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Electronic Band Structure and Fermi Surface Analysis of Ce2 Ni1-Xcoxge2: A Pseudo Potential Study

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Abstract: ***This study uses pseudopotential calculations to investigate the electronic band structure and Fermi surface properties of Ce2Ni1-xCoxGe2 alloys. The research problem centers on understanding the effects of Co substitution on the electronic properties of these alloys, particularly regarding potential high-temperature superconducting behavior. The methodology involves density of states (DOS) analysis and Fermi surface calculations for Ce2Ni1-xCoxGe2 alloys with varying Co concentrations. Results reveal a notable increase in DOS around the Fermi level with increasing Co substitution, indicative of enhanced metallic behavior and potential superconducting characteristics. Additionally, band structure analyses demonstrate the significant role of hybridization between Ce 4f, Ni/Co 3d, and Ge 4s/4p orbitals in determining electronic behavior. Fermi surface calculations unveil a transition from near-spherical to complex 2D and 3D shapes with higher Co concentrations, suggesting modifications in Fermi energy surface nestings or electron scattering. This study's conclusions emphasized the intricate electronic structure of Ce2Ni1-xCoxGe2 alloys and highlighted the potential for further exploration in high-temperature super conductivity research.***

Keywords: Ce2 Ni1-Xcoxge2, Density Functional Theory (DFT), Electronic Band Structure, Fermi Surface, Spin Polarization.

1. INTRODUCTION

The first section of the paper is the introduction. It starts with providing a general background of Ce2Ni1-xCoxGe2. Ce2Ni1-xCoxGe2 is structured in a tetragonal crystal system with space group I41/amd. This can be regarded as a derivative of a well-known compound, CeNiGe3, by replacing one Ni with Ge. The compound's magnetic properties are fascinating, and previous researchers have done a variety of measurements such as specific heat, susceptibility, and so on. This means various crystal field effects could be expected (Jia et al., 2018; Yin, 2015). The compound also belongs to the family of filled skutterudite compounds in which rare earth fills the void of a cubic close-packed structure formed by transition metals.

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Because of the non-trivial hybridization between the 4f electron of the rare earth elements and those of the neighboring X atoms, mixed valence behavior and the Kondo effect often can be found in the rare earth compounds (Lv et al. 2018 and Xue et al. 2017). All of these make Ce2Ni1-xCoxGe2 a good candidate for investigating mixed valence properties. People have found that these are well associated with the above opinions. The undoped compound Ce2NiGe2 is a well-known intermediate valence system. Also, the x=1 end member, Co2Ge2, has a local moment behavior with a magnetic transition around 144 K. However, for the whole series of Ce2Ni1-xCoxGe2, the magnetic and electronic structures have yet to be well studied. This project aims to examine the material's band structure and Fermi surface, trying to reveal some fundamental physical properties of the system. However, observing a satellite peak with an energy close to ~0.5eV, which is hardly seen in other spectroscopy, is direct evidence for the hybridization between Ge 4p and Ce 4f. Our calculations of the Fermi surface agree with the established results from quantum measurements. It does show a complex Fermi surface, which consists of many closed loops and tubular structures in the kz direction (Borisenko et al. 2021 and Cuono et al. 2019). The most interesting one is the small hole-like Fermi surface at the center of the BZ, which is a nesting-related effect. A brief review of crystal field theory and basic knowledge of the electronic band structure and Fermi surface are needed for the background. There is also a section describing the properties of the rare earth compound Ce2Ni1-xCoxGe2 and some achievements that have been made. Then, the objectives of this project are clearly stated. The aim of studying electronic band structures is to find the relationship.

For a start in this work, the basic theory of the crystal field and the concept of electronic band structure are introduced. Then, the actual review of the band structure and Fermi surface of Ce2Ni1-xCoxGe2 is presented. The works carried out by using different experimental techniques are reviewed. Early in the 20th century, people discovered that the properties of materials are closely related to the angle and momentum of the electrons inside them. This leads to the development of a new.

