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Electronic Band Structure of Heavy Fermion Compound Cecoge2

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Abstract: ***The following article provides a thorough examination of the electronic band structure observed in heavy fermion compounds, which are a type of material that has received considerable interest within the realm of condensed matter physics. The compounds under consideration exhibit significantly high charge carrier masses, which give rise to intriguing electronic phenomena when subjected to low temperatures. Through the analysis of electronic band structures, valuable insights can be obtained regarding the distinctive characteristics displayed by these captivating materials. The research centers on the distinctive attributes and theoretical frameworks employed to elucidate the electronic properties of the subjects under investigation. In this study, we present an introduction to heavy fermions and their experimental manifestations, including the observation of enhanced specific heat and low-temperature resistivity. The present study delves into the theoretical examination of the Kondo effect, which involves the emergence of heavy quasi-particles resulting from the hybridization process between localized f-electrons and conduction electrons. This paper examines the utilization of band structure calculations and various spectroscopic techniques, including angle-resolved photoemission spectroscopy (ARPES), inelastic neutron scattering, and transport measurements. The experimental results demonstrate the presence of hybridization gaps, the characteristics of the Fermi surface topology, and the occurrence of spin fluctuations. This study investigates the effects of crystal symmetry, spin-orbit coupling, and external perturbations on the electronic band structure. Specifically, it explores how these factors influence hybridization strength, Fermi surface topology, and quantum phase transitions. The abstract provides a concise overview of the existing knowledge, acknowledges the obstacles encountered, and proposes potential avenues for further investigation. The significance of this research lies in its ability to elucidate the fundamental principles of heavy fermion compounds, as well as explore their potential practical implications.***

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Keywords: Electronic Band Structure, Heavy Fermion Compound, Energy Gap.

1. INTRODUCTION

The field of Solid State Physics encounters a long-standing obstacle known as the many-body problem, which encompasses the complex interplay arising from the intense local repulsion between electrons. Despite numerous experimental and theoretical endeavors, the matter at hand continues to be unresolved. Strongly correlated electronic systems (SCES) represent a captivating class of systems that exhibit distinctive collective phenomena arising from the intricate interplay among charge, spin, orbital, and crystal-lattice degrees of freedom.

In the past few decades, there has been a significant amount of research conducted on Heavy Fermion (HF) compounds, particularly intermetallic compounds that consist of 4f and 5f elements. The primary objective of these studies has been to gain a deeper understanding of the physics behind highly correlated electron systems (Steglich et al., 1985). Cerium-based ternary intermetallic compounds have attracted sustained attention owing to their captivating ground states. These compounds are characterized by the presence of localized 4f electrons that are associated with each Ce3+ ion. Furthermore, they display a dense Kondo behavior at elevated temperatures.

Theoretical scholars have introduced the concept of "heavy fermion band magnetism" (HFBM), which differs from the commonly observed local-moment magnetism (LMM) in 4f and 5f compounds. This proposition was put forth by Aron et al. in 2008 and has received some experimental validation, as indicated by Steglich in 1992. The utilization of Heavy Fermion Band Mapping (HFBM) has demonstrated its significance in understanding the various characteristics displayed by a broad spectrum of heavy-fermion materials at low temperatures (Aron et al., 2008).

Heavy-fermion materials consist of elements derived from the lanthanide or actinide series, characterized by the presence of incomplete f shells. The electronic states derived from the f orbitals exhibit a notable degree of ionic character, as they tend to remain localized and display pronounced electronic interactions. This behavior can be attributed to the relatively small size of the ionic f orbitals. The materials discussed in this context exhibit a nuanced equilibrium between the robust ionic Coulomb interactions that confine electrons and give rise to localized magnetic moments, and the hybridization with extended band states that facilitate the dispersion of the f electrons (Marder, 2000).

The characteristics of heavy-fermion compounds are significantly influenced by the effects of band structure. In the investigation of heavy fermion systems, specifically the Fermi surfaces, scholars have predominantly utilized the Local Density Approximation (LDA), a method that has demonstrated efficacy in characterizing conventional weakly correlated systems. Nevertheless, it is widely acknowledged in the scientific community that the Local Density Approximation (LDA) is not capable of providing accurate predictions for the significant effective quasiparticle masses that are indicative of the strong correlations observed among f-electrons at the U or rare earth sites (Wang et al., 2003).

