

MAGNETIC ORDERING AND SPIN WAVE DYNAMICS IN TRANSITION METAL
ARSENIDES

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BY

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DISSERTATION

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Abstract

Metallic antiferromagnets have gained interest in recent times due to the possibility of being useful as a memory device. Arsenic forms a large pool of magnetic metals in combination with other transition metals that have largely been ignored so far. In this report, we discover a new ternary metallic arsenide in the Cu-Mn-As phase space, identify its chemical and magnetic structure, and characterize its electrical and magnetic properties. We also carry out the magnetic structure refinement of Mn_3As_2 from neutron powder diffraction data at different temperatures to understand the magnetic ordering in Mn-As compounds. Using inelastic neutron scattering measurements, we determine exchange interactions in Fe_2As , which has the same structure as CuMnAs, showing a highly 2D magnon character although the phonons are 3D. Finally, we report a magnetic-structural coupled transition across 300 K in tetragonal CuMnAs and determine the correct magnetic structure of the compound.

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Chapter 1

Introduction

1.1 Magnetic information storage

2 In information memory storage devices, there is typically a trade-off between the optimum
3 speed or response time and the complexity and size of memory storage [1]. Volatile memory
4 refers to temporary memory storage where the data is lost when the power is removed.
5 Volatile memory such as SRAM (static random access memory) and DRAM (dynamic random
6 access memory) are used as CPU caches and main memory respectively. SRAM has much
7 faster access times and does not require periodic refreshing. However, it requires four to six
8 transistors per bit as compared to one transistor and one capacitor in DRAM devices [2]. Non-
9 volatile memory (NVM) storage devices on the other hand, retain their data for a long period
10 of time until perturbed. Modern computers mostly use flash memory based solid state drives
11 (SSD) and magnetic hard disk drives (HDD) for storing large amounts of data permanently [2].
12 The first HDD was invented in 1956 by IBM and since then, has seen more than eight orders of
13 magnitude improvement in the storage density. However, the trilemma in magnetic recording
14 between poor thermal stability, coercive fields and signal-to-noise ratio has resulted in the
15 HDD reaching a saturation limit in their device performance [3]. Flash memory uses floating
16 gate MOSFETs (metal oxide semiconductor field effect transistors) to store memory and does
17 not contain any moving parts. Although SSD have dominated the NVM marketshare last few
18 years, there is an increasing need for alternative NVM technologies that are fast, low power
19 consuming and have high storage density [2].

20 One such emerging NVM is MRAM (magnetoresistive random access memory). Unlike
21 flash memory which uses electronic charge as a medium of memory storage, MRAM uses the
22 electronic spin degree of freedom to store information. Unlike charge based storage devices,
23 MRAM is stable against perturbations such as ionizing radiation [4]. MRAM devices consist
24 of cells with magnetic tunnel junctions (MTJ) that have two ferromagnet (FM) layers separated
25 by an insulating layer. One of the layer is pinned where the magnetization orientation is fixed
26 and acts as a reference layer. Depending on the orientation of the free layer, the tunneling
27 magnetoresistance (TMR) is high or low and hence, memory can be read out using electrical
28 currents [3]. Early MRAMs were written by induced fields from heavy currents passed on
29 the adjacent layer. With recent developments in spin transfer torque (STT) in ferromagnets,

30 it has become possible to write using electrical currents [5]. This has reduced the power
31 consumption significantly and made commercialization of MRAM devices possible [3,6].

32 **1.2 Antiferromagnets for potential applications as a memory unit**

33 Historically, antiferromagnets (AFM) have been used as inactive components in MTJ, primarily
34 in exchange biasing the pinned FM layer. However in 2010, Gomonay *et al.* [7] proposed
35 electrical switching of AFMs using STT by passing a spin polarized current injected from
36 a fixed FM layer through the AFM layer. The electrical current gets spin polarized in the
37 FM layer and transfers its angular momentum to the AFM moments to switch it from one
38 orientation to another. There are advantages to using AFM over FM in MRAM devices. AFM
39 are not easily affected by external magnetic fields and do not produce stray fields of their
40 own. They have smaller domains which would allow for higher storage densities [4]. Since
41 the precession frequency of AFM moments is determined the geometric mean of exchange
42 and anisotropy energies, the dynamics in AFM materials occur at THz timescales which is
43 two orders of magnitude higher than in FM [8]. Although the AFM can be switched using
44 electrical currents from parallel to perpendicular orientation with respect to the FM mag-
45 netization direction, the reverse process cannot be obtained using electrical current. High
46 magnetic fields above the spin flop transition of the AFM needs to be applied in order to
47 switch back the AFM to its original state [7].

48 Unlike previously discussed STT MRAM devices, spin orbit torque based electrical switch-
49 ing in broken inversion symmetry FM does not require the presence of a FM polarizer [9].
50 This concept of the presence of relativistic fields is applicable to AFM as well provided the
51 local moments do not sit on centrosymmetric sites. If the two sublattices are related to each
52 other by a center of inversion, then the current induced spin polarized fields are staggered
53 across the two sublattices [4,10,11]. This results in a uniform fieldlike torque experienced by
54 the order parameter. This is possible in bulk materials that are globally centrosymmetric but
55 locally non-centrosymmetric and the two sublattices are related to each other by a center of
56 inversion. It was initially demonstrated in the case of epitaxially grown tetragonal CuMnAs
57 thin films on GaP substrate [4] and since then, it has also been shown in Mn₂Au and CuMnAs
58 sputtered films as well [12,13]. Observation of electrical switching behavior in AFM requires
59 the presence of degenerate Néel vectors like in CuMnAs as shown in Fig. 1.1(a) as opposed to
60 compounds like MnF₂ where the Mn moments point along *c* in Fig. 1.1(b).

61 **1.3 Exploration of Cu-Mn-As phase space**

62 Compounds in Cu-Mn-As phase space have attracted a lot of attention in recent times mainly
63 due to the exotic properties of tetragonal and orthorhombic CuMnAs. As mentioned earlier,

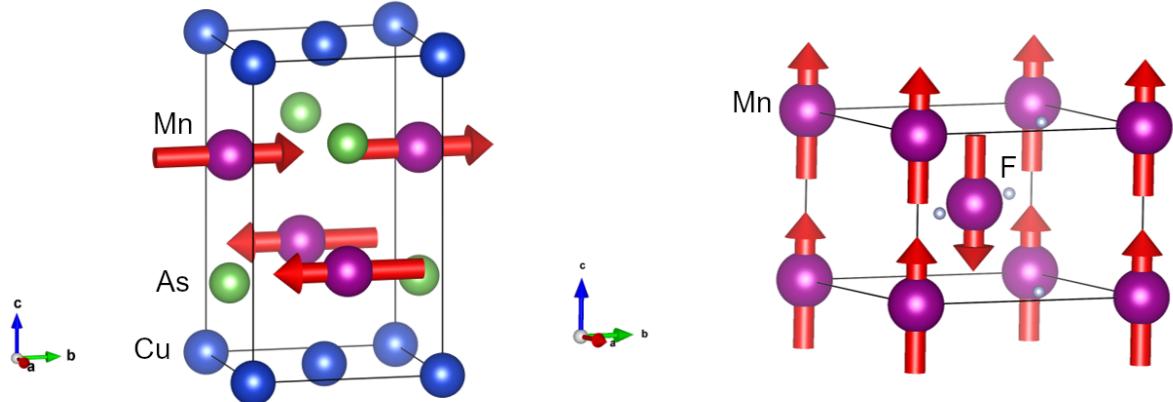


Figure 1.1: The magnetic structures of tetragonal CuMnAs and MnF₂ are shown in (a) and (b), respectively.

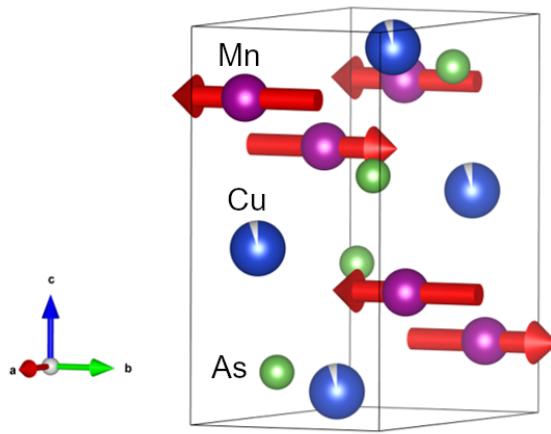


Figure 1.2: Magnetic structure of orthorhombic CuMnAs

tetragonal CuMnAs was the first antiferromagnet where electrical switching was supposedly demonstrated. Orthorhombic CuMnAs, shown in Fig. 1.2, was the first magnetic compound to be proposed as a Dirac semimetal. It is a special compound where the inversion and time reversal symmetry of the magnetic structure is broken but their combined symmetry (*PT* symmetry) is still preserved. Based on the orientation of the AFM order parameter, the compound changes from a conducting to an insulating phase. Hence, there are voltage based switching applications that have been proposed for this compound [14].

Despite the growing importance of the compounds in Cu-Mn-As system, the Cu-Mn-As ternary phase space has not been explored properly. There are four known ternary compounds including both the polymorphs of CuMnAs, orthorhombic CuMn₃As₂ and Cu₂Mn₄As₃ as shown in Fig. 1.3 [15–18]. Bulk orthorhombic CuMnAs can be grown us-

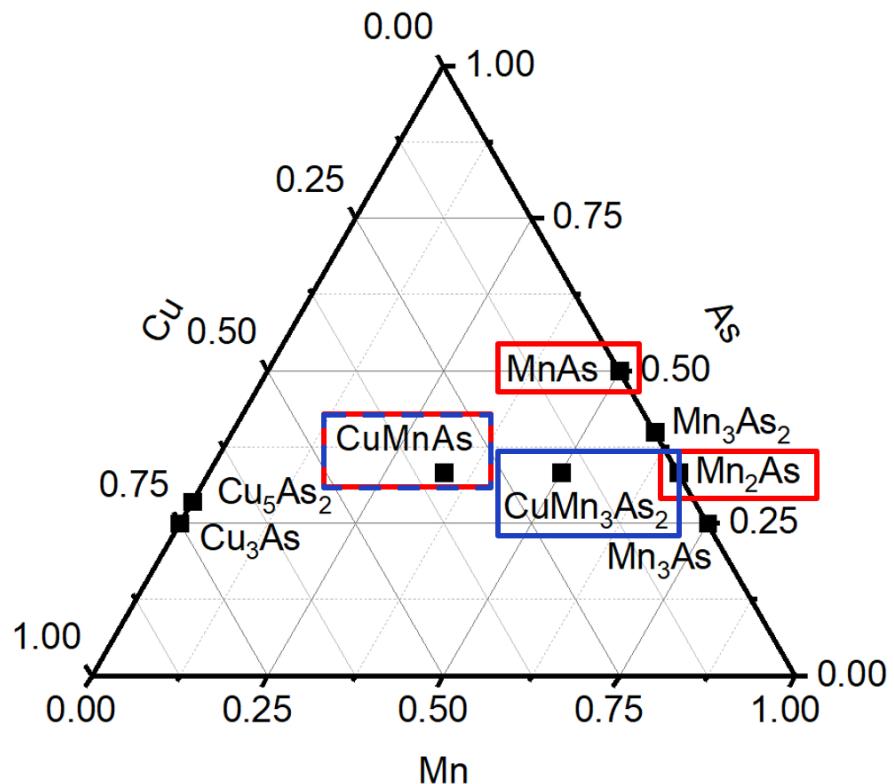


Figure 1.3: Cu-Mn-As ternary phase diagram highlighting some of the known ternary compounds in blue and known magnetic structures in red. Not all compounds in this system are shown here.

75 ing traditional solid state synthesis routes by Cu, Mn and As powders in stoichiometric ratio
76 and heating the powders to 1000°C. In order to synthesize pure bulk tetragonal CuMnAs,
77 we have to go off-stoichiometry and either substitute Mn with Cu or As [18]. Hence, it is
78 important to explore different regions in the Cu-Mn-As system and verify the stability of
79 different ternary compounds. The magnetic structures in the Cu-Mn-As system have also
80 not been identified for most of the compounds. Apart from the four Cu-Mn-As ternary
81 compounds, there are more than ten Mn-As binary compounds present in this system. The
82 magnetic structures are known only for the two previously mentioned CuMnAs compounds,
83 Mn₂As and MnAs as shown in Fig. 1.3 [16,17,19–22]. Since most, if not all, the binary Mn-As
84 compounds are metallic, there is a need to magnetically characterize the compounds and
85 identify their magnetic structures.

86 1.4 Exchange interactions in Cu₂Sb type structures

87 If we want to understand the electrical switching behavior in metallic antiferromagnets, we
88 should be able to quantify the fundamental energies such as magnetocrystalline anisotropy
89 and exchange interactions in materials like CuMnAs. CuMnAs has a Cu₂Sb structure type.
90 Other materials with this structure includes Mn₂As, Cr₂As, Fe₂As, CrMnAs, MnFeAs etc.
91 [23–25]. Although Mn₂As, Cr₂As and Fe₂As have the same structure, the magnetic ground
92 state is different in all three compounds. The strength and sign of direct exchange interactions
93 between two magnetic atoms is a result of the nature of orbital overlap between the two
94 magnetic atoms [24]. Since these materials are metallic, there are two contributions to indirect
95 exchange interactions. One contribution arises from superexchange interactions mediated by
96 As atoms and the other contribution comes from RKKY (Ruderman–Kittel–Kasuya–Yosida)
97 interactions [25]. It is important that we are able to determine what spin interactions are
98 relevant and how does it affect the magnetic ordering in these materials. It is also crucial that
99 we are able to verify the computational methods and the exchange coupling values obtained
100 from these methods so that we can use these methods for other systems as well.

Chapter 2

Theory of electrical switching in metallic antiferromagnets

101 Electrical switching in any magnetic compound is a series of events involving current induced
102 spin polarization (CISP) of charge carriers and different components of CISP exerting differ-
103 ent torque on the magnetic moments of the atoms. The nature of CISP is set by the crystal
104 symmetry. In previous studies of CuMnAs and Mn₂Au, it was stated that the compound
105 should globally centrosymmetric but locally non-centrosymmetric and the two sublattices
106 should be related to each other by a center of inversion [4,10,11]. Is this a necessary condition
107 for observing a staggered spin polarization configuration and can it be applied to general
108 cases? These are some of the questions we will answer in this chapter. Once we have deter-
109 mined the required symmetry criteria, we will filter out metallic antiferromagnetic candidates
110 from large databases of materials such as MPDS (Materials Platform for Data Science) and
111 ASM (ASM International), and analyze the effect of CISP on the torque experienced by the
112 order parameter.

113 2.1 Hidden spin polarization in centrosymmetric crystals

114 It has been known for quite some time that in materials (even non-magnetic) having large
115 spin orbit coupling (SOC) and lacking a center of inversion, magnetic fields are induced.
116 When materials possess structural inversion asymmetry such as in quantum wells and other
117 heterostructures, this effect is called the Rashba effect and it results in a helical type spin
118 texture. When this occurs in materials that lack bulk inversion symmetry, the effect is called
119 the Dresselhaus effect and it results in a unique spin texture [26]. Zhang *et al.* [26] argued that
120 since SOC is a relativistic effect, instead of considering the symmetry of the entire unit cell,
121 one should check for atomic site symmetry to understand SOC induced spin polarization.
122 Based on this argument, there are four cases possible as shown in Table 2.1.

123 R1 and D1 effects refer to conventional Rashba and Dresselhaus spin polarization respec-
124 tively. In materials that are globally centrosymmetric, hidden spin polarization is possible.
125 There is local spin polarization near non-centrosymmetric sites but when summed over the
126 entire unit cell, the net spin polarization is zero. This effect is called the R2 or D2 effect
127 corresponding to Rashba or Dresselhaus effect, respectively in centrosymmetric crystals. The
128 total spin polarization of the unit cell is the vector sum of all the local spin polarizations

Table 2.1: Different cases of spin polarization depending on the symmetry of atomic sites and the unit cell [26].