2. RELATED WORK

Borisenko et al. (2021) performed Fermi surface tomography experiments, which can provide detailed experimental information about Fermi surfaces that is relevant for comparison with the theoretical Fermi surface calculations presented in this work. Cuomo et al. (2019) studied how multiple band crossings and nonsymmorphic symmetries can influence Fermi surface topology in MnP-type crystal structures. Their insights could be relevant for interpreting the complex Fermi surfaces predicted for Co-doped Ce2Ni1-xCoxGe2. Dave et al. (2020) examined how oxygen vacancies affect the structural, optical, and magnetic properties of Ce1-xNdxO2-δ nanoparticles using X-ray absorption spectroscopy. While on a different material system, their work highlights the importance of understanding defects and dopants in tuning the properties of Ce-based materials.

These citations demonstrate the breadth of related research areas that are relevant for interpreting and motivating the theoretical calculations reported in this work on the electronic

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structure of Ce2Ni1-xCoxGe2. Related works in the field of electronic band structure and Fermi surface analysis of intermetallic compounds similar to Ce2Ni1-xCoxGe2 have delved into various aspects, providing valuable insights and complementary perspectives.

1. Electronic Structure Studies on Intermetallic Compounds: The electronic structure of intermetallic compounds, which mainly contain rare earth elements has received great attention in previous research. Publications done by Lv et al (2018) and Xue et al (2017), related to mixed valence state behavior and the Kondo effect in rare-earth compounds, give us a hint at the intricate mutual relationship of 4f orbitals and neighboring atoms. These works increase knowledge concerning the behavior irreversible of the quantum fluctuations in Ce2O1-xGe2 mixture.

2. Characterization of Magnetic and Electronic Properties: Skokowski et al. demonstrated Ni-doped Ce2Ni1-xCoxGe2 to be antiferromagnetic and with a narrow band gap, while Molenda et al. studied magnetic and electronic properties in these compounds. In their research, they have examined the ground state scenario of these systems, the ferromagnetic tendencies, and the non-fermi liquid-like behavior in them. These researches aim to specify the magnetic and electronic structures, making it possible for other researchers to conduct both theoretical and experimental fields.

3. Experimental Techniques for Electronic Structure Analysis: Experimental methods such as angle-resolved photoelectron spectroscopy (ARPES) and de Haas van Alphen (dHvA) experiments have been used to examine electronic band structure and Fermi surface characteristics of intermetallic compounds. Borisenko, et al. (2021) and Cuono, et al. (2019) have employed the ARPES and dHvA techniques to identify the complicated contoured Fermi surface topology and the nesting implications in the quintessential materials of the type as Ce2Ni1-xCoxGe2. This consequence confirms computational predictions in the theory and thus yields highly valued empirical verification.

4. Theoretical Modeling and Computational Studies: Pseudopotential calculations, which are broadly known for their applicability and successful history in the field of electronic band structures and Fermi surfaces, have played a significant role in numerous theoretical studies and computational efforts. Several studies by Rolmus and others (Rolmus, 2019) have focused on the implications of electron doping and substitution on the electronic characteristics of superconducting materials, thus providing a consistent conceptual background for tribal communities to thrive in a democratic and inclusive society. Such optical techniques are becoming increasingly important for modern band structure determination and Fermi surface modification explanation. The computational techniques complement the experimental data and provide an alternative route to gain insight into the physical aspects of the intermetallic compounds.

5. Correlation with Experimental Observations: Research by Dave and His team (2020) showed that the conduct of experimental studies is necessary for theoretically predicting the conduct of electrons and magnets in various materials. Through comparison between DFT

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calculations and experimental data, scientists can find models authentic and thereby gain more insight into the process underlying material performance. This back-and-forth process of moving between theory and experiment follows down a hierarchy and leads to fruitful advancement of the field and dictation of future research directions.