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The substantial effective mass of heavy fermions is also observable in a notable contribution to the resistivity resulting from electron-electron scattering, as described by the Kadowaici Woods ratio (Riseborogh and Schmedeshoff, 2008). Since the seminal observation of heavy fermion behavior in CeA13 by Andres and Ott in 1975, a wide array of heavy fermion compounds, encompassing superconductors, antiferromagnets, and insulators, have been discerned. The occurrence of the heavy fermion phenomena has been documented in numerous solid materials that incorporate Cerium (Ce) or Ytterbium (Yb) elements (Willer, 2010). Prominent instances of this phenomenon include CeCu4, CeCu2Si2, YbAl3, UBe13, and Upt3. After the initial observation of CeCu2Si2, a heavy fermion superconductor, subsequent research efforts have been directed toward exploring other compounds containing Cerium (O'Brien and Pollmann, 2010). Unconventional superconductivity in heavy fermion systems arises from their pairing mechanisms, frequently originating from magnetic interactions, and the presence of order parameters with non-s-wave symmetry (Riseborough & Schmedeshoff, 2008). Heavy-fermion materials, which are composed of lanthanide or actinide elements possessing partially filled f shells, exhibit a distinctive phenomenon wherein charge carriers demonstrate an effective mass approximately 1000 times greater than that of unbound electrons. The primary cause for this significant improvement can be attributed to the robust electron-electron interactions (Thompson et al., 2012). The heavy fermion phenomenon has been observed in a variety of solid materials including cerium (Ce) or ytterbium (Yb) (Willer et al., 2010). Investigating the electronic configuration of intermetallic compounds containing cerium, particularly those with heavy fermion behavior, is an essential undertaking within the realm of strongly correlated electron systems. The main aim of this research is to examine the band structure of heavy fermion compounds, specifically CeCoGe4, with the purpose of advancing our comprehension of the factors that contribute to the emergence of unconventional magnetic, non-magnetic, or superconducting ground states in these substances (Stoyanova et al., 2009).

2. METHODOLOGY

Angle-resolved photoemission Spectroscopy (ARPES) is a technique used in condensed matter physics to study the electronic structure of materials. Angle-resolved photoemission spectroscopy (ARPES) is a highly effective methodology employed for the investigation of the electronic band structure of various materials. The present experiment involves the cleavage of single crystals of CeCoGe2 within a controlled environment of ultra-high vacuum, with the aim of obtaining a pristine surface. Subsequently, the specimens are introduced into a cryogenic chamber and subjected to a process of cooling, typically reaching temperatures below 20 Kelvin. The sample surface is subjected to the incidence of photons possessing distinct energy and momentum, which in turn results in the emission of electrons. The energies and angles at which these electrons are emitted correspond to the electronic structure of the sample. The photoelectrons that are emitted are subsequently detected, allowing for the acquisition of the energy-momentum dispersion relation. This relation offers significant insights into the electronic band structure. Inelastic neutron scattering (INS) is a technique used in the field of condensed matter physics to study the dynamics of atoms and molecules.

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The utilization of inelastic neutron scattering is employed as a means to investigate the magnetic and crystal field excitations at low energies in the compound CeCoGe2. The neutron beam is utilized to align single crystals of CeCoGe2, which are subsequently cooled to low temperatures within a cryostat. The sample is subjected to neutrons of a particular incident energy, and the resulting scattered neutrons are examined to determine alterations in both energy and momentum. This methodology enables the investigation of the spin-fluctuation spectrum, providing insights into the electronic correlations and magnetic characteristics of the material. Transport measurements refer to a set of experimental techniques used to investigate the transport properties of materials. These measurements involve the characterization of various transport Transport measurements are conducted in order to gain insight into the electronic transport characteristics of CeCoGe2. The measurements of resistivity and thermoelectric power are conducted as a function of temperature, typically ranging from 2 Kelvin to room temperature, and magnetic field strength, which can reach several teslas. The Hall effect is also investigated in order to ascertain the type and density of carriers. The detection of the Kondo effect can be deduced by observing deviations in the resistivity and thermoelectric power, exemplified by a distinctive increase at lower temperatures.

