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First-Principles Study on Magnetic Nature and Electronic Behavior of Silver-Based Sulfide: Ag_3MnS_4

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Abstract: This work is about the electronic and magnetic character of the ternary silver-based sulfide (Ag_3MnS_4) crystallized in sulvanite type crystal structure with space group $P\bar{4}3m$ and space number 215. The mentioned characteristics has been examined by Generalized Gradient Approximation (GGA) with spin effect under Density Functional Theory (DFT). Four different magnetic phases have been considered to investigate the proper magnetic order for this system. As a result of calculations, it has been understood that, for Ag_3MnS_4 compound, the energetically most favored magnetic order is A-type antiferromagnetic. After the optimized structural parameters and relaxed atomic positions in its suitable magnetic order have been obtained, the electronic characteristic of this antiferromagnet system indicating semiconducting behavior due to the observed a small direct band gap (E_g = 0.325 eV) in both spin states, has been investigated. Also, this compound has thermodynamic stability and structural synthesizability due to its calculated negative formation energy values for all different type magnetic phases.

Key words: Semiconductor, Antiferromagnet, Ferromagnet, Density functional theory, Chalcogenide.

Gümüş-Tabanlı Sülfürün Manyetik Doğası ve Elektronik Davranışı Üzerine İlk-İlkeler Çalışması: Ag_3MnS_4

Özet: Bu çalışma, uzay grubu $P\bar{4}3m$ ve uzay numarası 215 ile sülvanit tipi kristal yapısında kristalize olan üçlü gümüş bazlı sülfidin (Ag_3MnS_4) elektronik ve manyetik karakteri ile ilgilidir. Bahsedilen özellikler Yoğunluk Fonksiyonel Teorisi (YFT) altında spin etkisi ile Genelleştirilmiş Gradyan Yaklaşımı (GGY) ile incelenmiştir. Bu sistem için uygun manyetik düzeni araştırmak için dört farklı manyetik faz düşünülmüştür. Hesaplamaların bir sonucu olarak, Ag_3MnS_4 bileşiği için, enerjisel olarak en çok tercih edilen manyetik düzenin A-tipi antiferromanyetik olduğu anlaşılmıştır. Optimize edilmiş yapısal parametreler ve uygun manyetik düzendeki relax edilen atomik pozisyonlar elde edildikten sonra, her iki spin durumunda da küçük bir direkt bant boşluğunun (E_b = 0.325 eV) gözlenmesi nedeniyle yarı iletken davranış gösteren bu antiferromanyetik sistemin elektronik özelliği araştırılmıştır. Ayrıca, bu bileşik, tüm farklı tip manyetik fazlar için hesaplanan negatif oluşum enerji değerlerinden dolayı termodinamik kararlılığa ve yapısal sentezlenebilirliğe sahiptir.

Anahtar kelimeler: Yarıiletken, Antiferromanyetik, Ferromanyetik, Yoğunluk fonksiyonel teorisi, Kalgonit.

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1. Introduction

Recently, compounds containing chalcogenide group elements such as sulphur, selenium or tellurium have attracted a lot of attention due to be used in many technological fields [1-8]. For this reason, such compounds have become the focal point of many scientists' experimental and theoretical studies [9-14]. Especially in literature, there are many experimental and theoretical studies [15-20] about copper-based (Cu_3TMCh_4) chalcogenide systems in which TM atoms are generally selected from transition metal elements and having sulvanite type cubic crystal structure conforming to $P\bar{4}3m$ space group (space number: 215) [21-22].

The compounds containing any chalcogen such as sulphur, selenium or tellurium element, show interesting electronic behaviors with different types of magnetic phases. In one of the previous theoretical studies, the electronic behaviors and magnetism natures in transition metal chalcogenide systems having zinc-sulfide structure, have been investigated [23-25]. Also, by Han *et al.*, the magnetic susceptibility measurements indicating suitable magnetic order which is antiferromagnetic for $KFeS_2$ and KFe_2S_3, which include single and double chains of FeS_4 tetrahedron, respectively were reported experimentally [26]. Furthermore, there are investigations on $Na_2MnGe_2Se_6$ and $K_2FeGe_3Se_8$ compounds which have semiconducting nature in antiferromagnetic order, both experimentally and theoretically [27-28]. Apart from those studies, the ternary copper-based chalcogenide series are powerful candidates for solar cell absorbers were reported [29]. Recently, another theoretical study, the mechanical properties of ferromagnetic zinc-based vanadium sulfide and telluride having half-metallic electronic nature indicating to be able to use for spintronic applications have been examined [30]. In this context, the discovery of particularly interesting magnetic nature and electronic behavior of sulvanite type new ternary silver-based sulfide system (Ag_3MnS_4) is the main source of motivation in this study.