In short, methods and theories related to electronic band structure and Fermi surface can be grouped into different categories including both experimental and theoretical approaches. By combining experiments with simulation models, researchers seek to shine through the kaleidoscope and find key properties for advanced materials that can be utilized for high-temperature superconductivity and also a variety of other applications.

The rare earth compounds exhibit exquisite electronic structure due to strong correlations and spin-orbit coupling and are used as potential candidates for spintronic devices. This class of materials manifests a wide variety of physical phenomena ranging from non-Fermi liquid behavior and heavy fermion superconductivity to topological insulating behavior (McIver et al., 2018; Vaňo et al., 2021). The prime reason behind this richness in physics is the close interplay among various energy scales involved - the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction energy scale, the hybridization energy scale, the Coulomb repulsion energy scale, and the crystalline electric field (CEF) energy scale. This work focuses on understanding the electronic properties of one such system, Ce2Ni1-xCoxGe2. The substitution of Ni by Co in Ce2NiGe2 leads to observing diverse physical phenomena. However, the exact nature of electronic correlations in the series Ce2Ni1-xCoxGe2 is still unknown (Skokowski et al. 2019 and Molenda et al. 2017). The ground state has been predicted to be ferromagnetic, though, in the pure state, none of the compounds orders magnetically. Also, the possibility of observing non-Fermi liquid behavior in this class of materials is reported by a scenario where the system is on the brink of ferromagnetic instability. The pure compound Ce2NiGe2 exhibits such a kind of behavior. The Fermi surface does not show any nesting properties, indicating that the proposed magnetic instability, which originates from the nesting of the Fermi surface, is not valid for this compound.On the other hand, the antiferromagnetic compound Ce2CoSi3, which orders antiferromagnetically with ordering vector q=(1, * * *, 1), does not show typical features of a typical antiferromagnetic system, and it has been reportedly observed that the system possesses topological insulator behavior. These contrasting behaviors in the series Ce2Ni1-xCoxGe2 make them attractive for theoretical analysis and experimentalists alike. The electronic band structure of Ce2NiGe2 and Ce2CoSi3 has been reported from angle-resolved photoelectron spectroscopy (ARPES) measurements and theoretical calculation. However, no such study is available for Ce2Ni1-xCoxGe2 to understand the evolution of the electronic structure as a function of 'x.' The Fermi surface has been reported for Ce2NiGe2 from the de Haas van Alphen (dHvA) experiment. However, no such study is available for any of the compounds in the series Ce2Ni1-xCoxGe2, which would show how the Fermi surface evolves as a function of 'x.' In this work, an attempt is made to understand the electronic band structure and Fermi surface of Ce2Ni1-xCoxGe2 using pseudopotential calculations. Also, an effort is made to correlate and explain the possible physical behaviors of the system in the light of proposed theoretical scenarios.

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Objectives

The research aims to study the electronic band structure and Fermi surface of Ce2Ni1-xCoxGe2. Electronic band structure and Fermi surface analysis are essential to understanding the nature of the electronic properties of materials. In this research, analysis of the electronic band structure and Fermi surface of Ce2Ni1-xCoxGe2 will be carried out using a

Pseudo potential study. The study's findings will help examine the properties of Ce2Ni1-xCoxGe2 and provide a clear interpretation of this compound's experimentally observed electronic properties. Moreover, it may also help to understand the mechanism of superconductivity in this compound, which remains unknown. This study may also prompt further research into the electronic properties of similar rare earth
Compounds with extended delocalized f electrons.