	All non-polar point groups	At least one polar point groups	All centrosymmetric point groups
Non-Centrosymmetric space group	D1 effect	R1/D1 effect	Not possible
Centrosymmetric space group	D2 effect	R2/D2 effect	No spin polarization

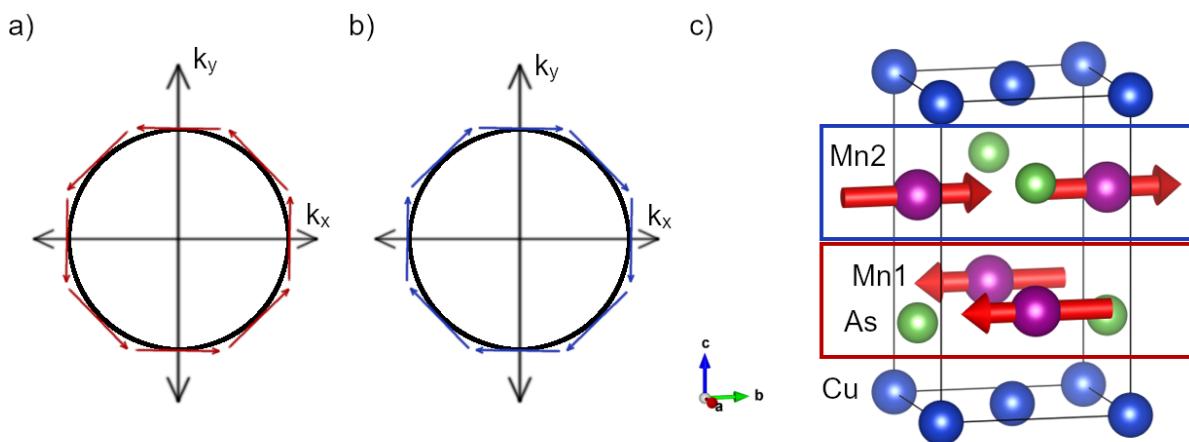


Figure 2.1: The schematic of the Fermi surface of the local sectors near Mn1 and Mn2 atoms are shown in (a) and (b), respectively. The magnetic structure of tetragonal CuMnAs is shown in (c) which also includes the highlighted local sectors.

129 in the unit cell. Non-centrosymmetric point groups can be further divided into polar and
 130 non-polar groups. Local Rashba effect requires the presence of polar point groups on atomic
 131 sites and the local Dresselhaus effect requires the presence of non-polar point groups at the
 132 atom sites. The presence of local spin polarization in centrosymmetric crystals opens the
 133 avenue for studying spin polarization in a larger group of compounds including metallic
 134 antiferromagnets.

135 **2.2 Finding metallic antiferromagnetic candidates with R2-D2
 136 effect**

137 In spin orbit torque based switching of metallic antiferromagnets, the same arguments apply
 138 as before except that we only care about the point group symmetry at the magnetic atom
 139 sites. For example, the magnetic structure of CuMnAs is shown in Fig. 2.1(c). Cu and As

140 atoms have no moments and sit on D_{2d} and C_{4v} sites, respectively. Since only the Mn atoms
141 have moments, we must take the site symmetry of Mn atoms into consideration. Mn atom
142 sites have C_{4v} point group symmetry which is polar. As seen in Fig. 2.1(a,b), the schematic
143 of the Fermi surface corresponding to the Mn layer has a Rashba-like spin texture. When
144 the current is applied, through inverse spin galvanic effect, there is a spin polarization of
145 the conduction electrons near Mn sites. The spin polarization is staggered across the two
146 Mn sublattices and through exchange coupling, a torque is experienced by the Mn moments.
147 From the example of CuMnAs above, we can search for compounds from databases that are
148 antiferromagnets or are likely to be antiferromagnets where the magnetic atoms sit on a polar
149 point group. Such a search can be made for compounds which are not complicated by the
150 presence of many magnetic sites with different point groups. The general case applicable for
151 all magnetic compounds will be considered in the following sections. Following is the general
152 procedure for extracting potential metallic antiferromagnet candidates from databases -

- 153 1. Search for known metallic antiferromagnets from database having tetragonal, trigonal
154 or hexagonal crystal system.
- 155 2. Remove duplicate and non-centrosymmetric compounds.
- 156 3. Identify the Néel temperature and magnetic ordering.
- 157 4. Filter out compounds having Néel temperature > 300 K.
- 158 5. Identify the nature of atomic site symmetry and select compounds.
- 159 6. Study available literature to see if any compounds can be synthesized as single crystals.

160 This procedure assumes that we are starting with a collection of known or possible metallic
161 antiferromagnets. This is true in case of compounds downloaded from MPDS. In case of ASM
162 database, the compounds are metallic but their magnetism is not known beforehand. We will
163 have to make some assumptions based on the chemical nature and stoichiometry of the ions
164 present in the compound in order to select possible antiferromagnets. Tetragonal, trigonal
165 or hexagonal crystal systems are preferred since they allow for the presence of multiple
166 degenerate axes for Néel vector orientation. It is still important to check if the magnetic
167 structure for the compound is known or not and if the Néel vector points along the degerate
168 axes. Carrying out the above mentioned steps for compounds in MPDS and ASM database
169 gives us a list of compounds in Table 2.2 that have been grouped together based on their
170 structure types.

171 The first group of compounds consist of materials in MoSi_2 structure type. Mn_2Au is a
172 well-known compound that has been extensively studied for electrical switching applications
173 [12, 27]. Cr_2Al powders can be prepared using traditional solid state synthesis routes by
174 heating to above 850°C [28]. Early neutron diffraction experiments suggest Cr moments align

Table 2.2: List of metallic antiferromagnetic candidates filtered out from MPDS and ASM database and their metal atom site symmetries

Structure type	List of compounds	Point group	Magnetism
MoSi ₂	Mn ₂ Au, Cr ₂ Al, Ni ₂ Ta	C _{4v}	Mn ₂ Au is a known candidate
HfFe ₆ Ge ₆	ScFe ₆ Ge ₆	C _{2v}	AFM with Néel vector along <i>c</i>
Mg ₃ Cd	Mn ₃ Ga, Mn ₃ Ge, Mn ₃ Sn, Fe ₃ Ga, Co ₃ Mo, Co ₃ W, Ni ₃ In, Ni ₃ Sn, Ni ₃ Zr	C _{2v}	Non-collinear AFM
IrIn ₃	CoGa ₃ , CoIn ₃ , FeGa ₃	C _{2v}	FeGa ₃ and CoGa ₃ are diamagnets
MoNi ₄	MoNi ₄ , WNi ₄	C _{1v}	Unknown
Ni ₂ Al ₃	Ni ₂ Al ₃ , Ni ₂ Ga ₃ , Ni ₂ In ₃	C _{3v}	Unknown

at 65° to the *ab* plane [29]. However, a later article indicates that the determined magnetic structure may not be correct [30]. Regardless of whether the moments align in the *ab* plane or not, Cr₂Al is an interesting candidate to study electrical switching behavior. ScFe₆Ge₆ is AFM at room temperature [31]. However, the Fe moments align along *c* and does not satisfy our criteria [32]. Compounds in the Mg₃Cd structure type contain Kagome lattice of magnetic atoms. Mn₃Sn and Mn₃Ge are known to have a non-collinear spin arrangement. They have become popular recently for showing large anomalous hall and spin hall effect behavior [33–35]. Electrical switching was also demonstrated in Mn₃Sn recently. In the fourth group of compounds, both FeGa₃ and CoGa₃ are known to show diamagnetic properties and hence they can be discarded [36–38]. The magnetism is unknown in the final two groups of compounds in MoNi₄ and Ni₂Al₃ structure types and most of these compounds can be synthesized by the arc melting process [39,40].

2.3 Components of torque from non-equilibrium CISP

The previous section dealt with relatively simple magnetic compounds that had only one magnetic atom site and we were concerned with the point group of the site to determine whether the inverse spin galvanic effect would be observed or not. In the simplest sense, antidamping-like STT is induced by spin hall effect (SHE) and fieldlike SOT is generated from inverse spin galvanic effect. However, incomplete absorption of the spin current from SHE by the FM layer may produce a fieldlike torque, and spin relaxation and damping may induce an antidamping like component to the SOT [11]. Using Kubo linear formalism, we

195 can write CISP $\delta S_a = \chi_a E$ where E is the applied electric field and χ_a is the linear response
 196 tensor for the sublattice a. χ_a can be further divided into three components:

$$\chi_a = \chi_a^I + \chi_a^{II(a)} + \chi_a^{II(b)} \quad (2.1)$$

197 where χ_a^I is the intraband term, and $\chi_a^{II(a)}$ and $\chi_a^{II(b)}$ are the interband terms. χ_a can also
 198 be broken down into even and odd terms:

$$\chi_a = \chi_a^{even} + \chi_a^{odd} \quad (2.2)$$

199 where $\chi_a^{even} = (\chi_a([M]) + \chi_a([-M]))/2$ and $\chi_a^{odd} = (\chi_a([M]) - \chi_a([-M]))/2$. From the
 200 symmetry of the operators and the matrix element, it follows that -

$$\chi_a^{even} = \chi_a^I + \chi_a^{II(b)} \quad (2.3)$$

$$\chi_a^{odd} = \chi_a^{II(a)} \quad (2.4)$$

201 We assume that the system only has a weak disorder and hence, we can neglect $\chi_a^{II(b)}$. χ_a
 202 also depends on the direction of the magnetic moments where \hat{n} is the direction of the Néel
 203 vector.

$$\chi_{a,i,j}(\hat{n}) = \chi_{a,i,j}^{(0)} + \chi_{a,i,j,k}^{(1)} \hat{n}_k + \chi_{a,i,j,k,l}^{(2)} \hat{n}_k \hat{n}_l + \dots \quad (2.5)$$

204 where the sum of the first term and every alternate term after that corresponds to χ_a^{even} and
 205 the sum of the remaining terms correspond to χ_a^{odd} . $\chi_a^{(0)}$ is usually dominant, independent
 206 of magnetization and contributes to field-like torque. $\chi_a^{(1)}$ contributes to anti-damping like
 207 torque and $\chi_a^{(2)}$ can be neglected if $\chi_a^{(0)}$ is not 0 [11]. The zeroth order term which contributes
 208 to a fieldlike torque consists of three components in the form of generalized Rashba and
 209 generalized Dresselhaus terms and a term that is proportional to the electric field. Similarly,
 210 first order term can also be broken into three different components [11]. The summary of the
 211 linear response tensor components is also provided in the Table 2.3

212 2.4 Spin polarization in CuMnAs, Mn₂Au and Fe₂As

213 Zelezny *et al.* [11] provides a python code *symmetr* for analyzing the linear response tensor
 214 for a number of observables such as current, spin, torque, position, spin current etc. and
 215 electric field. Using this code, we can test the reponse tensor of known compounds such
 216 as CuMnAs and Mn₂Au and also check for unknown compounds such as Fe₂As. Table
 217 2.4 shows the linear response tensor in case of CuMnAs or Mn₂Au. Both compounds have
 218 same spin polarization since they are both globally centrosymmetric and Mn atoms sit on
 219 C_{4v} point group sites. Let us first understand χ^{even} for all the different cases presented here.

Table 2.3: Summary of the linear response tensor components for the CISP observable and electric field

	χ_a^I	$\chi_a^{II(a)}$	$\chi_a^{II(b)}$
Component	Intraband	Interband (imaginary)	Interband (real)
Disorder $\Gamma \rightarrow 0$	Diverges	Constant	Zero
Cause	Non-equilibrium Fermi-Dirac distribution	Intrinsic change in carrier wave function	Change in carrier wave function due to disorder/defects
Alternate name	χ_a^{even} or χ_a^0	χ_a^{odd} or χ_a^1	
Dependence on magnetization	Independent	Dependent	
Torque	Field-like	Anti-damping-like	

220 Magnetism can be turned off to avoid including magnetization-based effects to the reponse
 221 tensor. Regardless of whether we toggle magnetism in Mn atoms or not, χ^{even} is 0 for the
 222 whole unit cell since it is centrosymmetric. When Mn magnetic moment is set to 0, χ^{even} for
 223 each sublattice corresponds to the response in conventional Rashba spin texture. Regardless
 224 of magnetism, the spin polarization in one site is opposite to that of another site as seen in
 225 the projected cases. When magnetism is turned on, $|\chi^{10}| = |\chi^{01}|$ is not valid anymore since
 226 we also have to consider higher terms in χ^{even} . In case of χ^{odd} , it is 0 when magnetization is
 227 turned off as also shown in Table 2.3. When magnetic moments are allowed, there is spin
 228 polarization along c direction.

229 Table 2.5 shows linear response tensor components in Fe₂As. Fe₂As is complicated by the
 230 presence of two different Fe sites. Fe1, Fe2, Fe5 and Fe6 atoms shown in Fig. 2.2 sit on D_{2d}
 231 site whereas Fe3, Fe4, Fe7 and Fe8 atoms sit on C_{4v} sites. The table only shows cases where
 232 Fe moments have not been considered. However, allowing magnetism would make the cases
 233 more general.

234 2.5 Acknowledgements

235 I would like to acknowledge two REU students, Scott Berens and Carmen Paquette, for
 236 compiling the list of metallic antiferromagnets from MPDS and ASM databases respectively.
 237 It saved me a lot of time and I was able to analyze the symmetry requirements on a much
 238 smaller list of compounds.

Table 2.4: Linear response tensor in CuMnAs and Mn₂Au assuming Mn moment to be 1 μ_B .

	χ^{even}	χ^{odd}
Magnetic Mn	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \chi_{02} \\ 0 & 0 & 0 \\ \chi_{20} & 0 & 0 \end{bmatrix}$
Magnetic Mn and for each sublattice	$\begin{bmatrix} 0 & \chi_{01} & 0 \\ \chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \chi_{02} \\ 0 & 0 & 0 \\ \chi_{20} & 0 & 0 \end{bmatrix}$
Magnetic Mn, when one projected onto another	$\begin{bmatrix} 0 & -\chi_{01} & 0 \\ -\chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \chi_{02} \\ 0 & 0 & 0 \\ \chi_{20} & 0 & 0 \end{bmatrix}$
Non-magnetic Mn	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Mn, for each sublattice	$\begin{bmatrix} 0 & -\chi_{10} & 0 \\ \chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Mn, when one projected onto another	$\begin{bmatrix} 0 & \chi_{10} & 0 \\ -\chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

Table 2.5: Linear response tensor in Fe₂As with Fe moments equal to 1 μ_B .