In this study, due to the fact that copper-based chalcogenide series as well as zinc-based chalcogenides can be used in similar types of technological applications, the electronic nature in suitable magnetic order of new silver-based sulfide Ag_3MnS_4 has been investigated. In addition, the magnetic nature and electronic behavior of sulvanite type new ternary silver-based sulfide system (Ag_3MnS_4) have been investigated by considering ferromagnetic phase and three types of antiferromagnetic orders as A-type, G-type and C-type. The spin-polarized electronic band structure of this compound has been calculated within GGA, which is of great importance in terms of technology and industry, has been given in the most suitable magnetic order, which is the A-type antiferromagnetic phase. The adding new compounds to ternary chalcogenides has great importance, as it has a semiconductor nature and therefore can be used in possible future technological applications. As we have searched from the literature, there is no detailed study on the stable magnetic phase and electronic nature of this compound yet.

2. Material and Method

The calculations have been carried out using the VASP (Vienna Ab initio Simulation Package) [31,32] with projector augmented wave (PAW) method [33] under density functional theory [34-35]. For the exchange and correlation terms in the electron–electron interaction, a Perdew–Burke–Ernzerhof (PBE) type functional [36] was used within the generalized gradient approximation (GGA). The valence electron configurations for *Ag*, *Mn*, and *S* atoms in the mentioned system are as follows: $5s^1 4d^{10}$, $3d^6 4s^1$, and $3s^2 3p^4$, respectively.

To obtain optimal structural parameters and relaxed atomic positions in primitive crystal cell of our composition, the optimization operation has been carried out with automatically generated 12×12×12 Monkhorst-Pack scheme [37] in the irreducible Brillouin zone that gives 56 k-points. The cut-off energy has been fixed at 900 eV for wave-functions in plane wave basis sets expansion of eigenfunctions. The quasi-Newton method has been performed to relax atoms in primitive cell of this system until the forces on each atom is less than 10^{-8} eV/Å and the energy tolerance has been taken 10^{-9} eV per unit cell in the iterative computation of the Kohn-Sham equations. The relaxed atomic positions of the atoms in the primitive cell of the ternary silver-based sulfide Ag_3MnS_4 and the optimal structural parameters of this compound have been obtained by minimizing forces and pressures on this composition. Then, to decide which magnetic order is more suitable for the mentioned compound, a 2×2×2 super-cell including 64 atoms for this composition has been generated and calculated total energies and volumes. Finally, the structural parameters and the electronic behavior of this system have been investigated for the most suitable magnetic phase detected.

3. Results

Before investigating the electronic and magnetic nature of ternary silver-based sulfide (Ag_3MnS_4) which has simple cubic structure and conforming $P\bar{4}3m$ space group and 215 space number, it has been performed optimization operation to obtain optimal atomic positions in primitive cell of this composition. The relaxed positions of atoms in the primitive cell including eight atoms and the crystallographic representation have been given in Figure 1.

As can be seen in the primitive cell, three silver atoms are located at 3d (0.5, 0, 0) Wyckoff [38] positions, one manganese atom is positioned in 1a (0, 0, 0) whereas sulphur atoms are placed on 4e (0.211, 0.211, 0.211) positions. After the optimization operation has been completed, a 2×2×2 super-cell including 64 atoms has been taken into account to decide the stable magnetic phase of our composition. Finally, electronic behavior of this chalcogenide system has been discovered in its most stable magnetic order.