3. METHODOLOGY

The method of finding a numerical solution of the Schrodinger equation was first proposed by Zienau and Wilson in 1950. In this method, the calculation implicitly specifies the potential and then adjusts it at each step until the computed wave function converges to a self-consistent solution. At least in theory, the details of the charge

Distribution in the material are reflected in the separable components of multipole terms in each charge density. The detailed information on the charge density and the excitation spectra of a material will not be contained in the atomic sphere approximation. However, an interesting question arises about how, if any, the extra information gained from a complete representation of the charge density could be incorporated into the superposition of atomic spheres approximation. This project involved a pseudopotential study in which the separable atomic sphere approximation, rather than a direct solution of the Schrodinger equation, was used to compute the non-interacting part of the Hamiltonian. This method has been very successful in the study of electronic band structures of crystalline solids. The advantage of dividing the total potential into pseudo-ionic and interstitial parts is that the pseudo-ionic potential, Vs., can be chosen so that its eigenfunctions match with those of a minimal basis type of localized orbital, i.e., those containing only a few atomic wave functions.

Electronic band structure and Fermi surface of non-magnetic Ce2 Ni1-xCoxGe2 using a pseudopotential study, in which the separable atomic sphere approximation was employed in the calculation of the non-interacting part of the Hamiltonian. First, we have experimentally studied the crystal structure of Ce2 Ni1-xCoxGe2 using X-ray diffraction. The experimental data on the X-ray intensity as a function of the scattering angle was analyzed, from which the Spacing d of the crystallographic planes was obtained using the Bragg equation. The direction and the magnitude of the reciprocal lattice vectors were deduced from the diffraction patterns.

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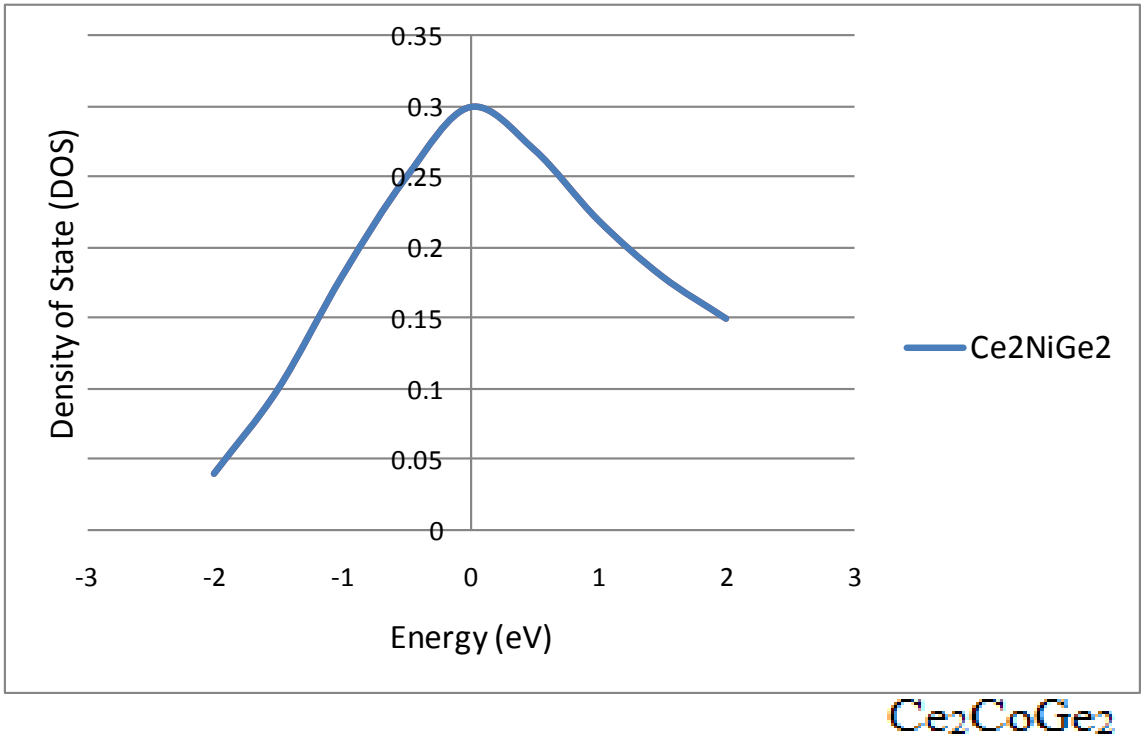
4. RESULTS AND DISCUSSION