	χ^{even}	χ^{odd}
Non-magnetic Fe	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Fe, for each sublattice 1 and 2	$\begin{bmatrix} 0 & \chi_{10} & 0 \\ \chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Fe, for each sublattice 3 and 4	$\begin{bmatrix} 0 & -\chi_{10} & 0 \\ \chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Fe, when 1 projected onto 2	$\begin{bmatrix} 0 & -\chi_{10} & 0 \\ 0 & -\chi_{10} & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Fe, when 3 projected onto 4	$\begin{bmatrix} 0 & \chi_{10} & 0 \\ -\chi_{10} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Non-magnetic Fe, when 1 projected onto 3	No relation	No relation

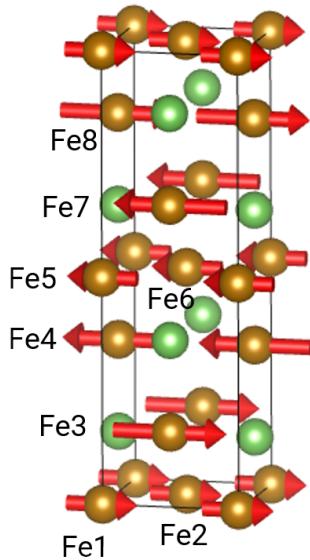


Figure 2.2: Magnetic structure of Fe_2As along with the Fe site numbers used in Table 2.5

Chapter 3

Materials synthesis and characterization

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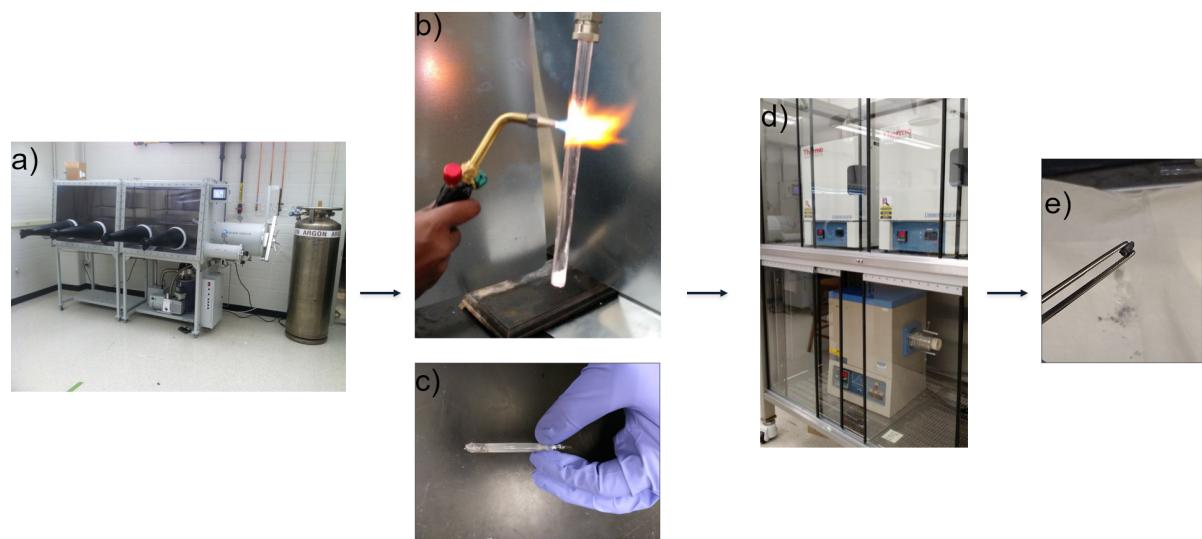


Figure 3.1: Electronic band structure

Chapter 4

Magnetic structure refinement from neutron diffraction measurements

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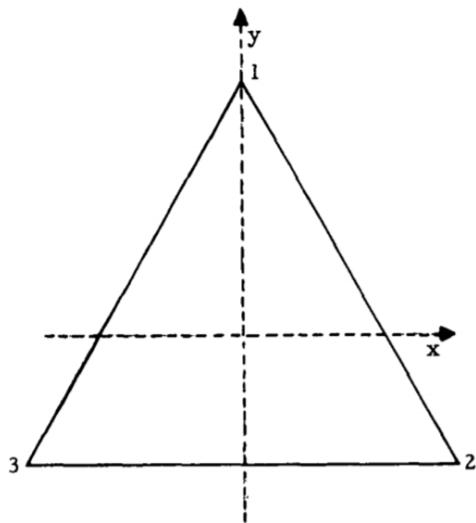


Figure 4.1: Electronic band structure

	E	C_3	C_3^2	σ_1	σ_2	σ_3
E	E	C_3	C_3^2	σ_1	σ_2	σ_3
C_3	C_3	C_3^2	E	σ_3	σ_1	σ_2
C_3^2	C_3^2	E	C_3	σ_2	σ_3	σ_1
σ_1	σ_1	σ_2	σ_3	E	C_3	C_3^2
σ_2	σ_2	σ_3	σ_1	C_3^2	E	C_3
σ_3	σ_3	σ_1	σ_2	C_3	C_3^2	E

Figure 4.2: Electronic band structure

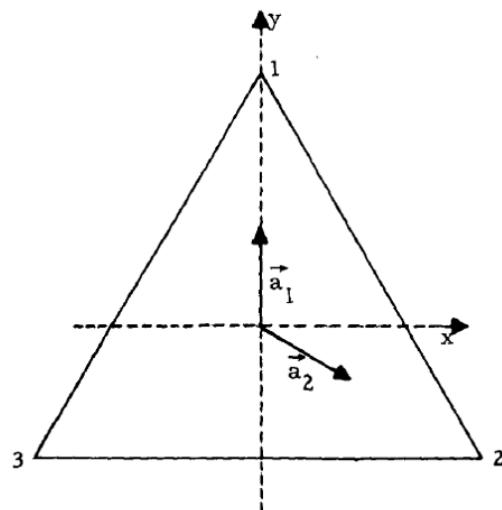


Figure 4.3: Electronic band structure

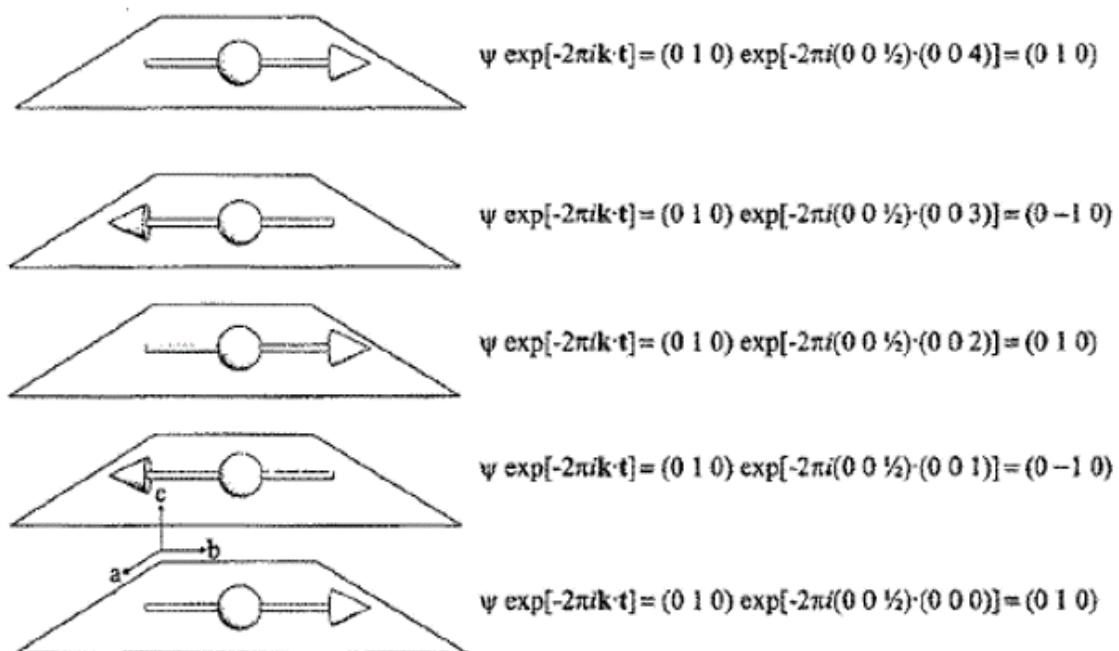


Figure 4.4: Electronic band structure

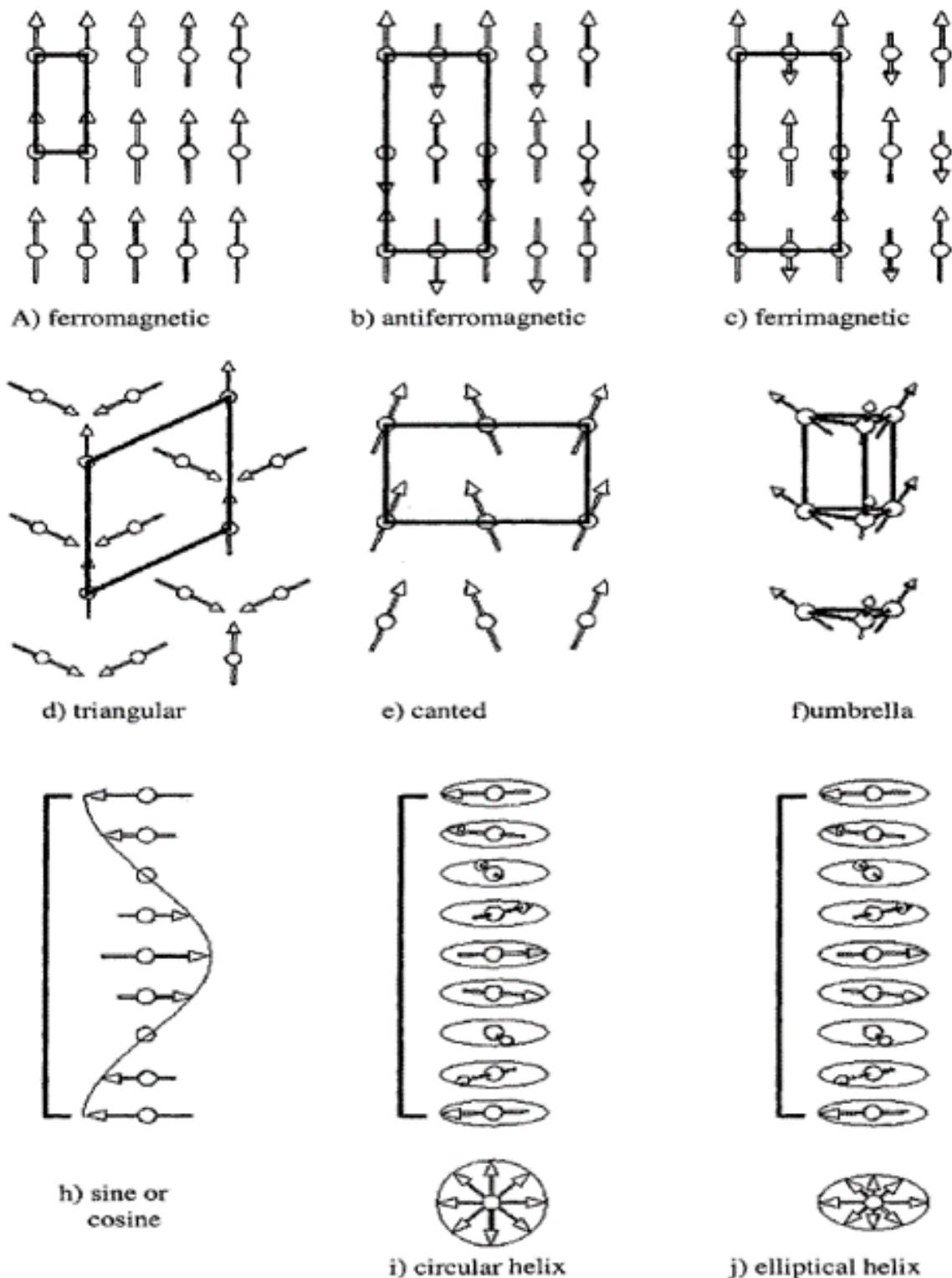


Figure 4.5: Electronic band structure

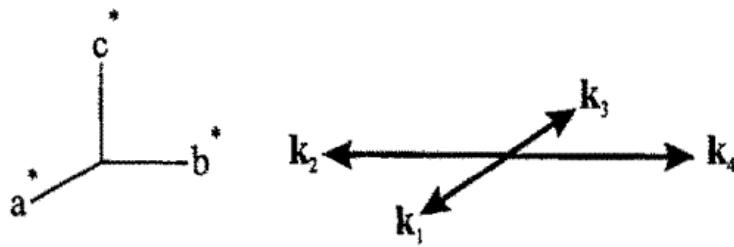


Figure 4.6: Electronic band structure

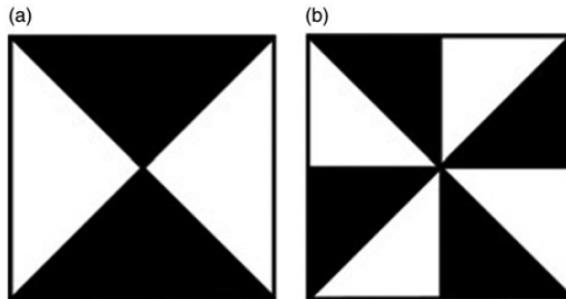


Figure 4.7: Electronic band structure

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Chapter 5

Discovery and magnetic frustration of hexagonal Cu_{0.82}Mn_{1.18}As

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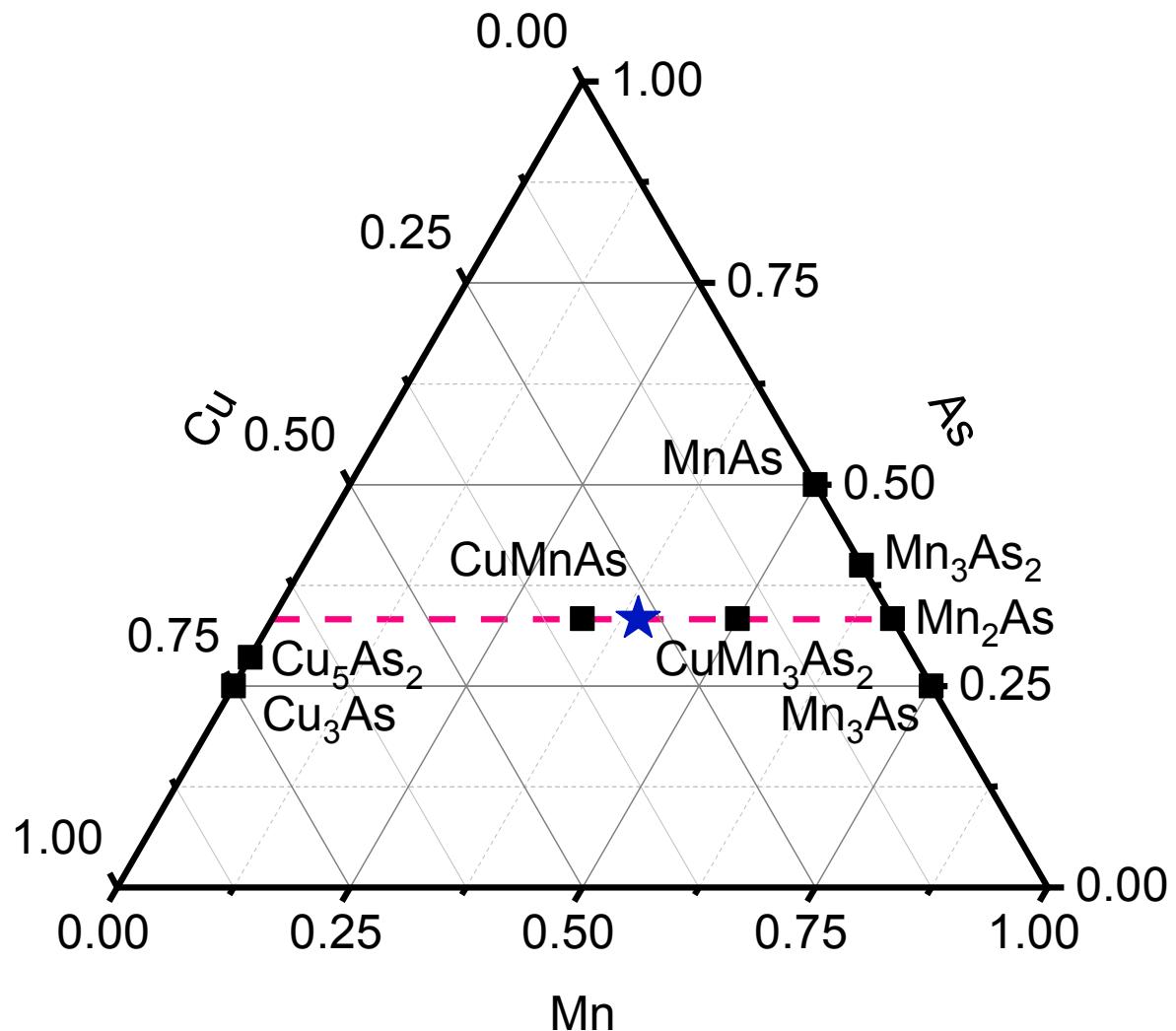