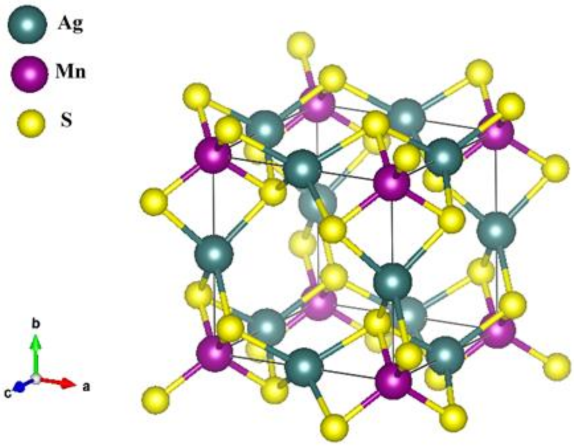

Figure 1. The crystallographic form of primitive cell designed by eight atoms ternary silver-based sulfide Ag_3MnS_4. The turquoise and purple colored atoms illustrate silver and manganese ions, respectively, while yellow atoms illustrate sulphur anions.

3.1. The Stable Magnetic Order and the Optimized Structural Parameters

The total magnetization of any solid crystal which has antiferromagnetic order approaches zero, although it consists of two ferromagnetic subsystems, each of which is mutually aligned and has large magnetization. For this reason, this type of crystal does not generate a magnetic field. In the literature, it is known that there are three types of antiferromagnetic orders: A-type, C-type and G-type. The directions of the magnetic moments of each antiferromagnetic order have a different arrangement of them to give zero total magnetization in each [39], as illustrated schematically in Figure 2.

In this study, in order to determine the suitable magnetic order of which the compound, the orientations of the magnetic moments of the manganese atoms in the produced supercell have been regulated in accordance with the above-mentioned adjustments and as seen in Figure 2 to be achieve zero total magnetization. Then, the formation energies (ΔE_f) which is usually used to verify the thermodynamic stability or structural synthesis of a crystal, for different type magnetic order of this system, have been calculated by using the internal energy differences. The formation energy (ΔE_f) has been calculated with the help of internal energy changes [40] as given in Equation 1:

$$\Delta E_f = E_{Ag_3MnS_4} - \left(3E_{Ag}^{bulk} + E_{Mn}^{bulk} + 4E_S^{bulk}\right) \tag{1}$$

where, $E_{Ag_3MnS_4}$ is the total energy of this compound. E_{Ag}^{bulk} , E_{Mn}^{bulk} and E_S^{bulk} are the ground state energies of *Ag*, *Mn* and *S* single crystals per atom. The negative value of formation energy indicates that the crystal is thermodynamically stable and structurally synthesizable. Also, for a solid crystal, if this computed energy value of its any structural or magnetic order is less than that of others, it can be considered that this order is energetically more favorable than others.

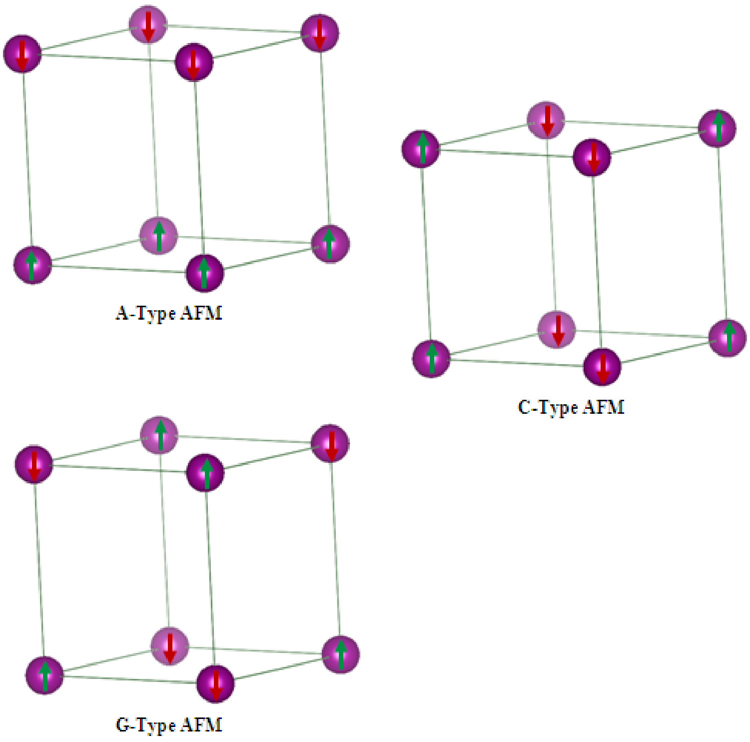

Figure 2. The spin orientation of the antiferromagnetic phases for a cubic crystal.