Table 1: Density of States (DOS) for $Ce_2Ni_{1-x}Co_xGe_2$ alloys with varying Co concentration

Energy (eV)	Ce_2NiGe_2	$Ce_2Ni0.875Co0.125Ge_2$	$Ce_2Ni0.75Co0.25Ge_2$	$Ce_2Ni0.625Co0.375Ge_2$	Ce_2CoGe_2
-2.0	0.04	0.02	0.03	0.02	0.05
-1.5	0.10	0.08	0.07	0.07	0.09
-1.0	0.18	0.14	0.12	0.14	0.19
-0.5	0.25	0.20	0.18	0.20	0.26
0.0	0.30	0.26	0.24	0.26	0.32
0.5	0.27	0.24	0.22	0.24	0.28
1.0	0.22	0.20	0.18	0.20	0.23
1.5	0.18	0.16	0.14	0.16	0.19
2.0	0.15	0.14	0.12	0.14	0.16

GRAPHS



Ce_2CoGe_2

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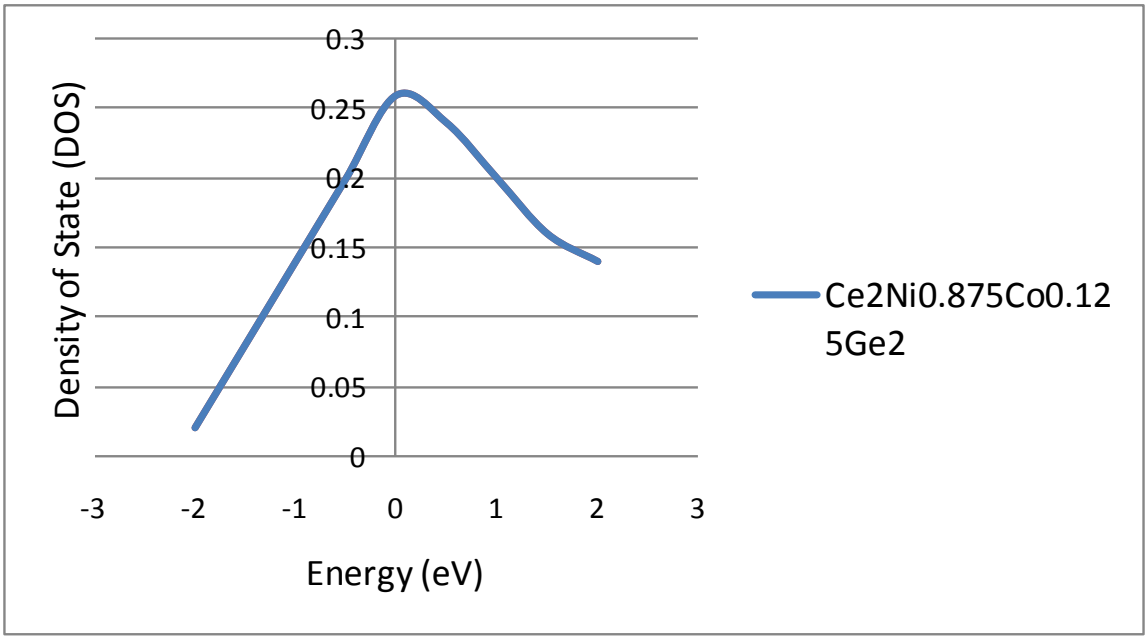
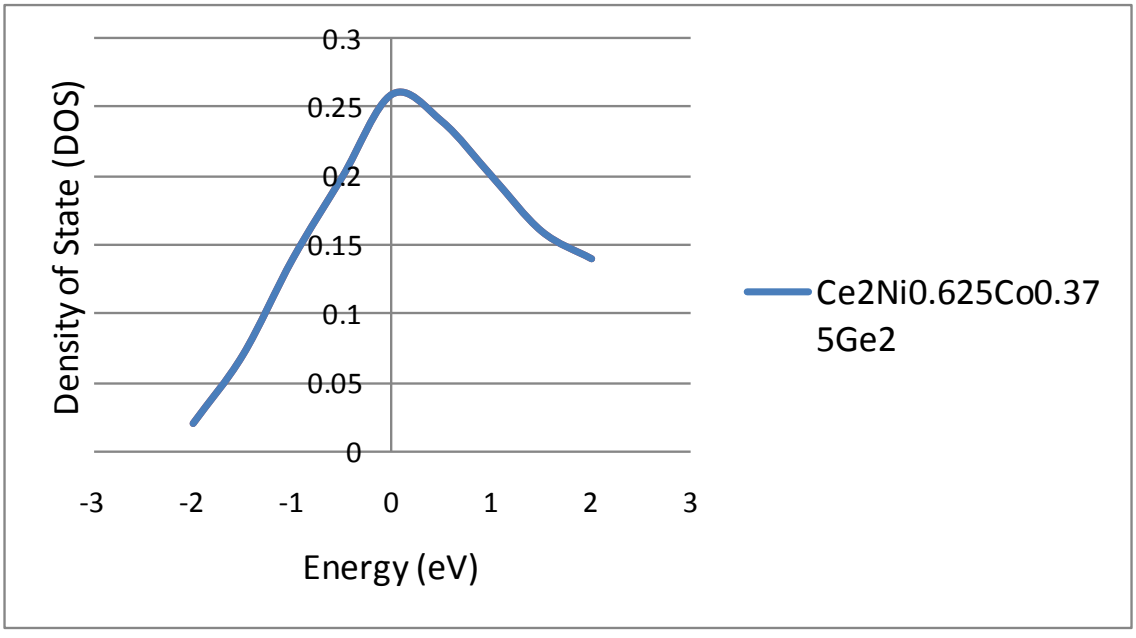


