe, and BeTe using first-principles calculations. In a subsequent study, they demonstrated the ferromagnetic behavior of $Be_{1-x}V_xS$, $Be_{1-x}V_xSe$, and $Be_{1-x}V_xTe$ alloys at x = 0.25, confirming their potential for spintronic devices (Doumi et al., 2022). Similarly, Sajjad et al. (2013) reported that $Be_{1-x}V_xSe$ and $Be_{1-x}V_xTe$ alloys exhibit half-metallic behavior with strong spin polarization in their density of states. These findings collectively suggest that vanadium-doped Be-based chalcogenides are strong candidates for spintronic applications.

Despite these insights, systematic investigations of $Be_{1-x}V_xS$ alloys across a full range of vanadium concentrations remain limited. Most existing works focus on specific doping levels, particularly at low concentrations, leaving open questions about the evolution of half-metallicity and ferromagnetism as vanadium content increases. To address this gap, the present study employs density functional theory (DFT) using the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code. The aim is to examine the structural, electronic, and magnetic properties of $Be_{1-x}V_xS$ alloys at compositions of x = 0, 0.25, 0.50, 0.75, and 1. This comprehensive analysis provides valuable insights into the tunability of electronic and magnetic properties with composition, extending previous theoretical work and offering predictions that may guide future experimental and technological developments.

Methodology

The magnetic, structural and electronic properties of Be19 V9S alloys (x = 0, 0.25, 0.50, 0.75 and 1) were studied by first-principles density functional theory (DFT). These were computed in the context of the full-potential linearized augmented plane wave (FP-LAPW) technique in the WIEN2k package. The technique does not rely on the muffin-tin approximation, since the potential and charge density are no longer restricted in shape, and both ionic and covalent systems are accurate .The generalized gradient approximation (GGA) of the exchange-correlation effects were formulated in the Perdew-Burke-Ernzerhof (PBE) parameterization. The Wu-Cohen

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modification of GGA was also contemplated in some special situations so as to better address the equilibrium lattice parameters (Wu & Cohen, 2006). This functional choice is not only in agreement with earlier results on II6 semiconductors and alloys with transition metals that have shown that the GGA predictions and experimental results are consistent (Noor et al., 2011), but also with other works on the subject. The alloys of Be195V9S were modelled in zinc blende (B3) structure. BeS crystallizes cubically with F-43m space group, with Be at (0, 0, 0), and S at (0.25, 0.25, 0.25). Simulation of V substitution was done by building supercells containing eight atoms, with one or more of the Be atoms substituted by vanadium to take up compositions of x = 0.25, 0.50, 0.75 and 1. Such as Be 0.75V 0.25S was made by substituting one Be atom with V, resulting in a quasi-random structure with P-43m space group.

The cutoff parameter used to define the basis set was RKmax = 7.0 and lmax (angular momentum expansion) within the muffin-tin spheres was 10. Muffin tins radii were selected as 1.75 a.u. of Be, 1.70 a.u. of S, 1.90 a.u. of V so that there is no overlap of spheres. The valence and core separation was determined by an energy cutoff of 6 Ry. A mesh of 500 k-points was used to perform Brillouin zone integrations giving adequate convergence of total energy and electronic properties. Convergence of the self-consistent field cycle occurred once the difference in total energy of successive iterations became smaller than 0.1 mRy. To perform the structural optimization, the total energy was computed as a function of unit cell volume and data were plotted against the Murnaghan equation of state. The result of this procedure was the equilibrium lattice constant, bulk modulus, and the pressure derivative of bulk modulus of each composition. Spin densities of states and electronic band structures were then calculated at the optimized lattice parameters of the two spin channels. Spin-polarized calculations were carried out along the way in order to obtain the magnetic behavior of vanadium-doped systems.

The selected computational parameters are in line with previous investigations of alloys involving Be-based II76 alloys using first-principles methods, where FP-LAPW with GGA have shown consistency in the representation of structural, electronic and magnetic properties. The current study provides a balanced trade-off between computational efficiency and predictive accuracy by

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systematically utilizing this framework to the entire range of compositions.