Table 1. The optimal lattice parameters, atomic bond distances, and the formation energies of Ag_3MnS_4.

Material	a (Å)	$d_{Mn\text{-}S}$ (Å)	$d_{Ag\text{-}S}$ (Å)	ΔE_f *(eV/f.u.)*
Ag_3MnS_4	6.055 (FM)	2.20796	2.51474	-6.577 (FM)
	6.054 (A-Type AFM)			-6.578 (A-Type AFM)
	6.012 (C-Type AFM)			-5.980 (C-Type AFM)
	6.024 (G-Type AFM)			-5.913 (G-Type AFM)

As presented in Table 1, for the future possible technological applications, the calculated formation energies of this compound indicate that it has structural synthesizability and is stable in thermodynamically in all different type magnetic phases. Also, the absolute value of the calculated formation energy for this compound in A-type antiferromagnetic order is greater than the energy values of other considered magnetic orders. Therefore, it has been decided that the magnetic nature of this compound is A-type AFM. After the optimization operation of the mentioned system, the ground state energy-volume values have been obtained and drawn graphs from these values as shown in Figure 3 by fitting the Vinet equation of state [41]. For this material, the obtained ground state energy has been well-converged and the asymptotic errors in fitting operation are smaller than almost one percent. The obtained some structural parameters for different type magnetic orders have been tabulated in Table 1.

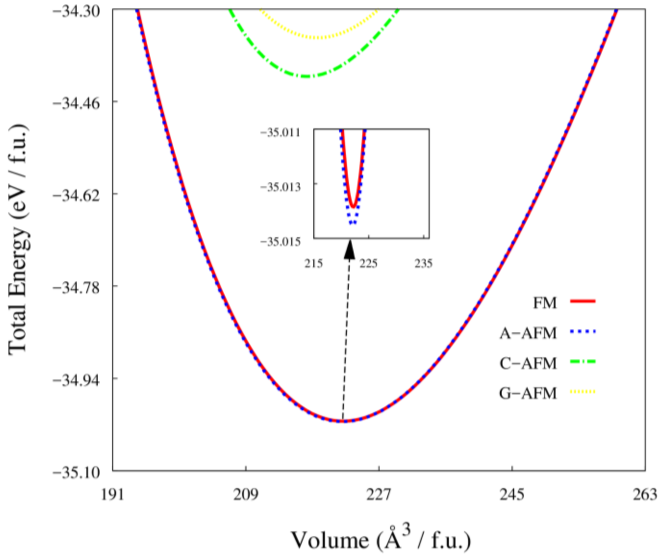

Figure 3. The total energy versus volume graphics for four different type magnetic phases of Ag_3MnS_4.

For the mentioned chalcogenide in this study, the energy-volume graphics show that, C-type and G-type antiferromagnetic phases have not suitability for our compound due to have much upper ground state energy values than A-type antiferromagnetic and ferromagnetic phases. Also, it can be clearly seen from the Figure 3 that, this material is most stable in A-type AFM order with slightly lower energy than FM order. For this compound, the energy-volume graphics and the formation energies are accordance with each other. For the compound mentioned in this study, as understood from the energy-volume graphs and calculated formation energies, the energy difference between A-type AFM and FM phases is very small. As we have searched from the literature, there is not detailed study or any investigation about this chalcogenide in literature for making any comparison. Furthermore, it can be said that Ag-S bond lengths are higher than Mn-S bond lengths in the primitive cell of ternary silver-based sulfide. Consequently, this compound with A-type AFM behavior, can be a good candidate for future possible technological applications since it has advantageous characteristics which is ordered in magnetically, but neighboring magnetic moments point in opposite directions providing zero total magnetization [42-43].