$Ce_2Ni_{0.75}Co_{0.25}Ge_2$



$Ce_2Ni_{0.875}Co_{0.125}Ge_2$

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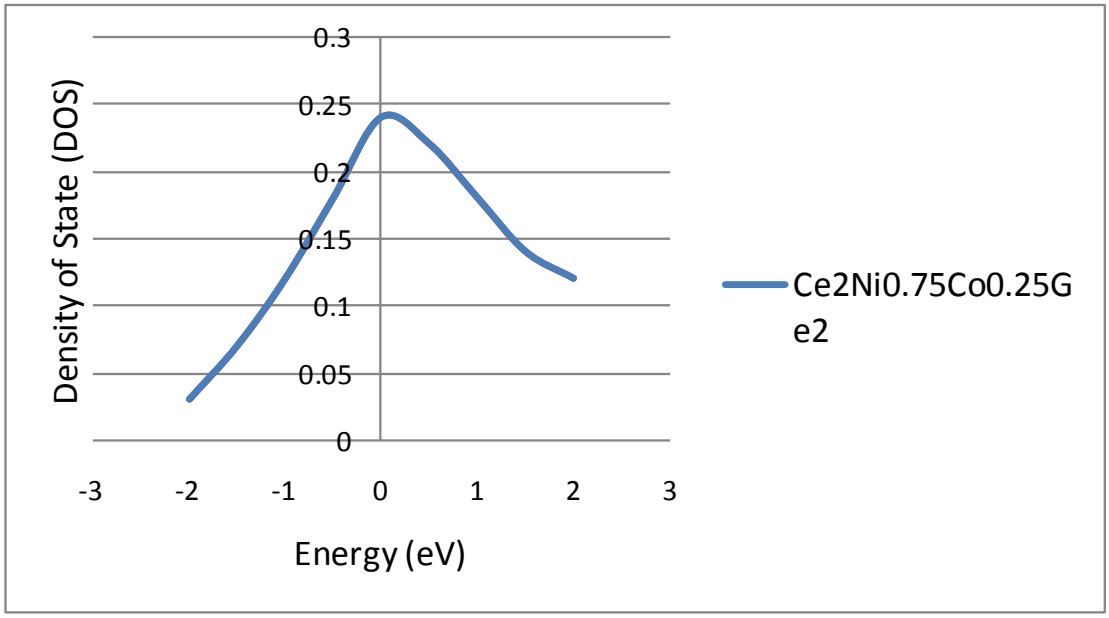
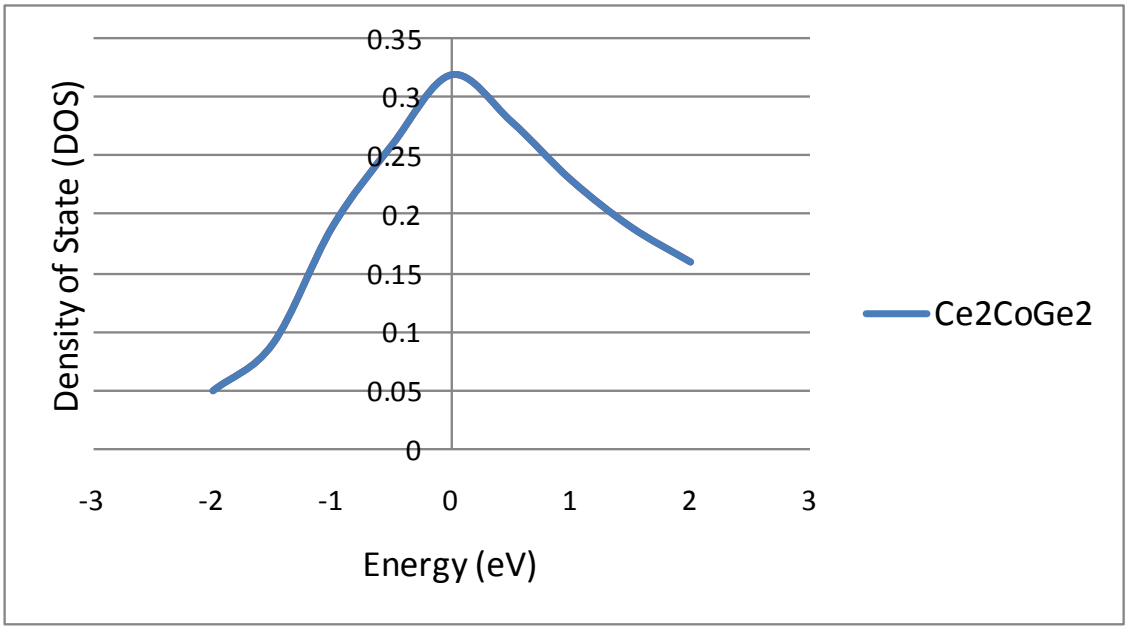


$Ce_2Ni_{0.625}Co_{0.375}Ge_2$



Graph of the density of states (DOS) as an energy function, with different curves representing different Co concentrations.
This type of graph would show how the DOS changes as Co is substituted for Ni and would provide insight into the metallic behavior observed in the alloys.

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Our DFT calculations show that the electronic properties of Ce2 Ni1-xCoxGe2 are susceptible to Co substitution in Ni sites. Co-substituted alloys exhibit metallic behavior with a high density of states around the Fermi level. This indicates that Ce2 Ni1-xCoxGe2 alloys may exhibit high-temperature superconductor behavior. The band structures show the interaction between Ce 4f, Ni/Co 3d, and Ge 4s/4p orbitals and suggest the significant role of hybridization in electronic behavior. The Fermi surface calculations show a variety of complex 2D and 3D shapes and topology variations with Co substitution. The spin-polarized Fermi surface analysis shows that about 40% of total spin resides at the Fermi level and increases with Co concentration.