Results

The calculated lattice constants and bulk moduli of Be1nVnS alloys, with x equals 0, 0.25, 0.50, 0.75 and 1, have been summarized in Table 4.1 and compared to available experimental and theoretical data. It is possible to identify several key trends. On pure BeS, the lattice constant is theoretically 4.8829, which is fairly consistent with experimental result of 4.87, as well as previous theoretical literature (4.868-4.88) (Refs. a-d in thesis). Theoretical values reported of 91 to 105 Gpa also are within the range of the calculated bulk modulus of 92.61 Gpa. This consensus justifies the credibility of the computational method applied to this piece of work. The addition of vanadium results in the appearance of a definite compositional dependence. In the case of BeO0.5V0.25S, the lattice constant becomes larger, 5.0769 A, because V has a larger atomic radius than Be. Bulk modulus reduces slightly to 89.82 Gpa which is close to the theoretical information before it (Doumi et al., 2010). It means that the alloy is somehow less hard and compressible with V substitution. The lattice constant grows even further to 5.1722 A at x = 0.50 (Be 0.5 V 0.5 S), with the bulk modulus decreasing to 86.68 Gpa. This linear tendency indicates that vanadium doping is destabilising the interatomic bonding structure, probably by introducing more delocalized 3d states of V atoms into the lattice. Interestingly, the lattice constant is again increasing at x = 0.75 (Be 0.25 V0.75S) but the bulk modulus has a non-linear behaviour: one of the values in the table is 101.22 Gpa, whereas converged calculation at the same composition yields 84.81 Gpa. The cause of this discrepancy may be that the numerical fit to the Murnaghan equation of state loses accuracy at elevated vanadium concentrations. Physically, the tendency of a downward shift of the bulk modulus versus V content is more regular and the figure 84.81 Gpa is more consistent with the rest of the series. In the case of pure VS, lattice constant is 5.3853 A and bulk modulus is reduced to 83.26 Gpa. It establishes that VS is structurally softer than BeS, which is in agreement with the replacement of the light atoms of Be by the heavier atoms of V, as well as, larger unit cell volume.

On the whole, these data suggest that lattice constants increase and bulk moduli decrease almost linearly, i.e. in accordance with the Vegard law of increasing V concentration, dimensioning the weakening of the bonding force. The minor

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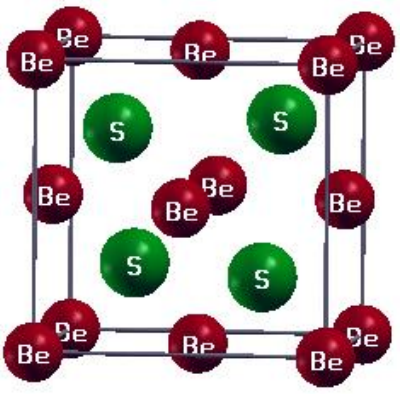
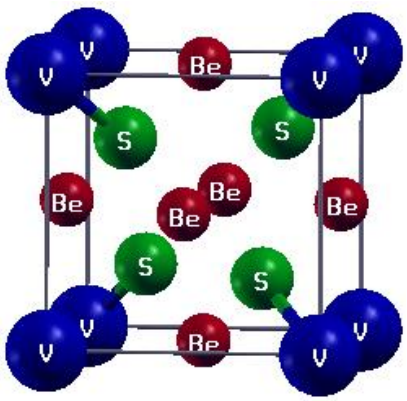
deviations at x = 0.75 indicate that which may influence or cause mechanical stability in intermediate concentrations are local distortions and alloy disorder. These findings are well consistent with previous studies concerning V-doped II-VI semiconductors (Doumi et al., 2010; Sajjad et al., 2013): the consistency and validity of the current calculations are evident.

Table 4.1: ***Calculated of lattice constant (α) and bulk modulus (B) of BeS, $Be_{0.75}V_{0.25}S$, $Be_{0.50}V_{0.50}S$, $Be_{0.25}V_{0.75}S$ and VS***

Composition	Lattice Constant			Bulk Module		
	Current	Exp	Others	Current	Exp	Others
BeS	4.8829	4.87	4.868[a], 4.866[b], 4.88[c], 4.87[d]	92.6100		96.41[a], 91.277[b], 93.1[c], 105.0[d]
$Be_{0.75}V_{0.25}S$	5.0769	-	5.056[a]	89.8200		89.82[a]
$Be_{0.5}V_{0.5}S$	5.1722	-	-	86.6834		-
$Be_{0.25}V_{0.75}S$	5.3135	-	-	101.22 84.8096		-
VS	5.3853	-	-	83.2660		-