3.2. The Observed Electronic Behaviors of Ag_3MnS_4 Sulfide

In order to explore the electronic behavior of ternary silver-based Ag_3MnS_4 chalcogenide, spin-polarized electronic band structure and total density of state calculated under the GGA approach has been plotted along the high symmetry directions for both spin-up and spin-down states in the Brillouin zone as given in Figure 4. As seen from this figure, ternary silver-based sulfide (Ag_3MnS_4) which has A-type antiferromagnetic nature, behaves as semiconductor material since the observed electronic band structure having a little direct band gap (E_g = 0.325 eV) at Γ point in both up and down spin states.

The total and partial density of electrons in orbitals of atoms in the composition have been drawn as given in Figure 5. For this compound, it has been seen that, the dominancy of *p*-subshells of sulphur (*S*) namely chalcogen atoms in the valence band below Fermi energy, while *3d* states of manganese (*Mn*) atoms have dominancy in the conduction band above Fermi energy. In the valence band of the sulfide (Ag_3MnS_4) system, there are strong hybridizations, especially near the Fermi level (almost between -0.3 eV and 0 eV), between full-filled *4d* states of silver (*Ag*) atoms and *p*-subshells of sulphur (*S*) atoms. Also, in the same band for this compound, almost between -0.3 eV and -1.5 eV, there are strong hybridizations too between *d*-orbitals of manganese (*Mn*) and silver (*Ag*) atoms and *p*-subshells of sulphur (*S*) atoms. Furthermore, in the conduction band of this composition, the hybridizing is between *p*-subshells of sulphur (*S*) atoms and *d*-subshells of manganese (*Mn*) and silver (*Ag*) atoms in almost between 0.3 eV and 1 eV and between 1.3 eV and 1.5 eV. In addition, it can be understood from this graphic that, filled *3s* states which are shown with red lines and have very low density of states around Fermi energy, of sulphur atoms in sulfide composition have no noticeable effect on bonding properties between atoms in Ag_3MnS_4 compound. This means that these states do not have a dominancy role in inter-atomic bonding in the composition and on the formation of the mentioned system. In this regard, the electronic behavior of Ag_3MnS_4 sulfide can be chiefly defined by *d*-subshells of silver (*Ag*) and manganese (*Mn*) atoms which are transition metals, and *p*-subshells of sulphur (*S*) atoms and hybridizations between them.

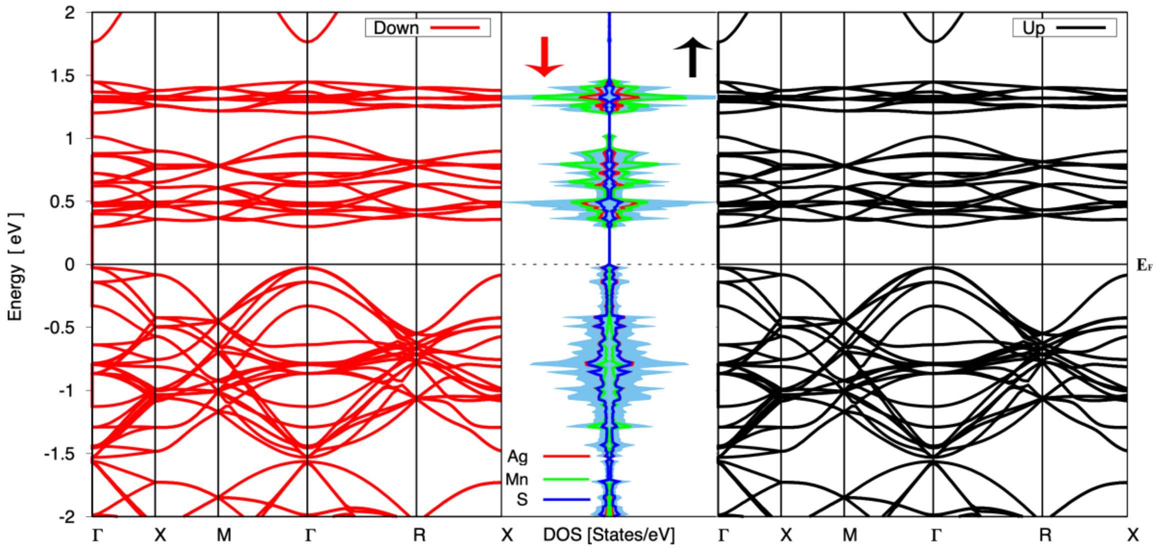

Figure 4. The band structure under spin polarization with the total DOS of sulvanite type Ag_3MnS_4.