Figure 5.1: Electronic band structure

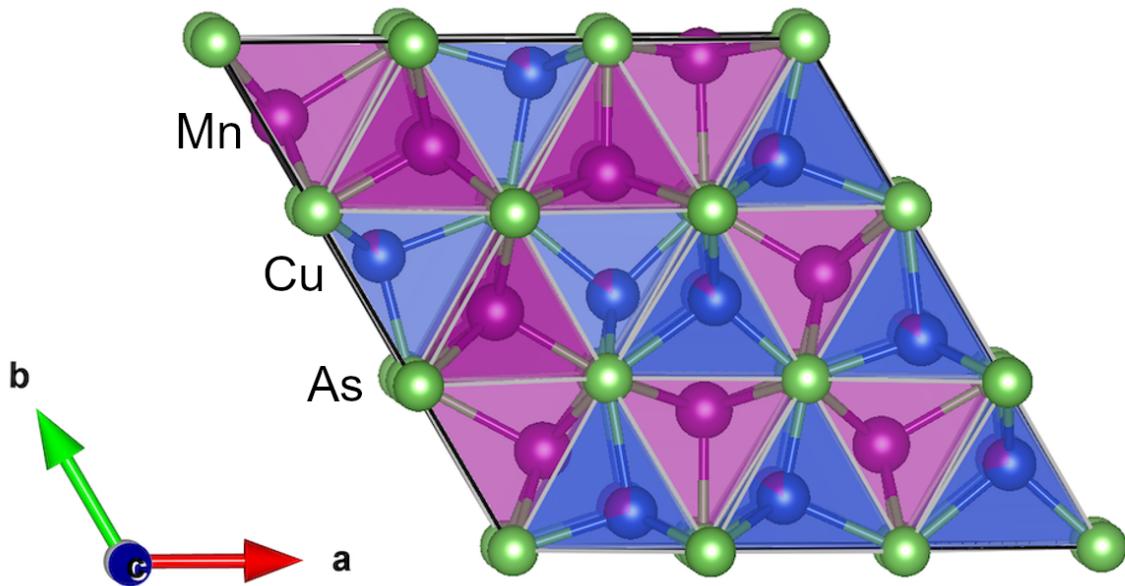


Figure 5.2: Electronic band structure

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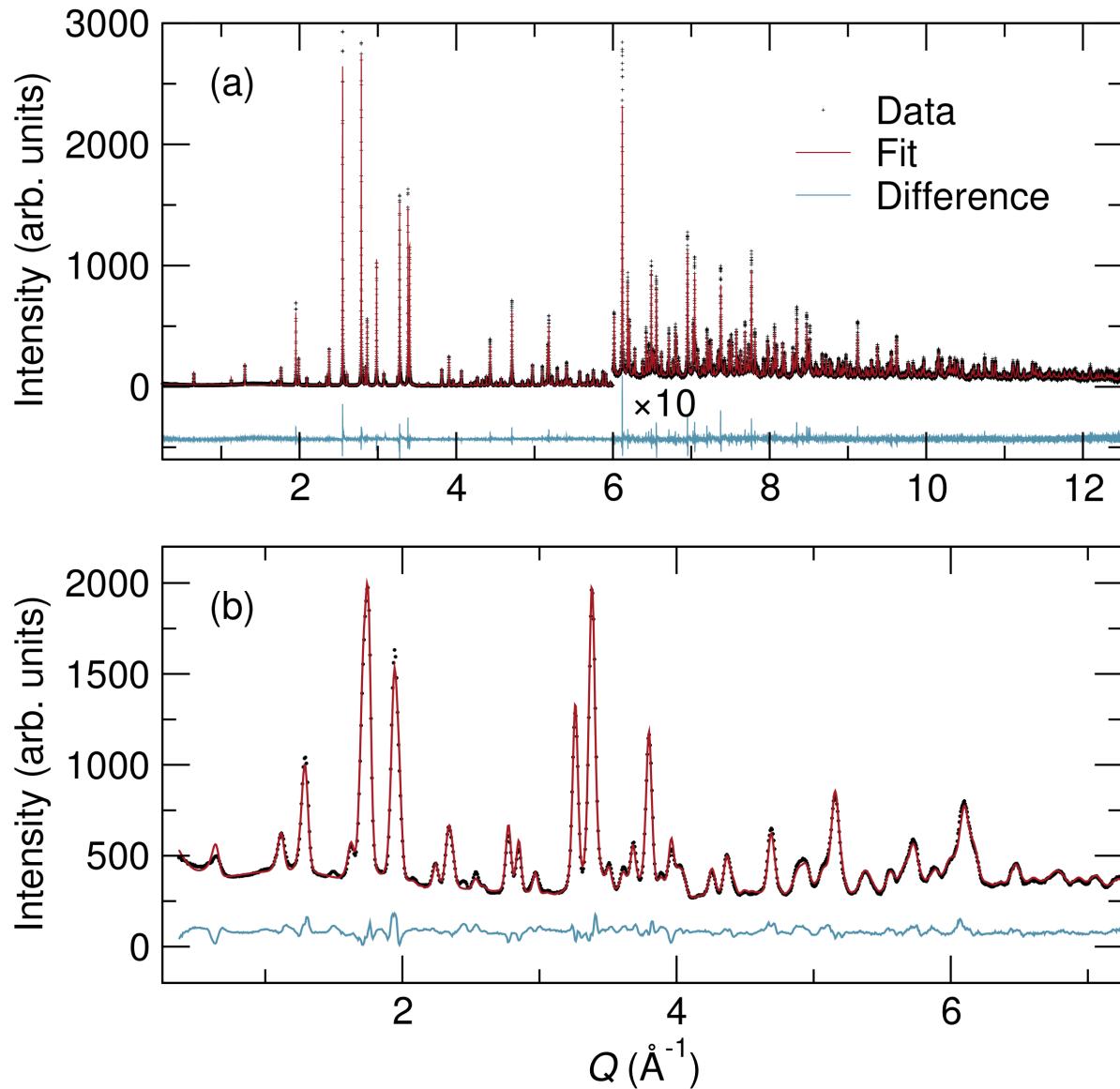


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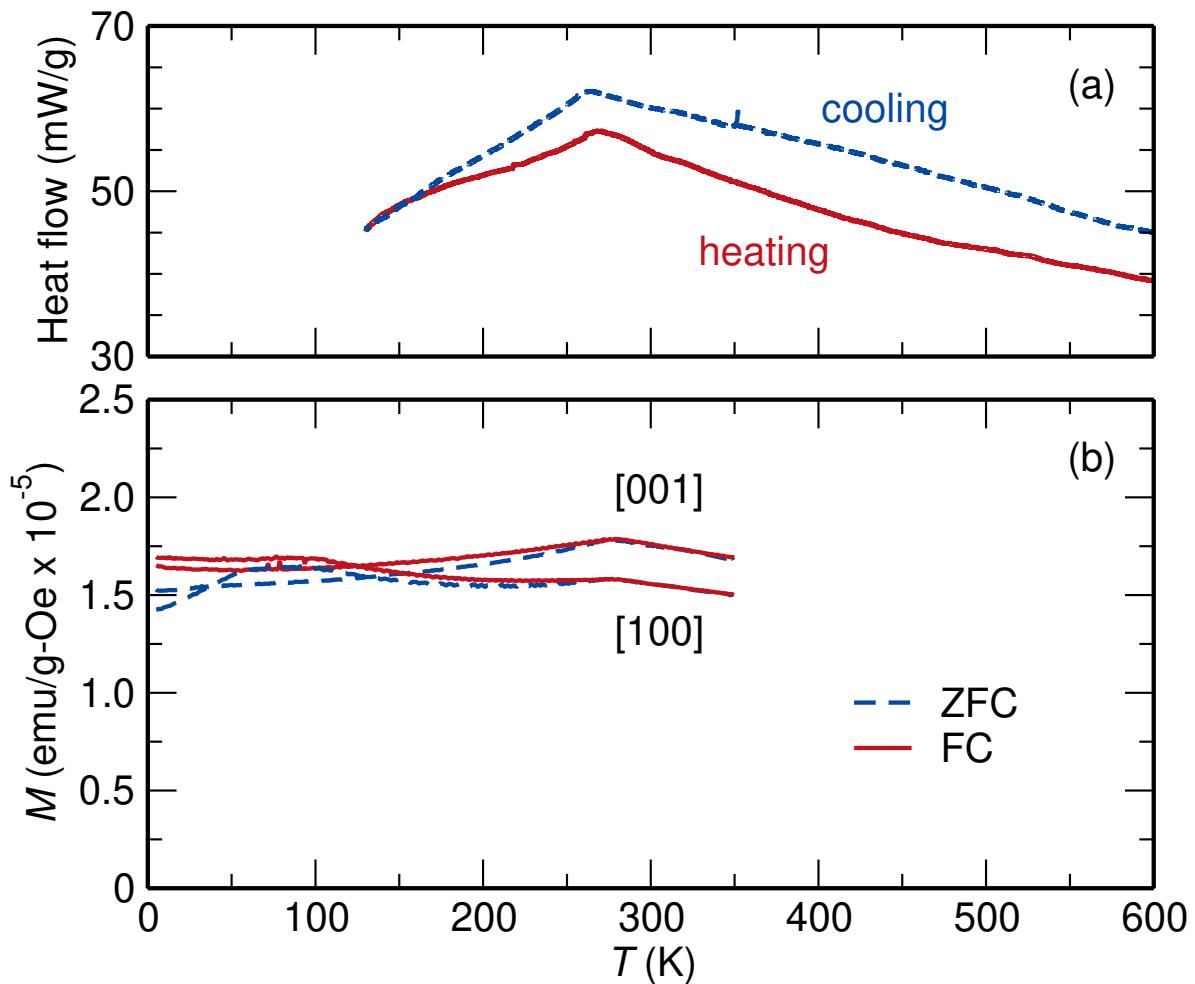


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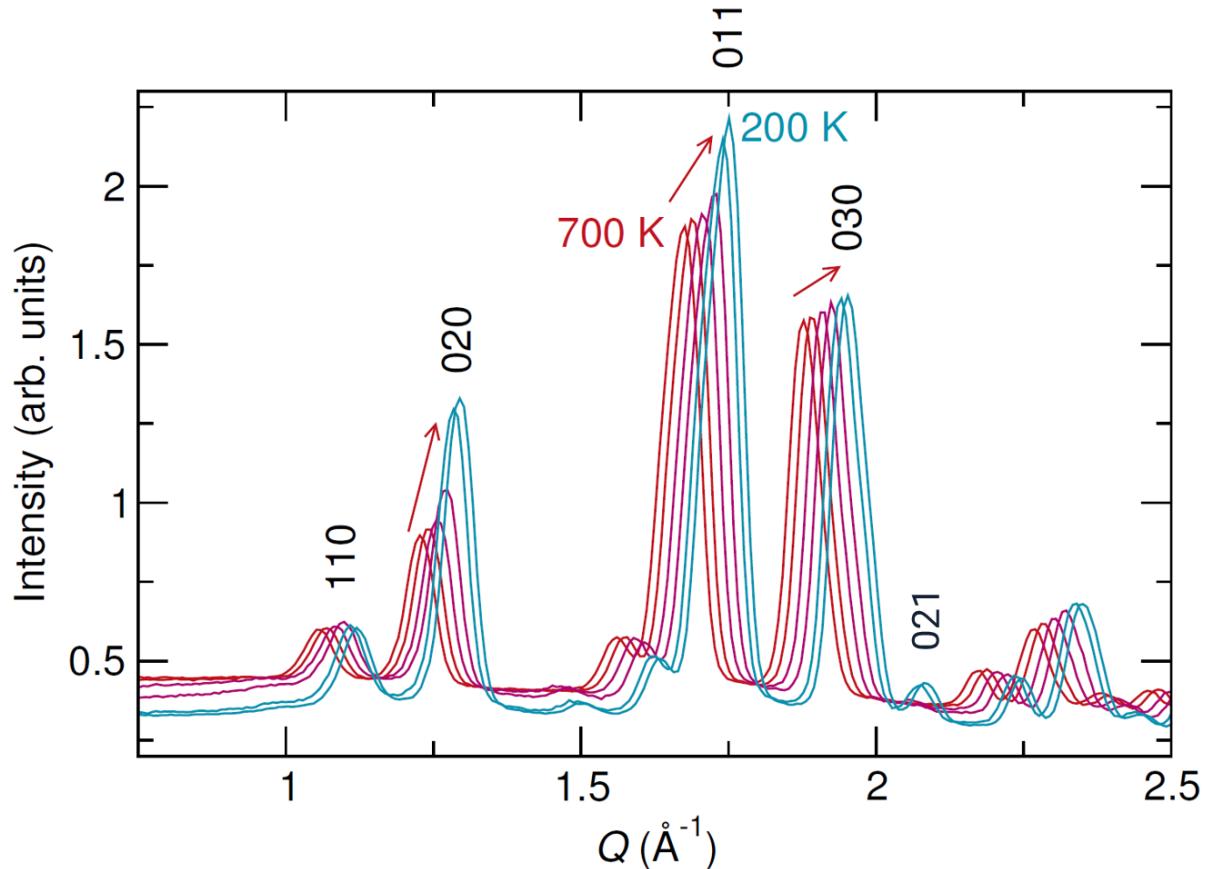


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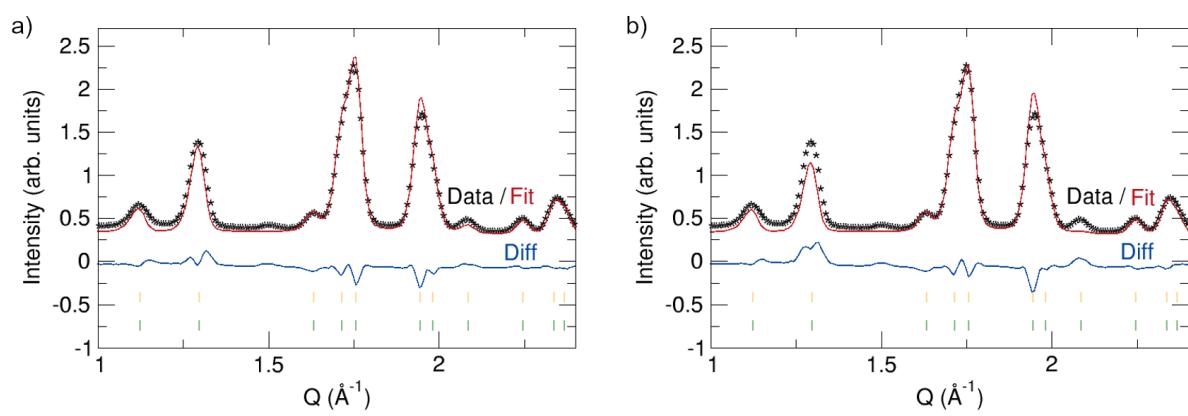


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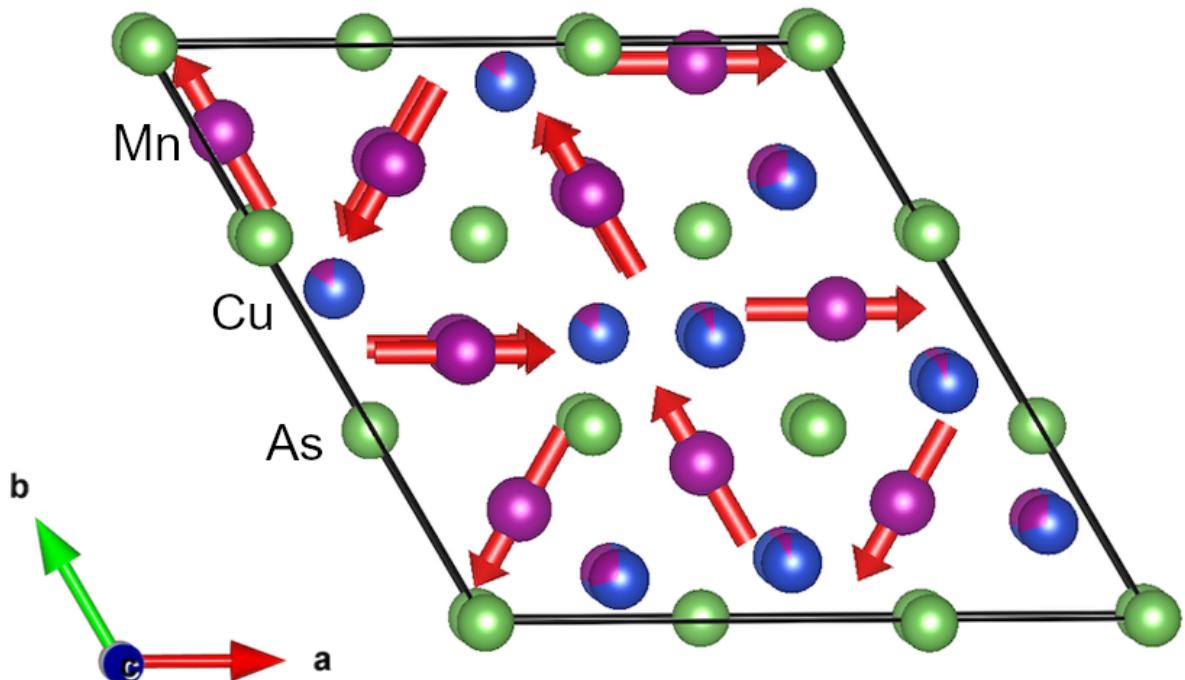