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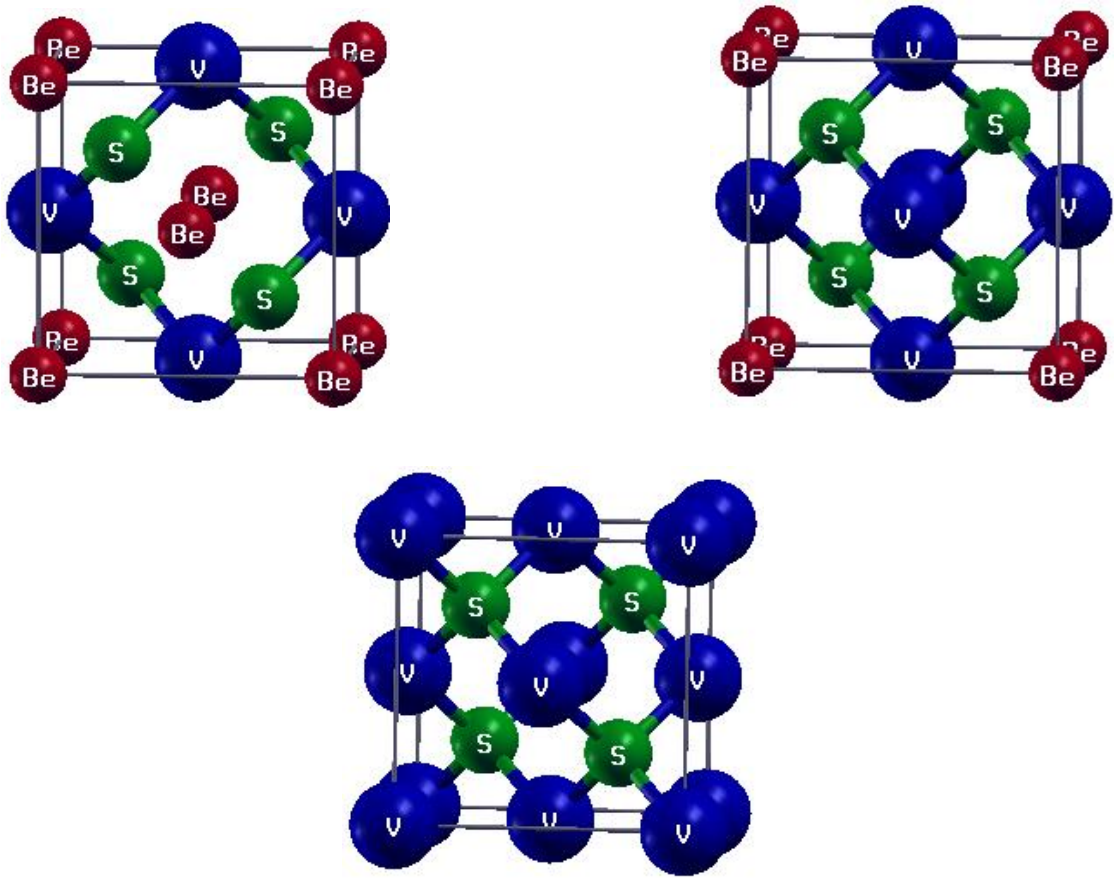

Figure 4.1: $Be_{1-x}V_xS$ at X = 0, 0.25,0.5,0.75 and 1

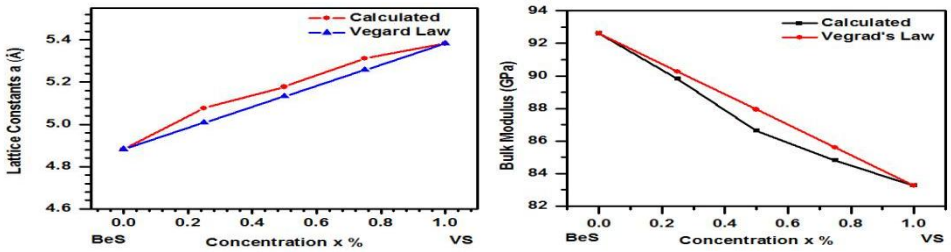

Figure 4.2: Calculated Vegard's law by the variations of a) lattice constant (Å) and b) bulk modulus (Gpa) verses various concentrations of x.