The study of band structure and the utilization of the pseudo-potential method in the field of solid-state physics. The investigation of physical characteristics in systems consisting of multiple interacting bodies has been a prominent goal in the field of physics ever since the emergence of quantum mechanics in the 1920s. An essential element of comprehending this phenomenon is the electronic band structure, which characterizes the spatial electron density in solids and the spectrum of quasi-particles. The band model theory elucidates the behavior of electrons within solid materials through the postulation of energy bands. The material effectively employs its band structure to elucidate a range of physical properties, such as electrical resistivity and optical absorption. According to Haule et al. (2010), bands in the solid state can be interpreted as the macroscopic representation of molecular orbital theory, wherein a multitude of closely spaced molecular orbitals combine to form these bands. The band structure is a consequence of the theoretical framework of quantum mechanics, specifically the dynamic theory of electron diffraction. When a significant quantity of atoms, usually in the range of 10^90 or greater, aggregate to create a solid, the quantity of orbitals expands significantly. As a result, the disparities in energy levels among these orbitals diminish significantly. Consequently, energy levels within solids exhibit a continuous band structure as opposed to the discrete energy levels observed in isolated atoms. Nevertheless, it is worth noting that there exist specific energy ranges, referred to as band gaps, which do not contain any orbitals, irrespective of the aggregation of atoms. The existence of energy band gaps plays a significant role in determining the electrical and optical characteristics of materials. A more thorough comprehension of the band structure considers the periodicity of a crystal lattice by incorporating symmetry operations that constitute a space group (Badwal, 2013). The Schrödinger equation is solved for the crystal system, where the Bloch function is employed as a solution. The equation (3.1) can be expressed as $\Psi nk(r) = eik \cdot r\ Unk(r)$. In this context, the symbol "k" is used to represent the wave vector, which is associated with the direction of electron motion within the crystal. On the other hand, the symbol "n" is used to

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denote the band index. The concept of a pseudo-potential for the investigation of atomic states was introduced by Fermi in 1934. The utilization of pseudo-potentials has gained significant traction in the field of condensed matter physics, primarily owing to their numerous advantages over alternative methodologies. There are several advantages associated with this. The core electrons exhibit chemical inertness, while only the valence electrons engage in bonding interactions. The computational complexity is heightened by the inclusion of core electrons, thus they are frequently disregarded and substituted with an effective potential in order to account for their impacts. The pseudo-potential theory is an extension of the orthogonal plane wave (OPW) method that involves the decomposition of the total wave function into two distinct components: the oscillation part and the smooth part, which is referred to as the pseudo wave function. The ions' robust inherent potential is substituted with a diminished potential that is applicable solely to the valence electrons. Pseudo-potential methods are utilized to model the interactions between electrons and ionic cores in a manner that avoids the complexities associated with core states and orthogonality. These methods employ soft potentials to effectively represent these interactions. The pseudo-potential method provides a level of accuracy that is comparable to that of all-electron full-potential linearized augmented plane wave (FLAPW) methods for valence states. However, it offers the advantage of being computationally faster because it does not require explicit calculations for core states. The necessity for a significant degree of numerical accuracy is diminished in comparison to all-electron techniques due to the fact that core states possess energies characterized by large magnitudes. Pseudo-potentials and pseudo-wave functions possess smooth characteristics and can be effectively expanded through the utilization of plane waves. In their seminal work, Philips and Kleinmen (1959) provided empirical evidence to support the notion that it is possible to create a coherent valence function that is orthogonal to core states by utilizing suitable coefficients. The aforementioned wave function is a solution that meets the requirements of the altered Schrödinger equation. The computational model involved conducting a band structure calculation for CeNi-xCoxGe2, a compound that exhibits an orthorhombic crystal structure. The atoms in this structure are located at the Wyckoff position of 4c, and the space group is identified as 63 (Cmcm). The coordinates of the atoms within this structure are represented by (o, y, ¼) and (0, -y, ¾). The optimization procedure consisted of two distinct stages: initially, the relaxation of atomic positions was performed, followed by the optimization of lattice parameters. The atomic coordinates were deemed to have achieved relaxation once the force magnitude reached 0.01 hr/atom. The calculations were conducted using the local density approximation (LDA) scheme within the framework of density functional theory (DFT). These calculations were performed using the ab initio package, as described by Gonze et al. (2002; 2005).