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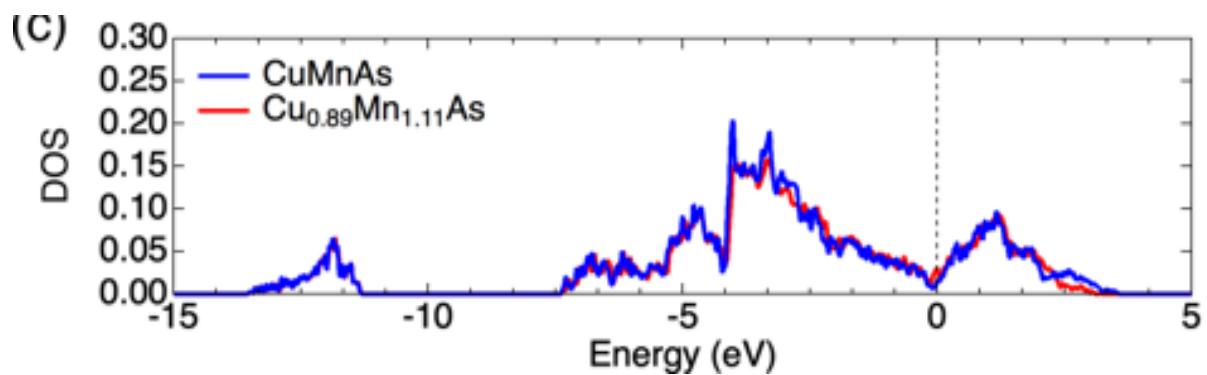


Figure 5.8: Electronic band structure

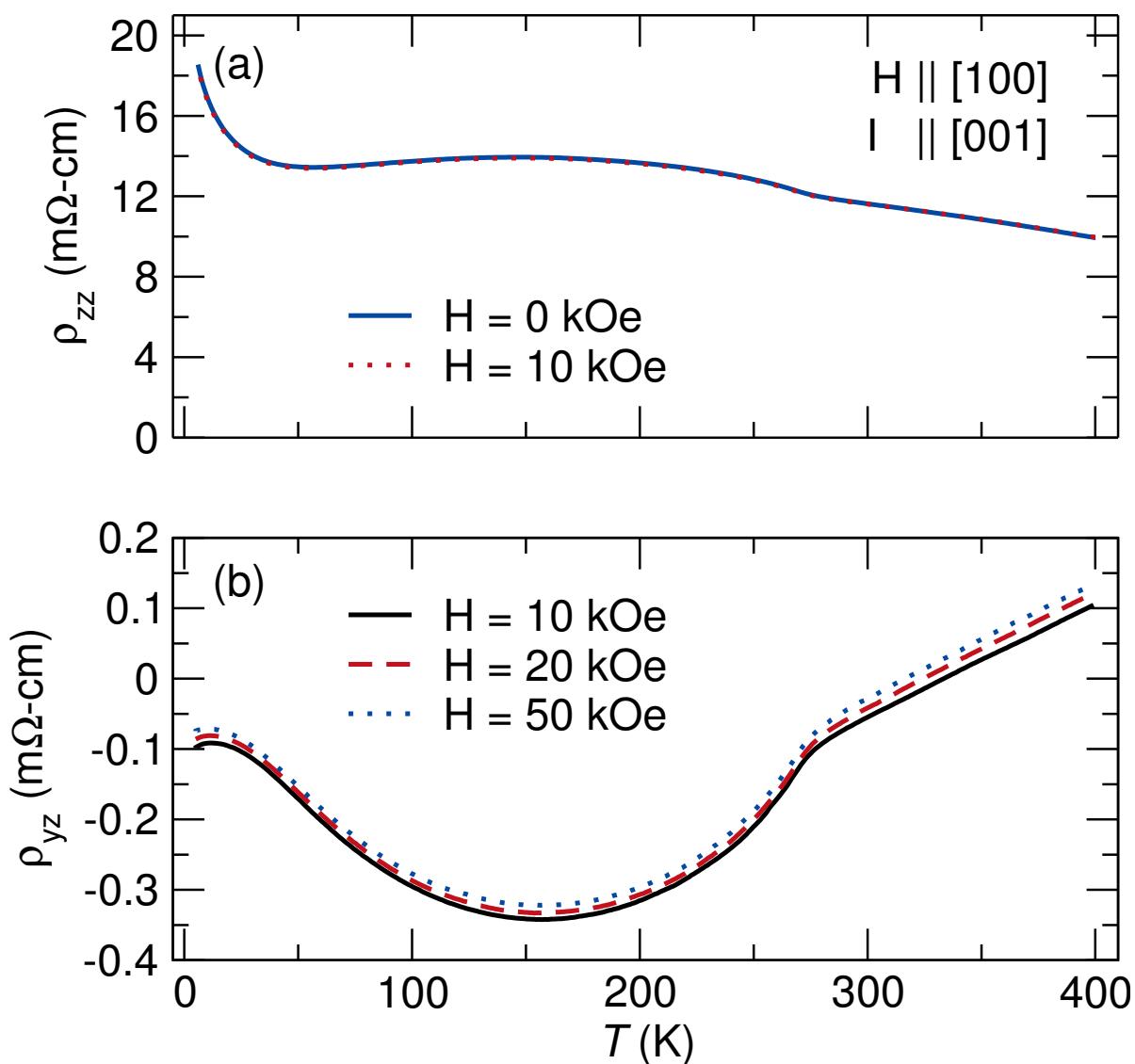


Figure 5.9: Electronic band structure

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Chapter 6

Two step magnetic ordering in monoclinic Mn₃As₂

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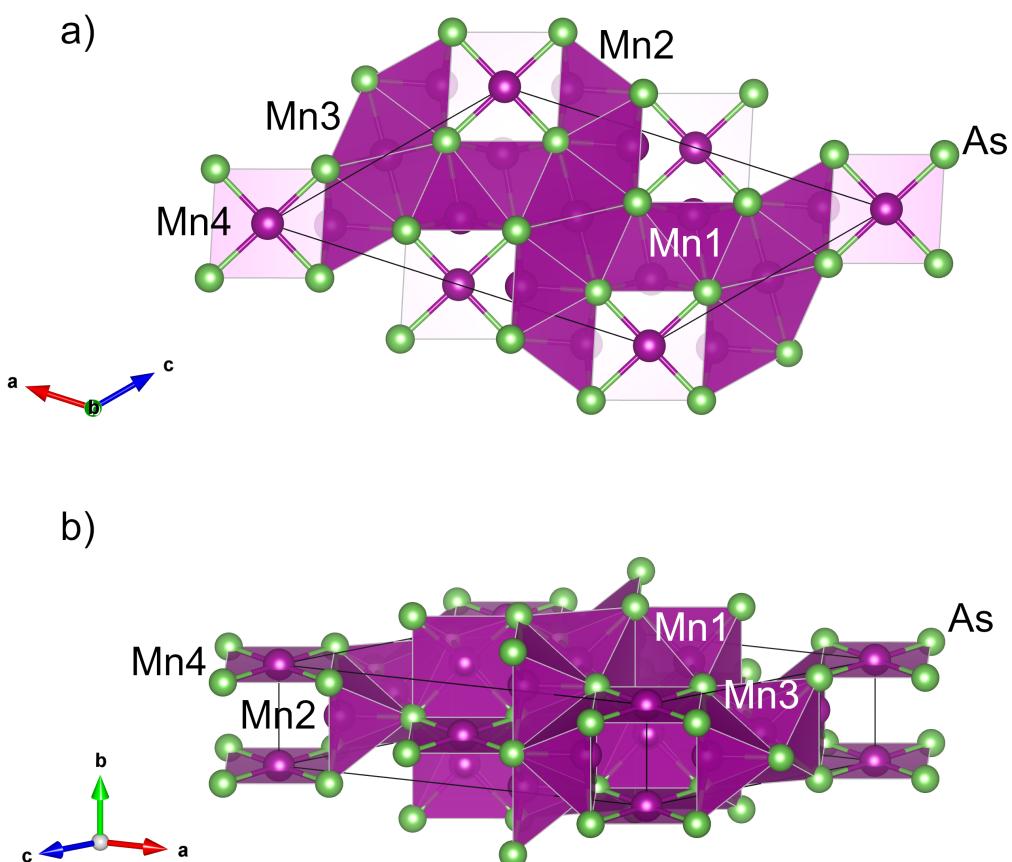