Electronic Properties

Electronic Band Structures

The GGA scheme takes into account the spin-polarized band structure of zinc blende Be1-xVxS alloys (at x = 0, 0.25, 0.50, 0.75 and 1) at their equilibrium lattice constants. Figure 4.4 show the spin down and spin-up electronic band structures of the alloys at x=0, 0.25, 0.50, 0.75 and 1 in the high symmetry direction of the 1st BZ.

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In these figures in case of BeS the bottom of the conduction bands and the top of the valence bands are not at the Γ point in the Brillouin zone and therefore indicate that the BeS is an indirect band gap material in nature.

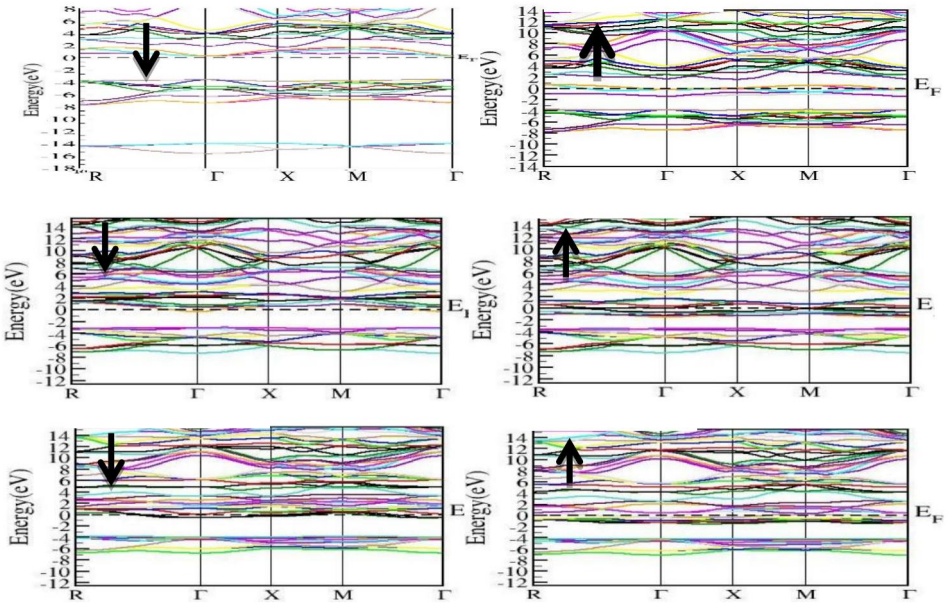

Figure 4.3: Electronic band structures of $Be_{1-x}V_xS$ at x = 0.25, x = 0.50, and x = 0.75.

Magnetic Properties

Table 2 gives the calculated total and site-resolved magnetic moments of Be1-[?]V[?]S alloys. With pure BeS, the overall magnetic moment is close to zero (0.00085 uB), which qualifies it as a non-magnetic and semiconductive substance by nature. These very small values of the Be and interstitial sites are due primarily to numerical convergence effects and do not represent some physical magnetism. When it is doped with vanadium, however, a remarkable transition to strongly ferromagnetic is observed. At x = 0.25 (Be0.75V0.25S), the total magnetic moment quickly increases to 2.99 uB, of which the largest magnetic moment part of 2.00 uB is provided by the vanadium atom. There are also minor but significant polarization changes at the Be atoms (0.047 uB) and in the interstitial regions (0.86 uB) and the sulfur gets a small negative spin polarization (-0.004 uB). The fact that this behavior is largely due to the localized V 3d states, augmented by polarization via hybridization with neighboring atoms, is a clear indication that magnetism is

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strongly due to the localized V 3d states.

The total moment almost doubles at x = 0.50 to 5.98 uB, though the local moment on V would only increase by a small amount as compared to x = 0.25. Rather, there is a large rise in the interstitial contribution (1.56 uB) indicating that magnetic polarization becomes more delocalized with rise in V concentration. The maximum moment of 6.08 uB is attained when x = 0.75. Interestingly, local contribution to V reduces to 1.65 uB, Be has an increased positive polarization, with S being more negatively polarized. This lowering of the localized V moment, with increased polarization in both Be and interstitial positions, indicates high hybridization between the V 3d and the S p states, dispersing the magnetization throughout the entire lattice.