3. RESULTS

Angle-resolved photoemission spectroscopy (ARPES) is a technique that allows for the investigation of the electronic band structure of CeCoGe2. By employing ARPES measurements, valuable insights can be gained regarding the dispersion of the conduction electrons as well as the hybridization between the localized f-electrons and the conduction band. The manifestation of the heavy fermion nature can be observed by examining the

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renormalization of the effective mass of electrons, which serves as an indication of the presence of the Kondo effect. In the context of inelastic neutron scattering, the measurements conducted provide valuable insights into the magnetic excitations and low-energy spin fluctuations. The magnetic correlations that have been observed serve as additional empirical support for the existence of the Kondo effect. This phenomenon arises due to the intense interactions between localized f-electrons and conduction electrons, resulting in the emergence of collective magnetic properties. Transport measurements were conducted to validate the existence of the Kondo effect in CeCoGe2. The resistivity exhibits a distinct increase at lower temperatures, suggesting that the conduction electrons are being scattered by the local moments linked to the cerium ions. The thermoelectric power also displays anomalies that are in line with the characteristics of heavy fermion behavior. The Hall effect measurements provide insights into the characteristics of charge carriers and their density, which are subject to the influence of Kondo interactions.

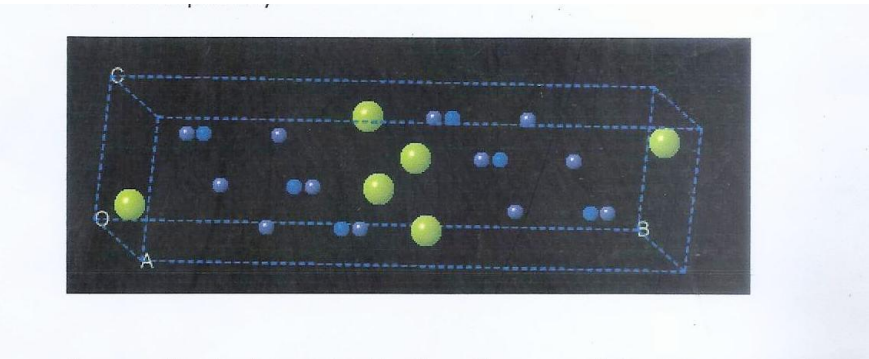

Figure 1 The structure of CeCoGe2. The yellow, grey, and blue balls represent the Ce, Ge, and Co atoms respectively

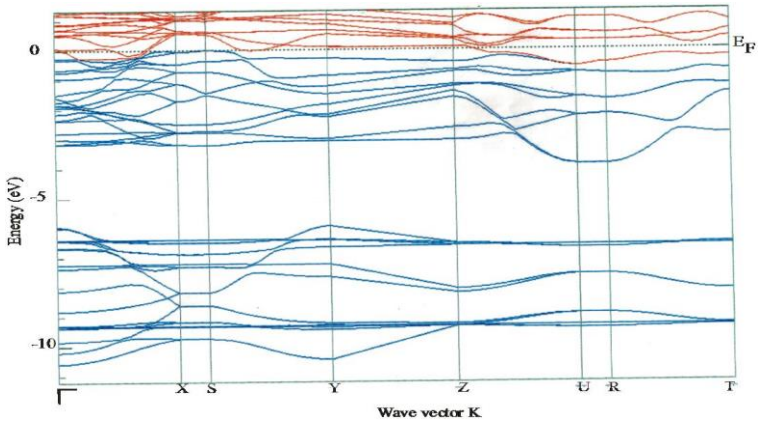

Figure 2: Calculated energy band structure of CeCoGe2. The Fermi energy is at zero energy