Figure 6.1: Electronic band structure

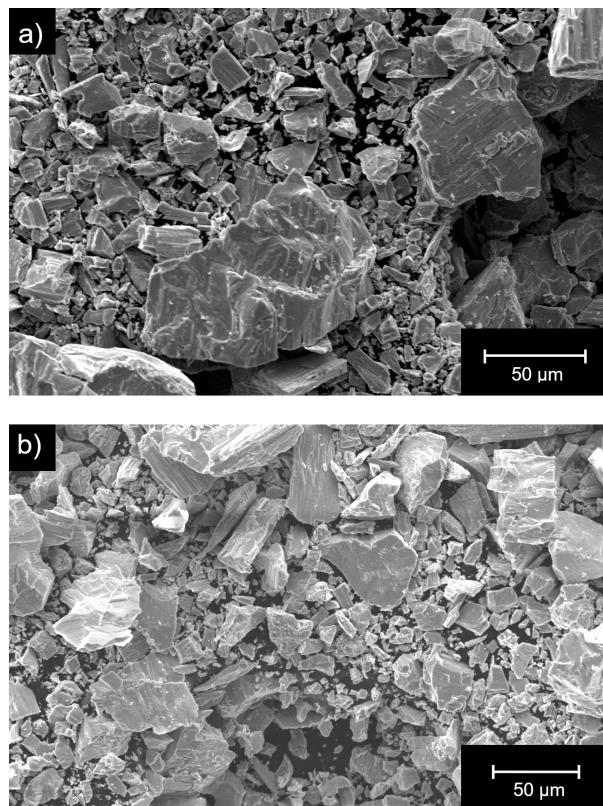


Figure 6.2: Electronic band structure

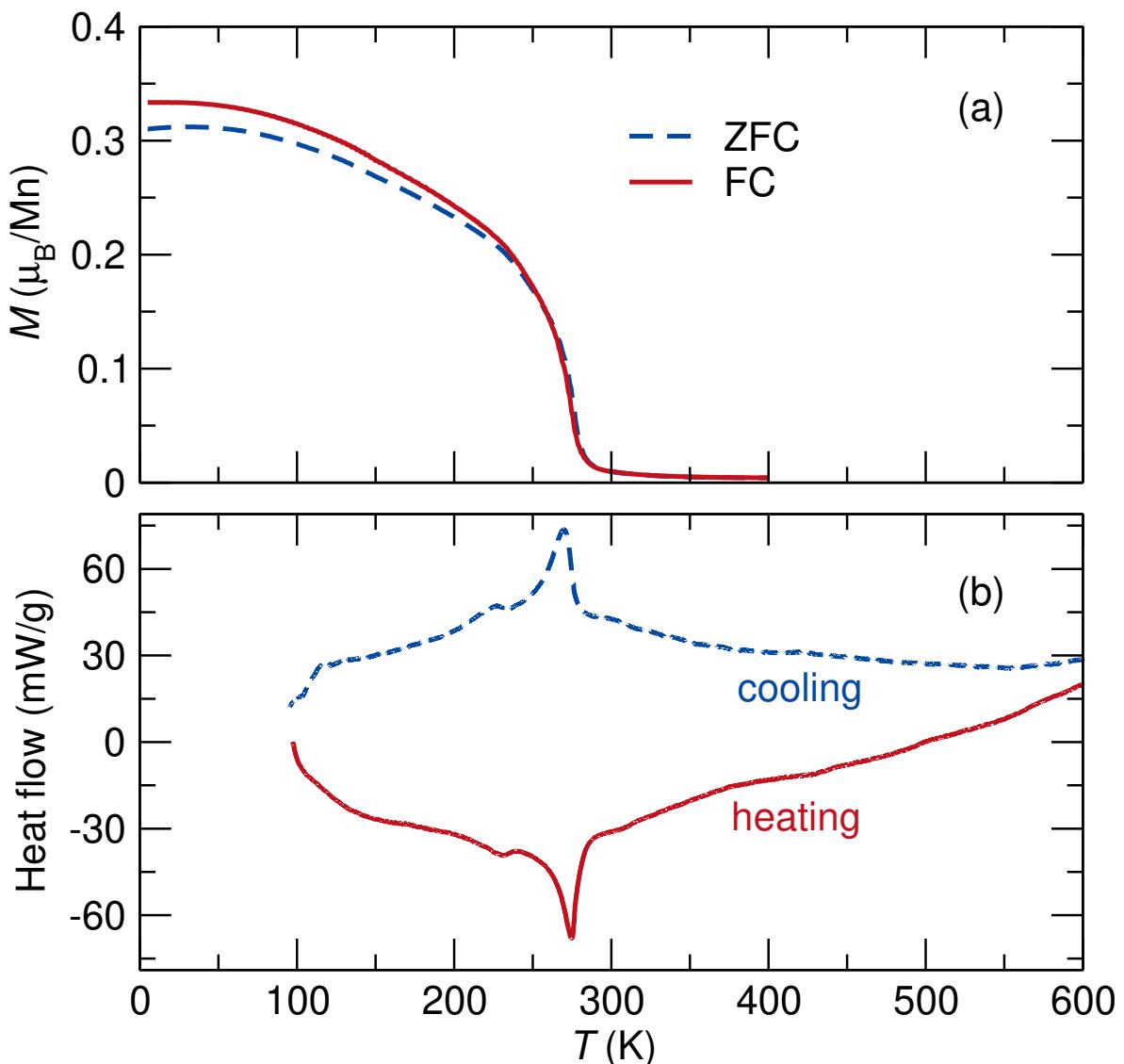


Figure 6.3: Electronic band structure

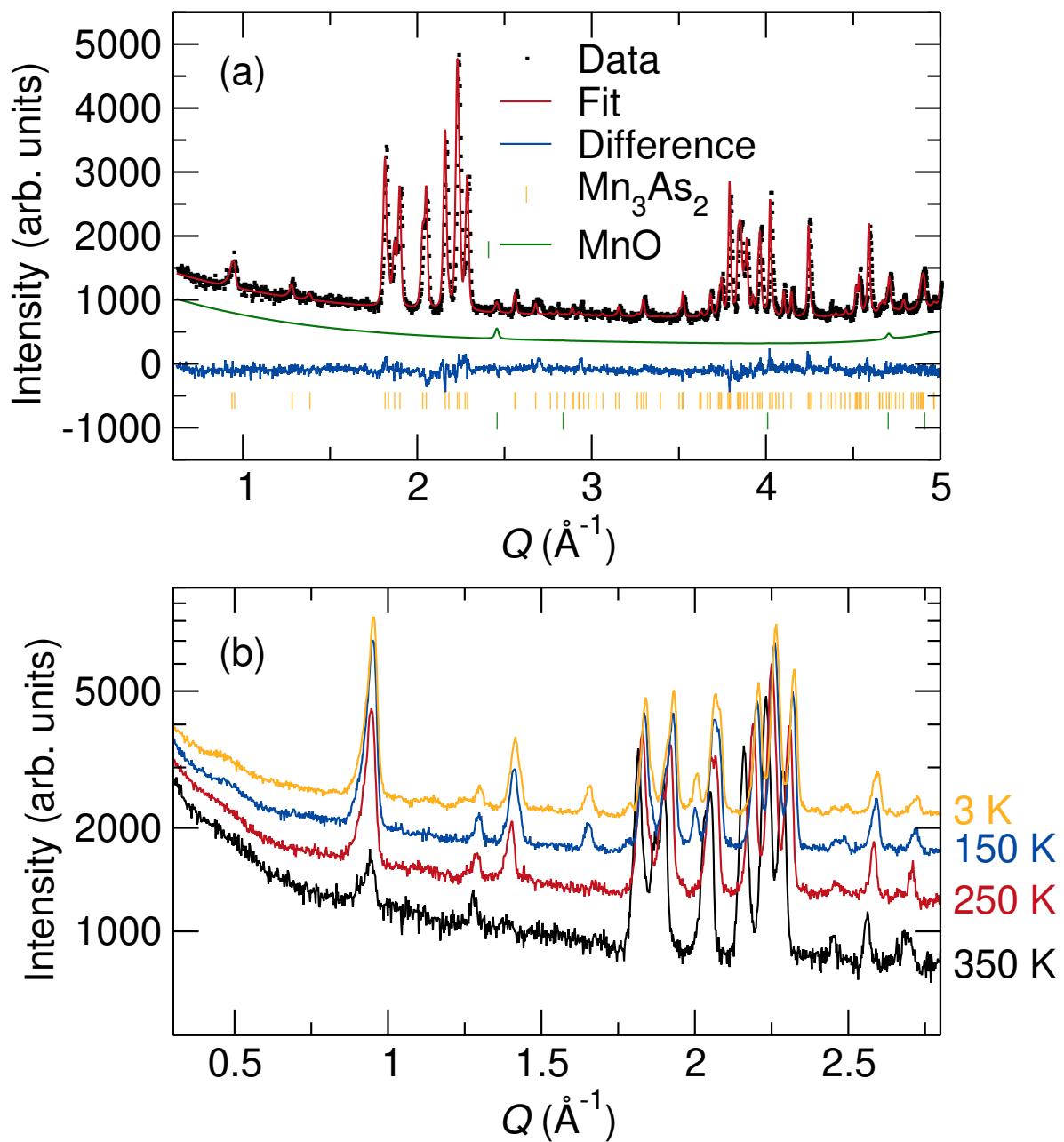


Figure 6.4: Electronic band structure

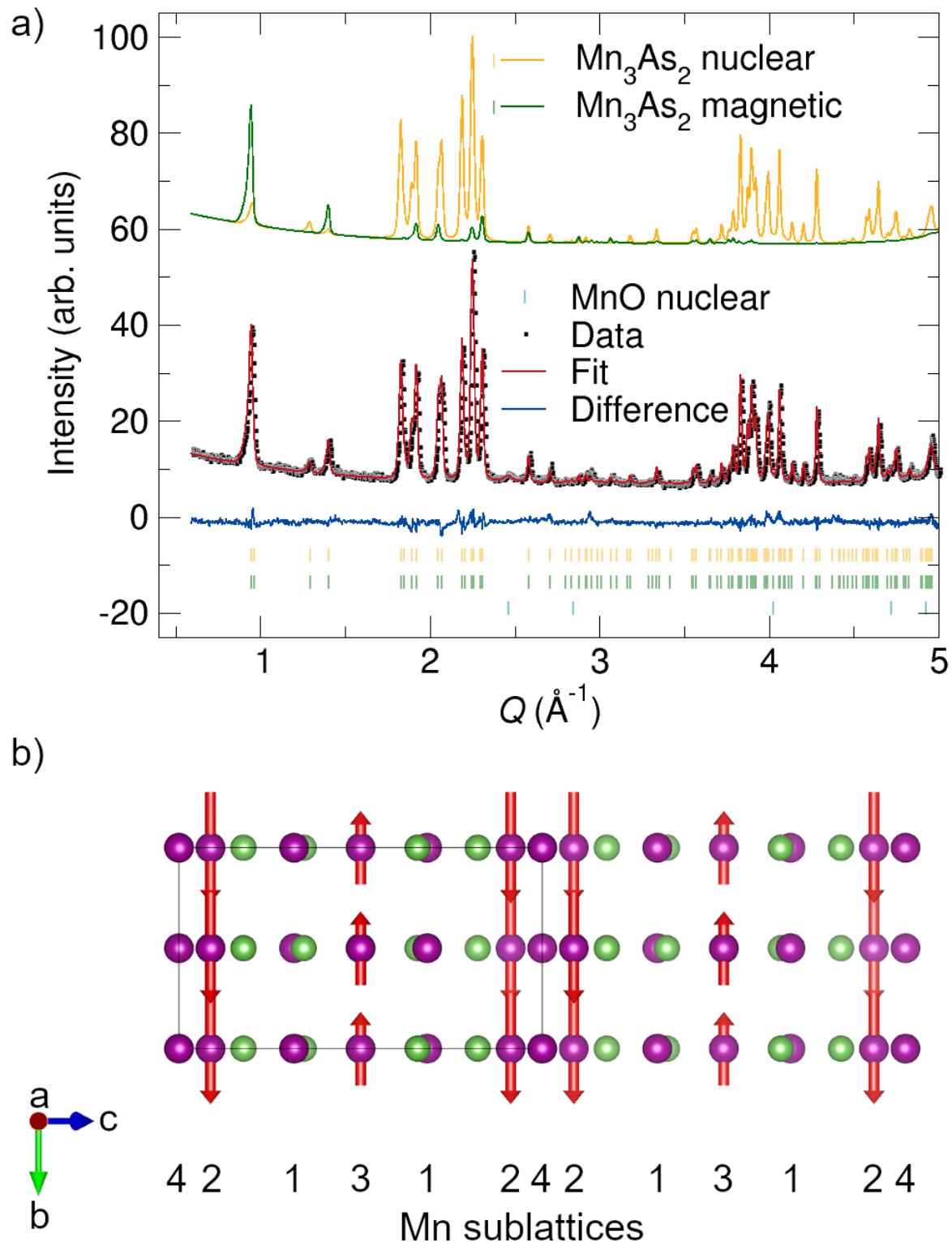


Figure 6.5: Electronic band structure

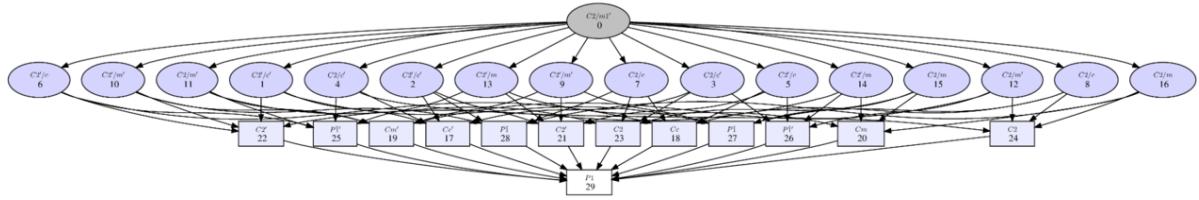


Figure 6.6: Electronic band structure

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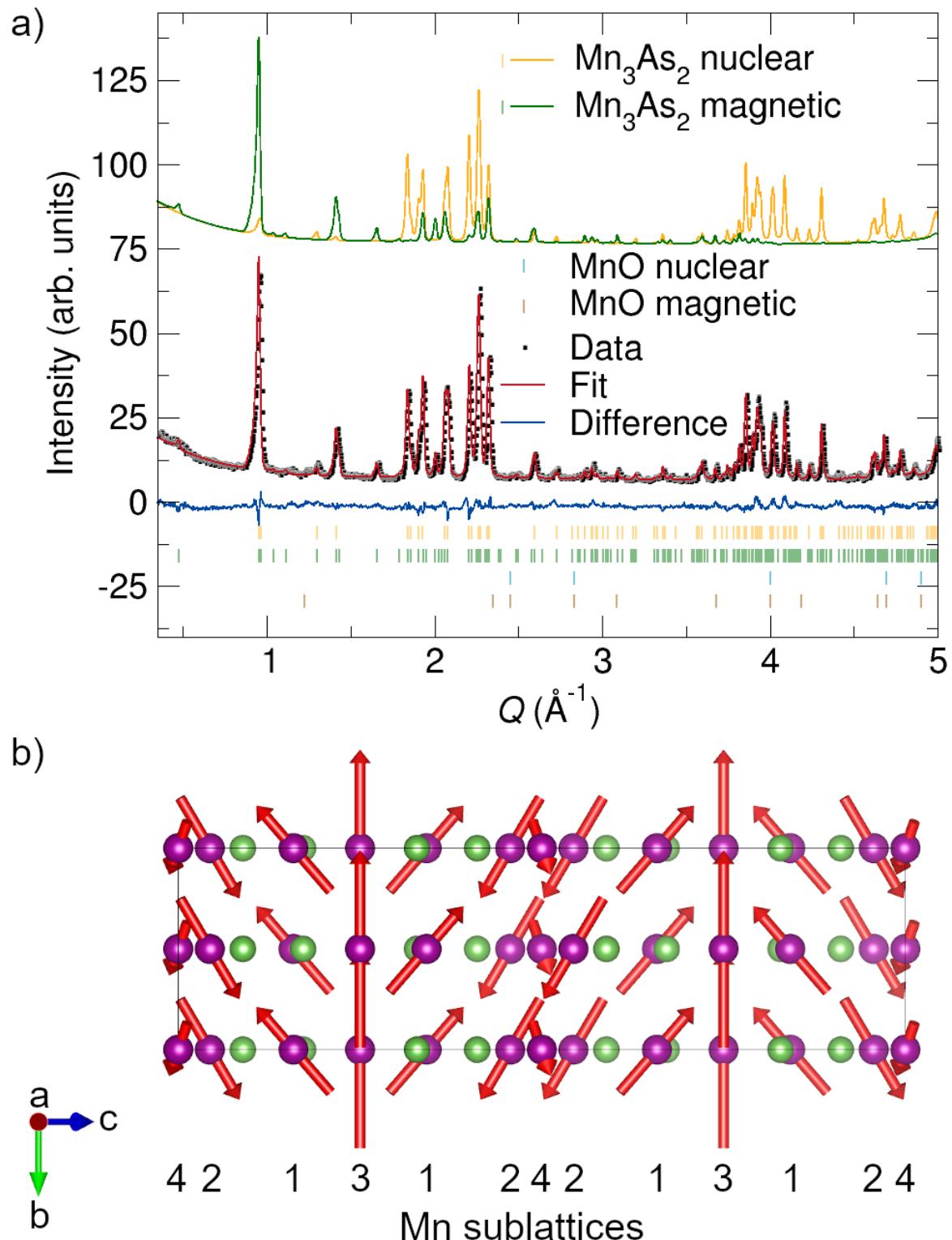