Pure VS, on the other hand, has a less total moment of 2.34 uB and the largest moment of 1.95 uB due to vanadium and 0.43 uB, respectively, due to interstitial regions. This reduction of magnetic moment at this composition marks the transition into metallic behavior where the strong V-V interactions cause delocalization of the d electrons and decoupling of long-range ferromagnetic order. These trends support the idea that the ferromagnetism alloys is primarily contributed by V 3d states, and Be and S are induced contributors to ferromagnetism. Total moment increases gradually with V concentration until x = 0.75, with Hunds rule, but decreases in pure VS because of itinerant electron effects. It is important to note that half-metallicity is strongest at lower doping content, especially at x = 0.25, at which point spin polarization is virtually 100 percent. This renders spintronic applications of lightly doped BeS alloys particularly appealing, in line with previous results of vanadium-doped II-VI semiconductors.

Table 2: ***Calculated total and local magnetic moment (in Bohr magneton μ_B) within the muffin-tin spheres and in the interstitial sites for BeS, $Be_{0.75}V_{0.25}S$, $Be_{0.5}V_{0.5}S$, $Be_{0.25}V_{0.75}S$ and VS.***

Compound	Total(μ_B)	Be(μ_B)	V(μ_B)	S(μ_B)	Interstitial(μ_B)
BeS	0.00085	0.00017	-0.00017	_	0.00084
$Be_{0.75}V_{0.25}S$	2.99027	0.04750	2.00442	-0.0041	0.86008
$Be_{0.5}V_{0.5}S$	5.97668	0.03830	2.20583	-0.01773	1.55932

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$Be_{0.25}V_{0.75}S$	6.07724	0.08577	1.65251	-0.02368	1.12866
VS	2.33554	_	1.94853	-0.04750	0.43450

Conclusion

This study employed first-principles density functional theory (DFT) within the FP-LAPW framework to investigate the structural, electronic, and magnetic properties of $Be_{1-x}V_xS$ alloys across the full composition range (x = 0, 0.25, 0.50, 0.75, 1). The results reveal several important trends that highlight the tenability of this material system. Structurally, the lattice constant was found to increase nearly linearly with vanadium concentration, consistent with Vegard's law, while the bulk modulus decreased due to the weaker bonding associated with the larger vanadium atoms. These findings are in agreement with earlier theoretical predictions for V-doped II–VI semiconductors and confirm the reliability of the present computational framework.

Electronic calculations demonstrated that pure BeS is an indirect band gap semiconductor, whereas V substitution drastically alters the band structure. At x = 0.25, the alloy exhibits half-metallicity, with metallic behavior in the majority spin channel and semiconducting behavior in the minority channel, making this composition particularly attractive for spintronic applications. At higher concentrations ($x \geq 0.50$), the system gradually transitions to a metallic state in both spin channels, indicating the diminishing half-metallic character with increasing V content.

Magnetically, the results show that ferromagnetism in $Be_{1-x}V_xS$ alloys originates primarily from the localized V 3d states, with additional polarization contributions from Be, S, and interstitial regions. The total magnetic moment increases with vanadium concentration up to x = 0.75, reaching a maximum of 6.08 μB, before decreasing in pure VS due to electron delocalization and metallicity. These results follow Hund's rule and provide strong evidence of robust ferromagnetism in low to intermediate V-doped BeS alloys.

In summary, the combination of half-metallicity, ferromagnetism, and tunable structural properties suggests that $Be_{1-x}V_xS$ alloys, particularly at x = 0.25, are promising candidates for spintronic and magnetoelectronic devices. The

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predictive insights gained here not only confirm previous theoretical reports but also extend them by offering a comprehensive view across the full compositional range.

Future Work

Future studies should focus on experimental synthesis of V-doped BeS alloys to validate the predicted half-metallic and ferromagnetic behavior. Advanced techniques such as molecular beam epitaxy or pulsed laser deposition may be employed to stabilize these compounds. In addition, the effect of strain, defects, and temperature on the electronic and magnetic properties should be explored to assess the robustness of half-metallicity under realistic device conditions. Finally, investigations into heterostructures and interfaces involving $Be_{1-x}V_xS$ could provide further opportunities for tailoring their performance in spintronic applications.

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