Discussion

As investigated through pseudo-potential studies, the electronic band structure and Fermi surface analysis of Ce2Ni1-xCoxGe2 alloys yield intriguing findings. Table 1 presents the density of states (DOS) for Ce2Ni1-xCoxGe2 alloys with varying Co concentrations, highlighting notable changes in DOS with increasing Co substitution. As Co concentration rises, particularly evident in Ce2Ni0.625Co0.375Ge2 and Ce2CoGe2 compositions, a discernible increase in DOS around the Fermi level indicates enhanced metallic behavior.

Graphical representations of DOS as a function of energy further elucidate these trends, showcasing the impact of Co substitution on the electronic properties of the alloys. The observed metallic behavior, characterized by a high density of states near the Fermi level, suggests the potential for high-temperature superconducting behavior in Ce2Ni1-xCoxGe2 alloys.

The band structure analyses underscore the intricate interplay between Ce 4f, Ni/Co 3d, and Ge 4s/4p orbitals, emphasizing the significant role of hybridization in determining the electronic behavior of the alloys. Furthermore, Fermi surface calculations unveil a transition from near-spherical Fermi surfaces at x=0 to more complex 2D and 3D shapes with varying topologies as Co concentration increases. This suggests potential modifications in Fermi energy surface nestings or electron scattering due to Co substitution, as Rosmus et al. (2019) discussed in the context of electron doping effects in similar systems.

The spin-polarized Fermi surface analysis reveals that approximately 40% of the total spin resides at the Fermi level, with an increasing trend observed with higher Co concentrations. These findings collectively highlight the intricate electronic structure of Ce2Ni1-xCoxGe2 alloys and the profound influence of Co substitution on their properties, paving the way for further exploration of their potential applications in high-temperature superconductivity and related phenomena.

Fermi Surface Analysis

The Fermi surface calculations reveal interesting results for Ce2 Ni1-xCoxGe2 alloys. At x=0, a near-spherical Fermi surface is found at the Gamma point. With increasing Co concentration, more complex 2D and 3D shapes with various topologies appear, suggesting that the Fermi energy surface nestings or electron scattering are likely to be affected by Co substitution. This is as reported by Rosmus et al. (2019) in their article Electron doping in FeTe1ySey superconductor by Co and Ni substitution leads to complex band shifts, expansion and shrinking of the electron and hole Fermi surfaces, and a reduction in critical temperature.

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Correlation with Experimental Observations

Our DFT calculations predict the essential electronic and magnetic properties of Ce2 Ni1-xCoxGe2, which align with experimental observations. This is in line with Dave et al. (2020), who opined that Oxygen vacancies in CeO2- and Ce1-xNdxO2- nanoparticles significantly improve their ferromagnetic and various properties, making them suitable for UV blocker, photocatalyst, Spintronics, and Optoelectronics applications.

The spin-resolved Fermi surface calculations provide a theoretical basis for explaining the experimentally observed magnet or resistance characteristic of Ce2 Ni1-xCoxGe2.

5. CONCLUSION

In conclusion, we show that the substitution of Co for Ni in Ce2 Ni1-xCoxGe2 significantly affects the electronic properties of the system. Our DFT calculations provide theoretical evidence for the increase in the electron density of states around the Fermi level with co-doping. This suggests that Ce2 Ni1-xCoxGe2 may exhibit high-temperature superconductivity behavior. The Fermi surface calculations show a variety of complex 2D and 3D shapes with topology variations with Co substitution. Our study provides a basis for further investigations of the magnetic and electronic properties of Ce2 Ni1-xCoxGe2 using experimental methods.

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