Figure 6.7: Electronic band structure

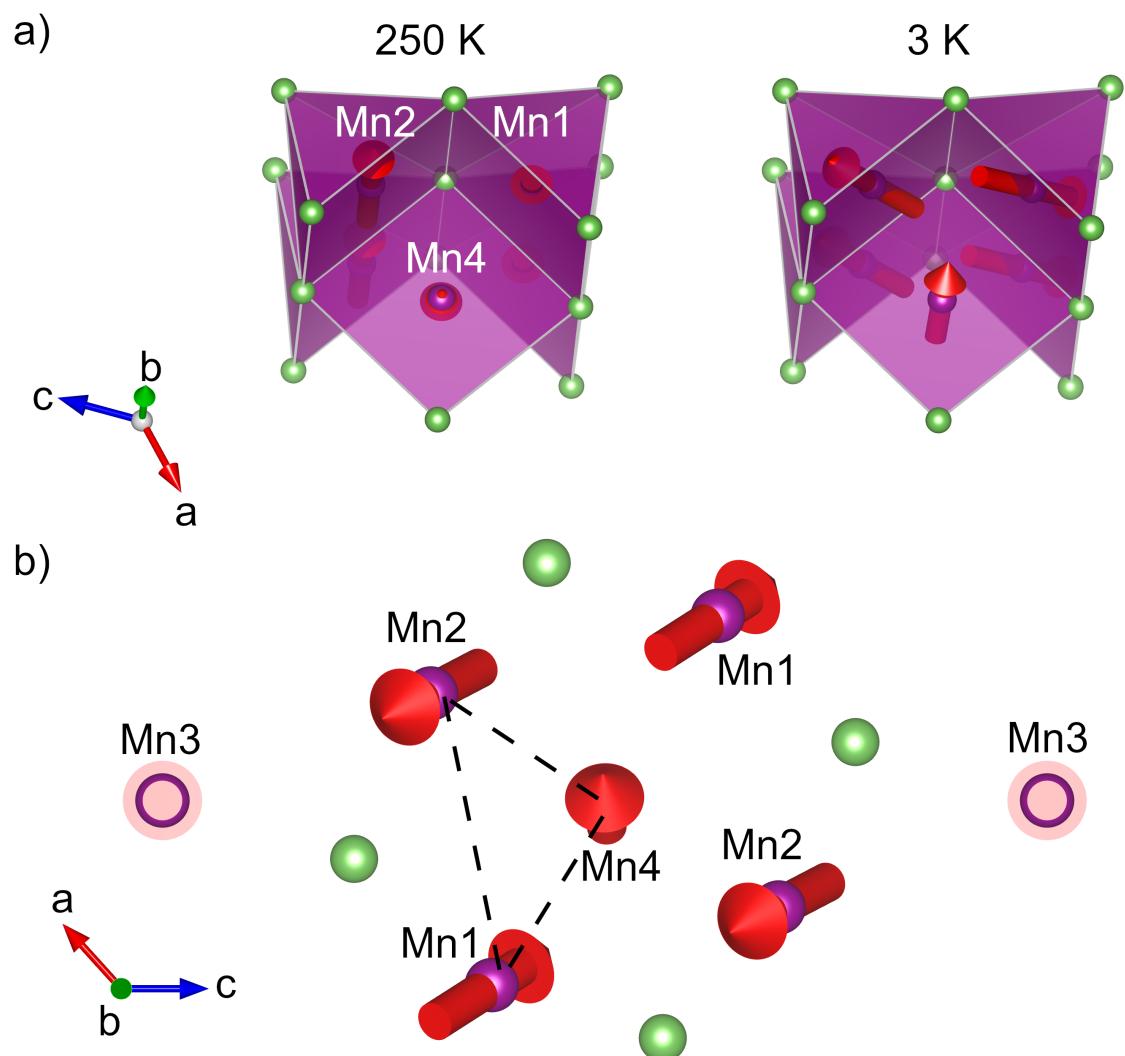


Figure 6.8: Electronic band structure

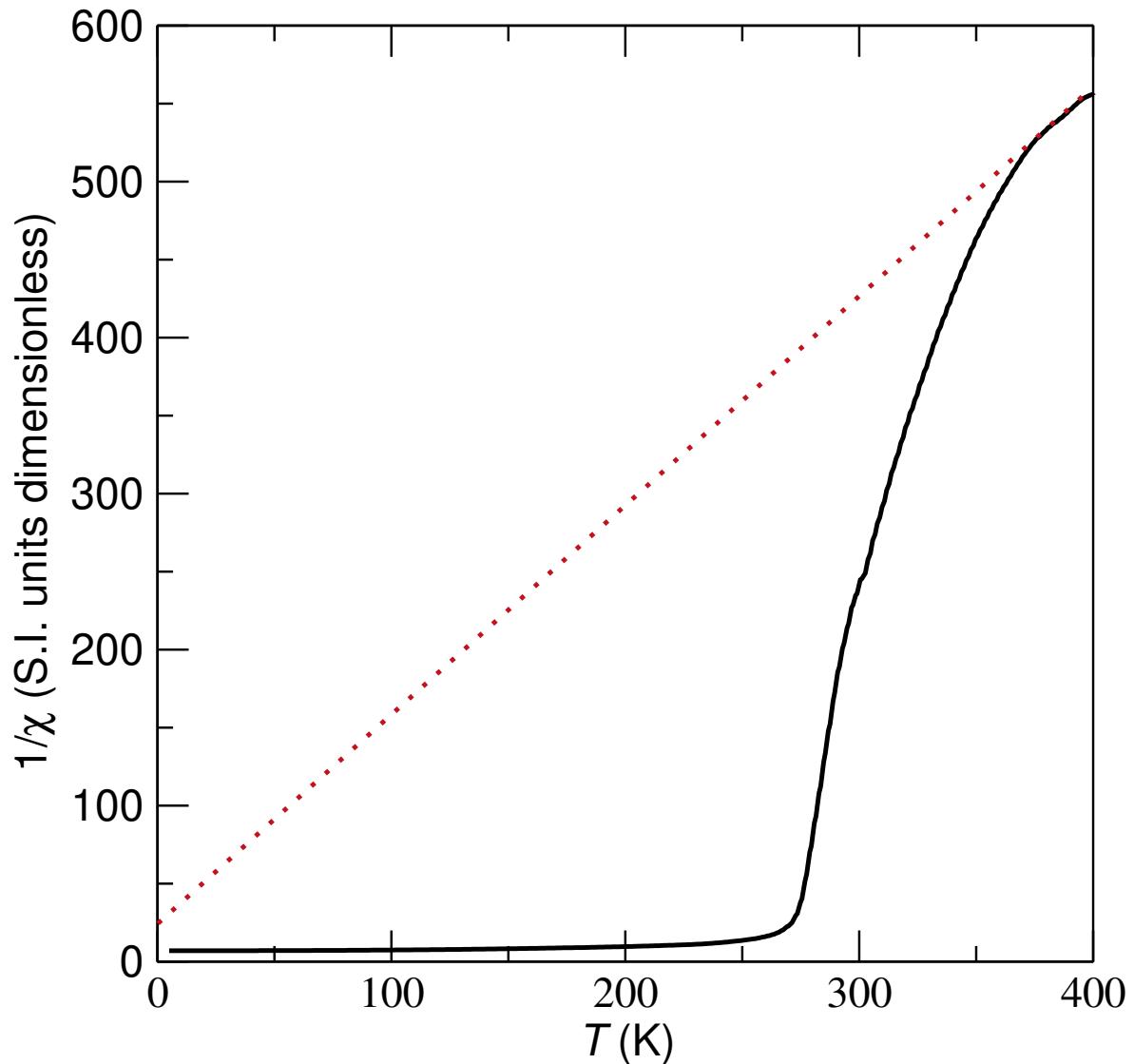


Figure 6.9: Electronic band structure

Chapter 7

Spin canting in tetragonal CuMnAs

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Chapter 8

Exchange interactions in Fe₂As probed by inelastic neutron scattering

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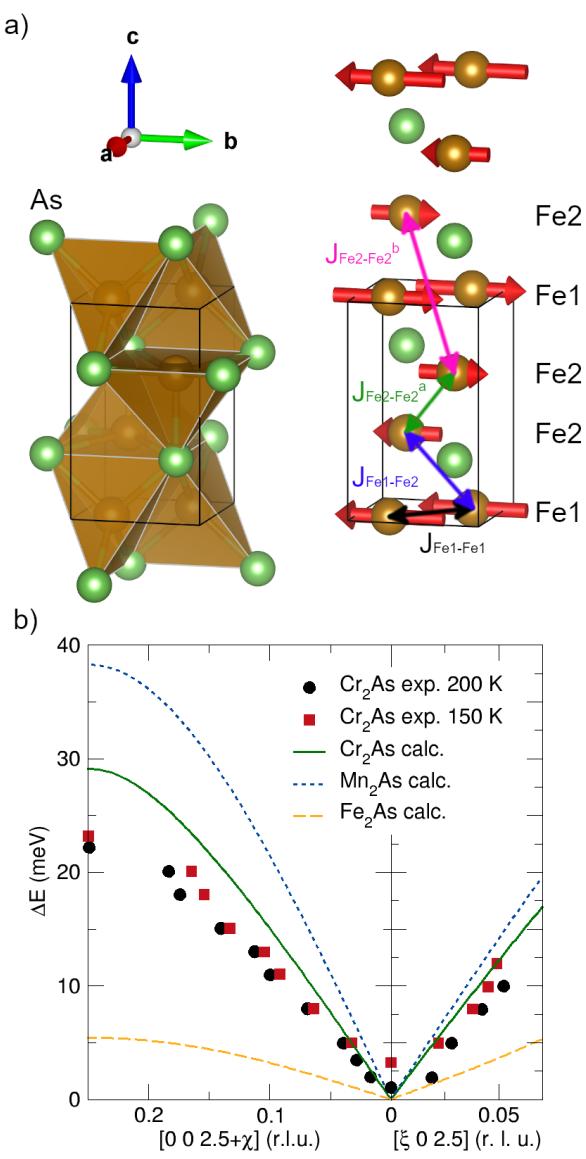


Figure 8.1: Electronic band structure

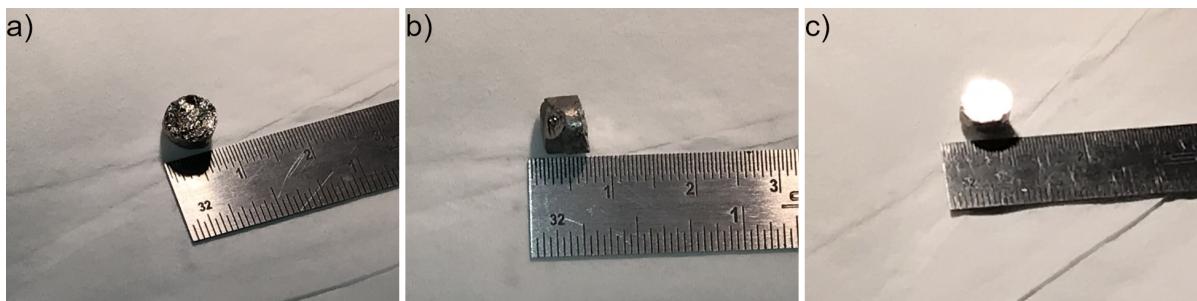


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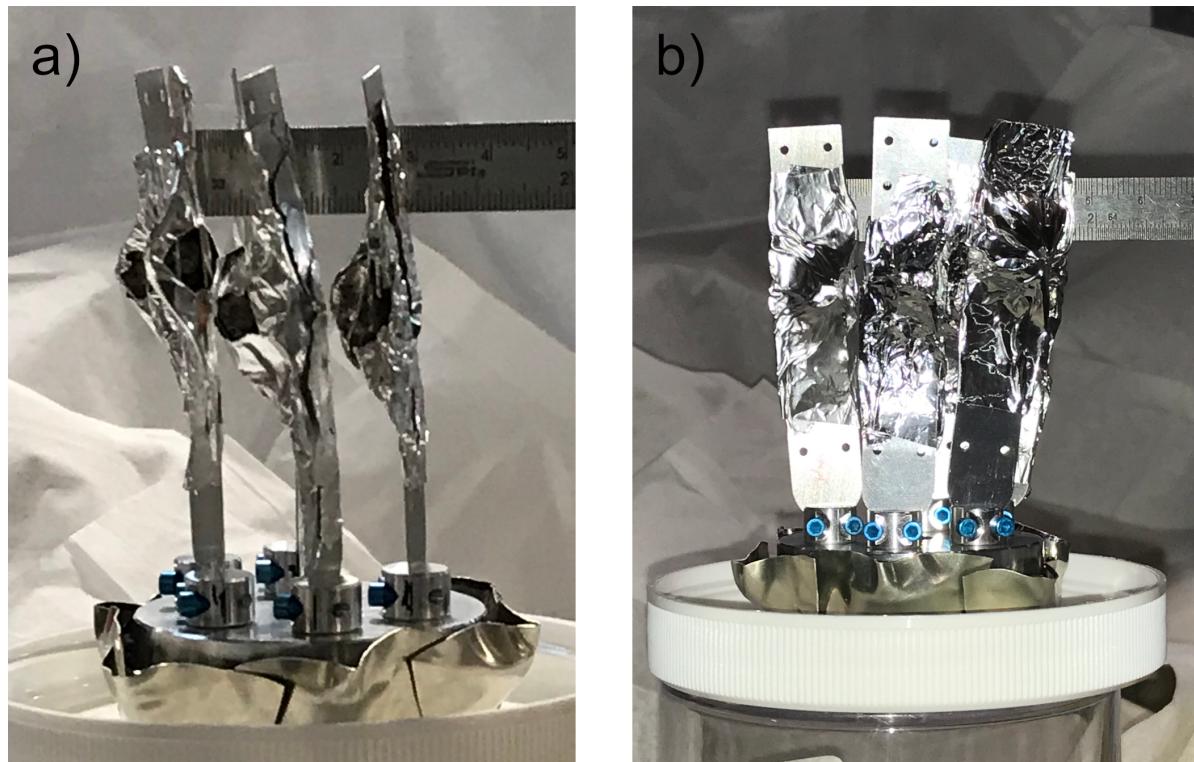


Figure 8.3: Electronic band structure

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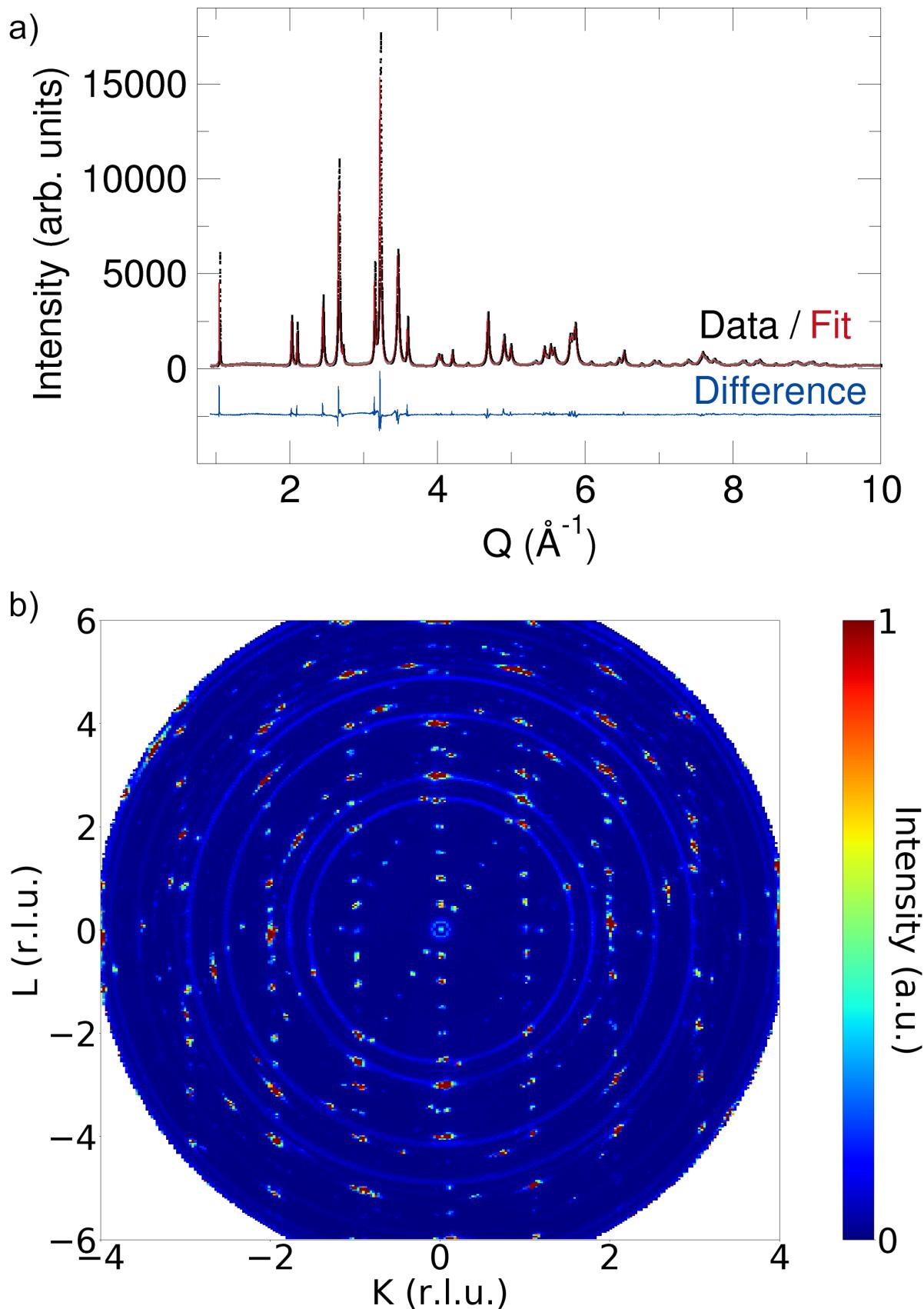


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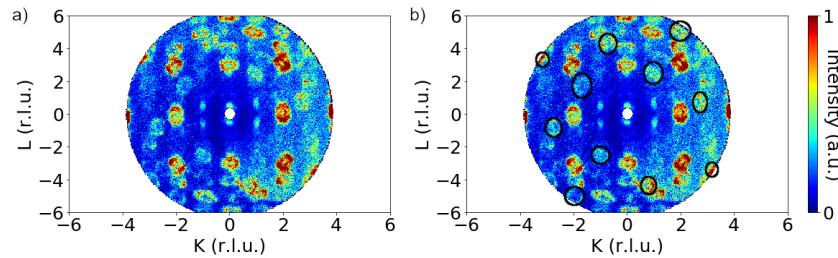


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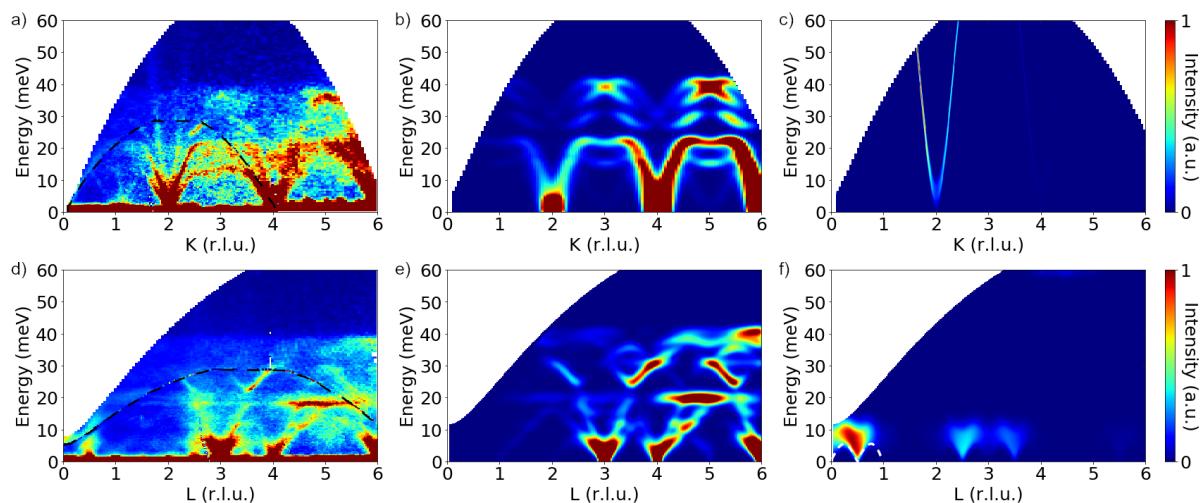


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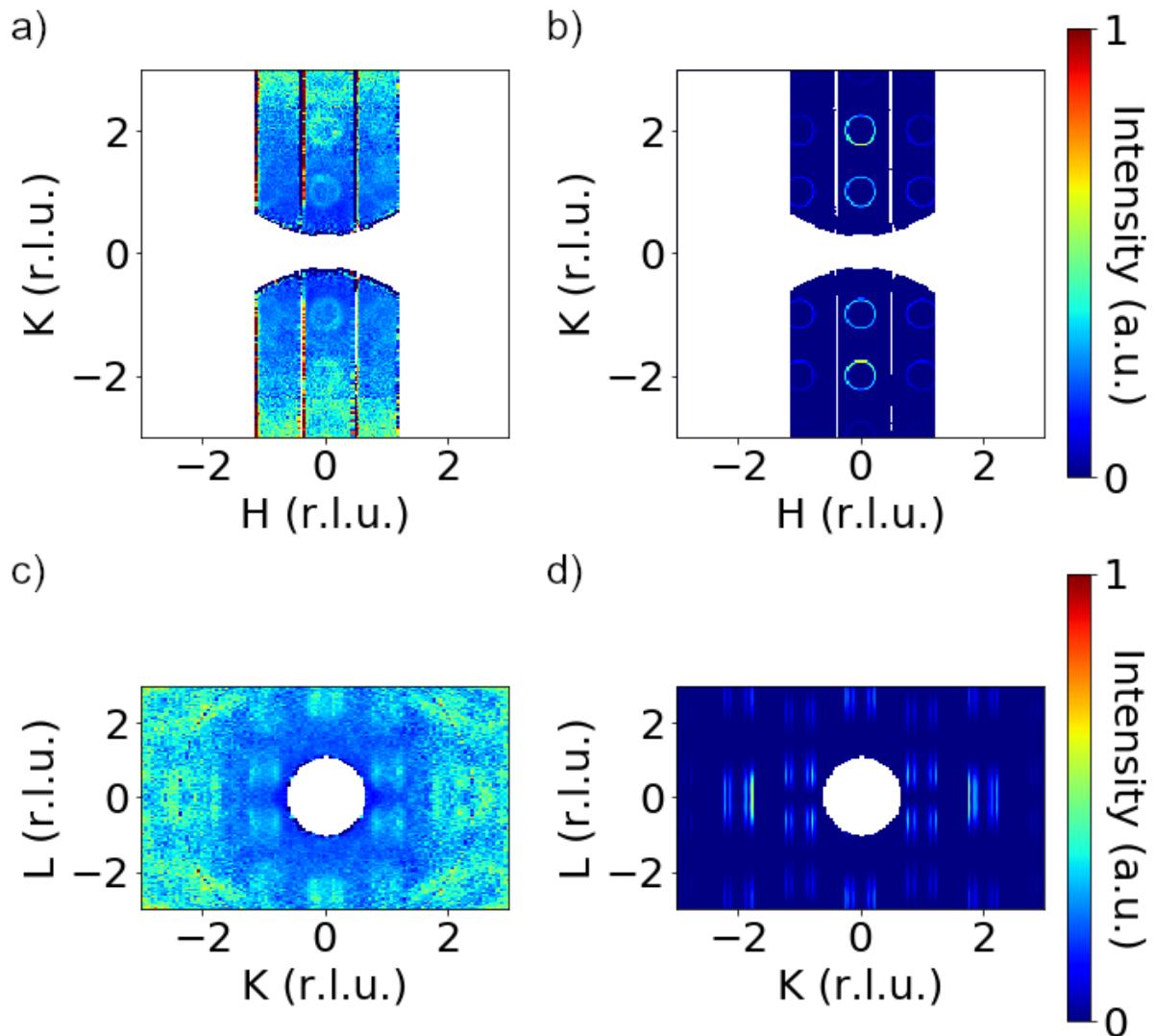