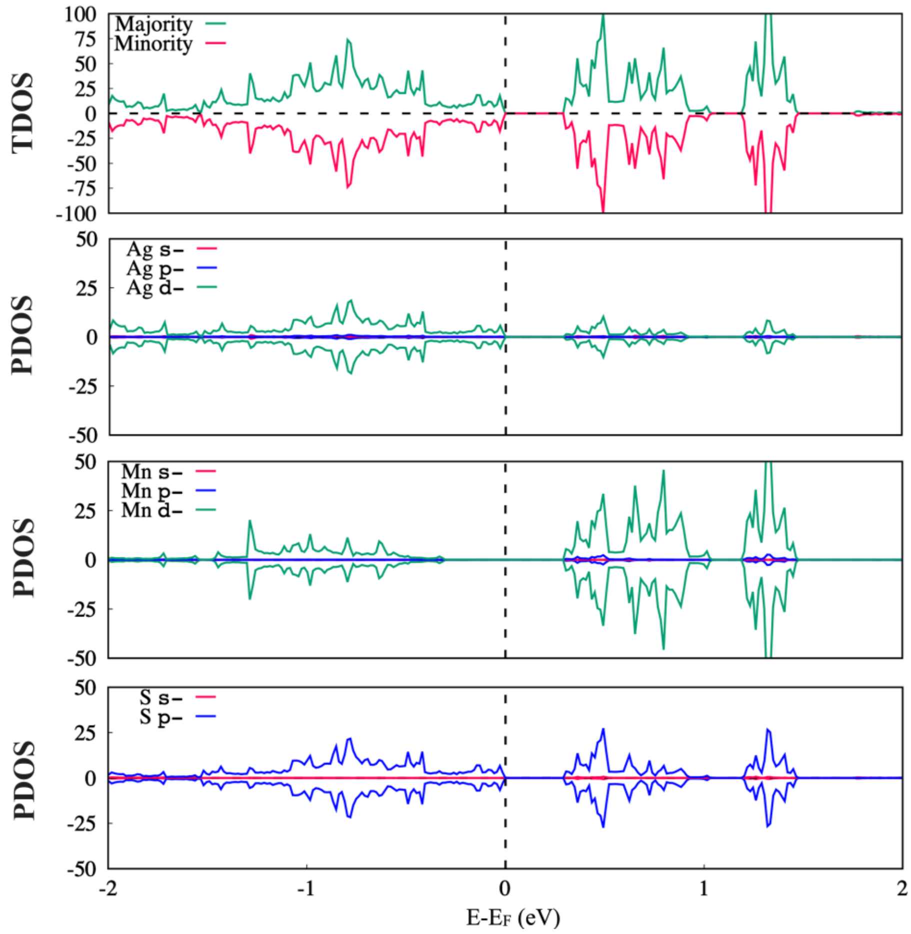

Figure 5. The total and the atom projected DOS for Ag_3MnS_4 under spin polarization.

4. Conclusion

In the study, the suitable spin orientation and the electronic character of sulvanite type silver-based sulfide (Ag_3MnS_4), which conforms to $P\bar{4}3m$ space group and 215 space number, has been examined in elaborated. For different spin orientations, the formation energies and energy-volume graphics indicate that, the magnetic nature of this ternary silver-based sulfide system is A-type antiferromagnet. This magnetic nature of Ag_3MnS_4 sulfide is make it so essential for the future technological applications. The selected material for the present study behaves like a semiconductor because there is a same band gap in up and down spin states (E_g = 0.325 eV) in the calculated band structure within GGA. The observed semiconducting electronic band structure of new ternary silver-based sulfide (Ag_3MnS_4) is promising for using in some applications in technology and industry.

Author Statement

Author 1 Aytaç Erkişi: Investigation, Original Draft Writing.
Author 2 Gökhan Sürücü: Investigation, Validation, Review and Editing.

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Conflict of Interest

As the authors of this study, we declare that we do not have any conflict of interest statement.

Ethics Committee Approval and Informed Consent

As the authors of this study, we declare that we do not have any ethics committee approval and/or informed consent statement.

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