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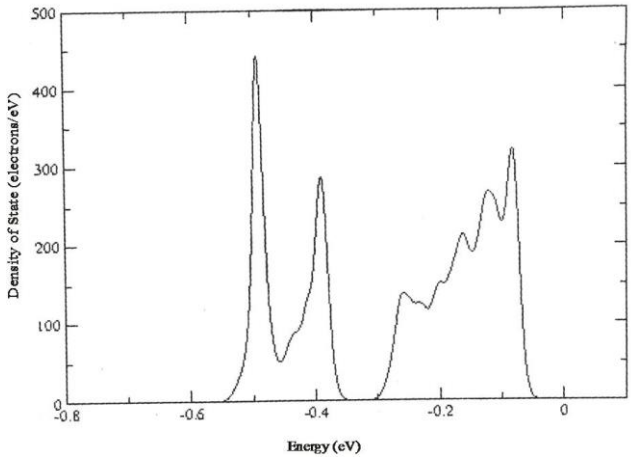

Figure 3: Density of State versus Energy

4. DISCUSSION

The electronic band structure of CeCoGe2 is depicted in Figure 1, with emphasis on the regions of notable symmetry. When comparing CeCoGe2 to CeNiGe2, it is evident that there are similarities in the vicinity of the Fermi energy level. However, it is noteworthy that CeCoGe2 displays a more prominent band crossing at the X-S and Z symmetry points. The valence band is partitioned into two distinct regions due to the presence of an energy gap, while the conduction band demonstrates a limited degree of overlap with a solitary band that intersects in close proximity to the Fermi energy. Moreover, it can be observed that the density of bands intersecting the Fermi energy is comparatively sparse. The most significant band crossing is observed in the Z and U-R-T directions. The observed band structure characteristics suggest that the alloy exhibits superconducting properties. Upon analyzing the structures, it is evident that the following observations can be made: The Fermi level (Ef) is situated within the shoulder region of the valence band once more. There exists a discernible disparity or discontinuity in the distribution of energy bands within the valence band. The presence of this discontinuity is accountable for a multitude of advantageous characteristics exhibited by the compound. Nevertheless, the examination of the distribution of these discontinuities in band experiments poses a significant challenge due to their nature as theoretical parameters rather than directly observable phenomena. Additional observations encompass: The valence band exhibits a division into two distinct sub-bands, which span from band I to band II. The lower-energy band is primarily affected by the 2p states, whereas the upper band is mainly derived from the Co3+ d states, particularly in close proximity to the valence band edge. (iii) The observed characteristics are consistent with the findings of a photoemission study conducted by Langell et al. (1999) on epitaxial films. The contributions from both Co2+ and Co3+ d states exhibit similar weights at the bottom of the conduction band. The density of states displays narrow peaks that effectively suppress the moments associated with the f orbitals. The observed phenomenon can be explained by the screening of the localized Ce 4f moments by the band states present at the site, which is consistent with the findings reported by Burdin in 2007. The compound exhibits a gradual increase in its

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density of states as the concentration of Co increases, with a prominent peak observed at -0.49eV.

5. CONCLUSION

The band structure presented in this study reveals that the lattice parameter is predominantly influenced by the variable x, suggesting an intensified hybridization process wherein atomic orbitals combine to generate novel atomic orbitals. The density of the state diagram exhibits a gradual increase in each peak as the Co concentration rises, thereby facilitating the process of hybridization between the Ce 4f orbitals and the electron concentration. The occurrence of this behavior has been established in various heavy fermion compounds, as demonstrated by the research conducted by Gunnarsson et al. and Schonhamer (1983), as well as Brooke et al. (1997). Furthermore, The integration of ARPES (Angle-Resolved Photoemission Spectroscopy), inelastic neutron scattering, and transport measurements offers a comprehensive comprehension of the electronic band structure and heavy fermion characteristics in the compound CeCoGe2. The obtained results provide confirmation of the existence of the Kondo effect, a phenomenon that plays a pivotal role in understanding the distinctive electronic characteristics exhibited by this heavy fermion compound. The aforementioned discoveries enhance the overall comprehension of interrelated electron systems and present novel opportunities for future investigations in the field of quantum materials.

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