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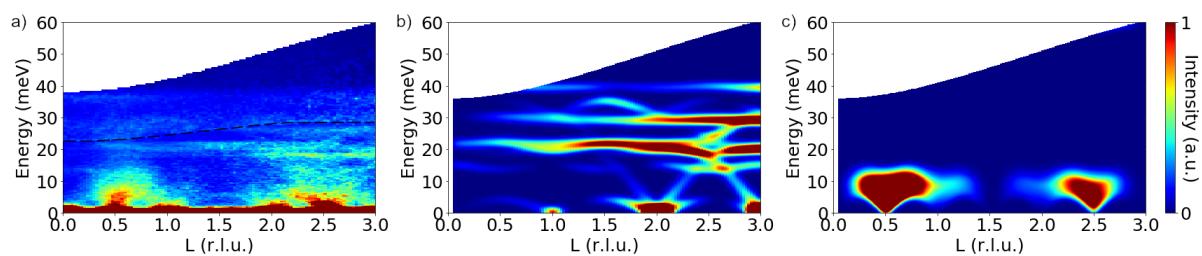


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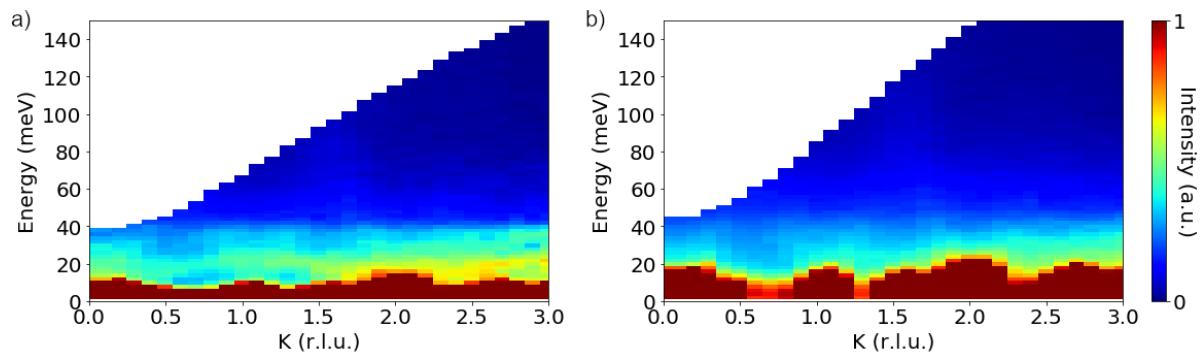


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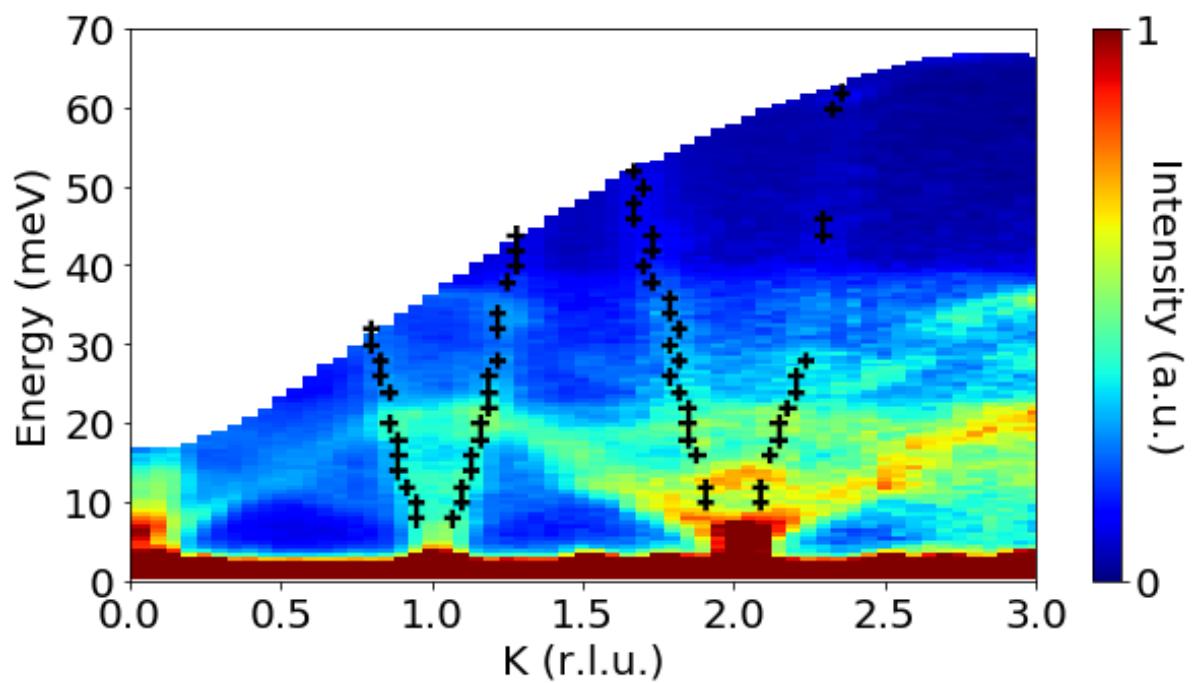


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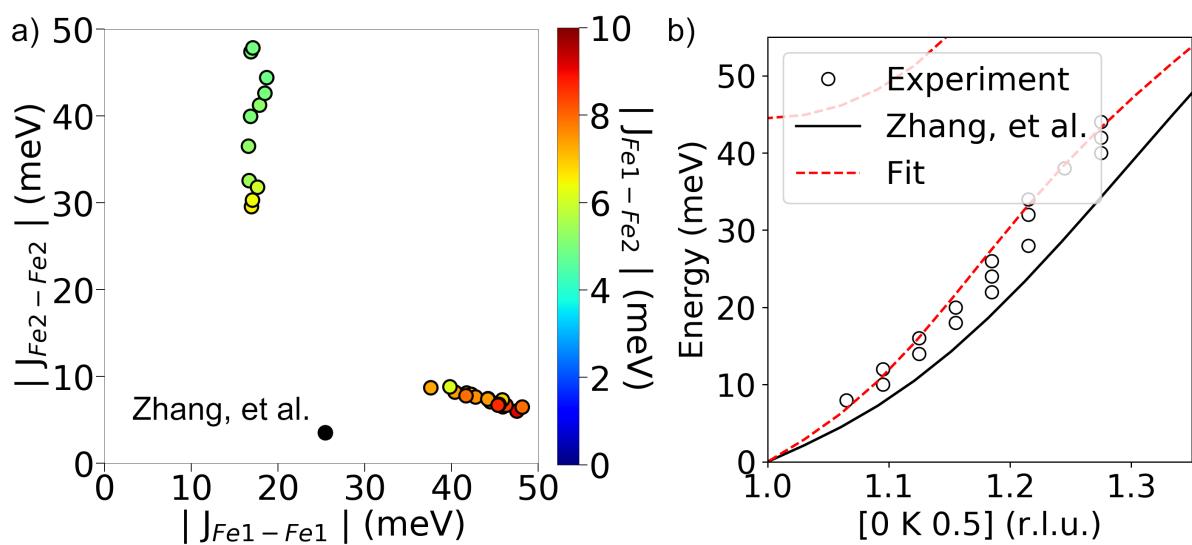


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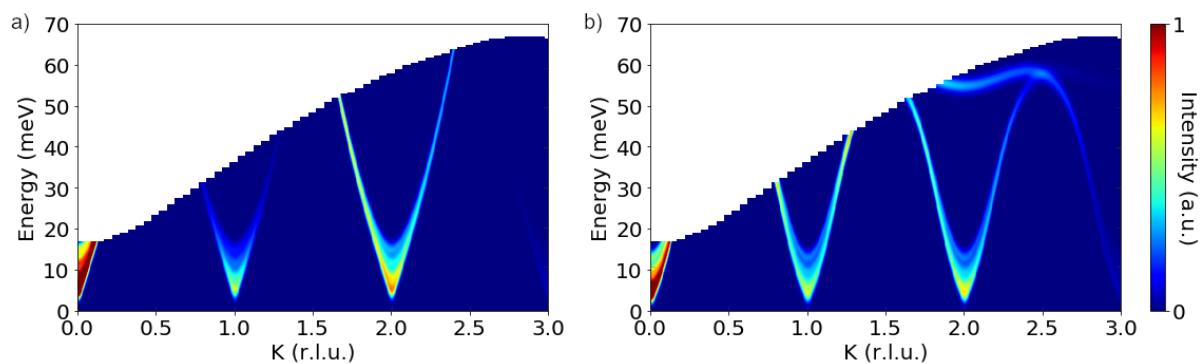


Figure 8.12: Electronic band structure

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Chapter 9

Conclusions

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References

- [1] W. Toy and B. Zee, *Computer Hardware/Software Architecture*, vol. First Edit. 1986.
- [2] J. S. Meena, S. M. Sze, U. Chand, and T. Y. Tseng, "Overview of emerging nonvolatile memory technologies," *Nanoscale Research Letters*, vol. 9, pp. 1–33, 2014.
- [3] K. M. Krishnan, *Fundamentals and Applications of Magnetic Materials*, vol. First Edit. 2016.
- [4] P. Wadley, B. Howells, J. Zelezny, C. Andrews, V. Hills, R. P. Campion, V. Novak, K. Olejnik, F. Maccherozzi, S. S. Dhesi, S. Y. Martin, T. Wagner, J. Wunderlich, F. Freimuth, Y. Mokrousov, J. Kunes, J. S. Chauhan, M. J. Grzybowski, A. W. Rushforth, K. W. Edmonds, B. L. Gallagher, and T. Jungwirth, "Electrical switching of an antiferromagnet," *Science*, vol. 351, pp. 587–591, 2016.
- [5] C. Chappert, A. Fert, and F. N. Van Dau, "The emergence of spin electronics in data storage," *Nature Materials*, vol. 6, pp. 813–823, 2007.
- [6] S. Bhatti, R. Sbiaa, A. Hirohata, H. Ohno, S. Fukami, and S. N. Piramanayagam, "Spintronics based random access memory: a review," *Materials Today*, vol. 20, pp. 530–548, 2017.
- [7] H. V. Gomonay and V. M. Loktev, "Spin transfer and current-induced switching in antiferromagnets," *Physical Review B - Condensed Matter and Materials Physics*, vol. 81, p. 144427, 2010.
- [8] S. A. Siddiqui, J. Sklenar, K. Kang, M. J. Gilbert, A. Schleife, N. Mason, and A. Hoffmann, "Metallic antiferromagnets," *Journal of Applied Physics*, vol. 128, p. 040904, 2020.
- [9] A. Manchon and S. Zhang, "Theory of nonequilibrium intrinsic spin torque in a single nanomagnet," *Physical Review B - Condensed Matter and Materials Physics*, vol. 78, p. 212405, 2008.
- [10] J. Železný, H. Gao, K. Výborný, J. Zemen, J. Mašek, A. Manchon, J. Wunderlich, J. Sinova, and T. Jungwirth, "Relativistic néel-order fields induced by electrical current in antiferromagnets," *Physical Review Letters*, vol. 113, no. 15, pp. 1–5, 2014.
- [11] J. Železný, H. Gao, A. Manchon, F. Freimuth, Y. Mokrousov, J. Zemen, J. Mašek, J. Sinova, and T. Jungwirth, "Spin-orbit torques in locally and globally noncentrosymmetric crystals: Antiferromagnets and ferromagnets," *Physical Review B*, vol. 95, p. 014403, 2017.

- [12] M. Meinert, D. Graulich, and T. Matalla-wagner, "Electrical Switching of Antiferromagnetic Mn₂Au and the Role of Thermal Activation," *Physical Review Applied*, vol. 9, p. 64040, 2018.
- [13] T. Matalla-Wagner, M. F. Rath, D. Graulich, J. M. Schmalhorst, G. Reiss, and M. Meinert, "Electrical Neél-Order Switching in Magnetron-Sputtered CuMnAs Thin Films," *Physical Review Applied*, vol. 12, p. 064003, 2019.
- [14] Y. Kim, K. Kang, A. Schleife, and M. J. Gilbert, "Voltage-induced switching of an antiferromagnetically ordered topological Dirac semimetal," *Physical Review B*, vol. 97, p. 134415, 2018.
- [15] A. N. Nateprov, V. C. Kravtsov, V. Fritsch, and H. von Löhneysen, "Structure and properties of the tetragonal phase of MnCuAs," *Surface Engineering and Applied Electrochemistry*, vol. 47, pp. 540–543, 2011.
- [16] F. MáčA, J. Mašek, O. Stelmakhovych, X. Martí, H. Reichlová, K. Uhlířová, P. Beran, P. Wadley, V. Novák, and T. Jungwirth, "Room-temperature antiferromagnetism in CuMnAs," *Journal of Magnetism and Magnetic Materials*, vol. 324, pp. 1606–1612, 2012.
- [17] P. Wadley, V. Novák, R. P. Campion, C. Rinaldi, X. Martí, H. Reichlová, J. Zelezny, J. Gazquez, M. A. Roldan, M. Varela, D. Khalyavin, S. Langridge, D. Kriegner, F. Máca, J. Masek, R. Bertacco, V. Holy, A. W. Rushforth, K. W. Edmonds, B. L. Gallagher, C. T. Foxon, J. Wunderlich, and T. Jungwirth, "Tetragonal phase of epitaxial room-temperature antiferromagnet CuMnAs," *Nature Communications*, vol. 4, p. 2322, 2013.
- [18] K. Uhlirova, R. Tarasenko, F. J. Martinez-Casado, B. Vondrackova, and Z. Matej, "Synthesis and single crystal study of CuMn₃As₂ and Cu₂Mn₄As₃," *Journal of Alloys and Compounds*, vol. 650, pp. 224–227, 2015.
- [19] V. Hills, P. Wadley, R. P. Campion, V. Novak, R. Beardsley, K. W. Edmonds, B. L. Gallagher, B. Ouladdiaf, and T. Jungwirth, "Paramagnetic to antiferromagnetic transition in epitaxial tetragonal CuMnAs (invited)," *Journal of Applied Physics*, vol. 117, p. 172608, 2015.
- [20] P. Wadley, V. Hills, M. R. Shahedkhah, K. W. Edmonds, R. P. Campion, V. Novák, B. Ouladdiaf, D. Khalyavin, S. Langridge, V. Saidl, P. Nemec, A. W. Rushforth, B. L. Gallagher, S. S. Dhesi, F. MacCherozzi, J. Železný, and T. Jungwirth, "Antiferromagnetic structure in tetragonal CuMnAs thin films," *Scientific Reports*, vol. 5, p. 17079, 2015.
- [21] A. E. Austin, E. Adelson, and W. H. Cloud, "Magnetic Structures of Mn₂As and Mn₂Sb_{0.7}As_{0.3}," *Journal of Applied Physics*, vol. 33, pp. 1356–1357, 1962.
- [22] G. E. Bacon and R. Street, "Magnetic Structure of Manganse Arsenide," *Nature*, vol. 175, p. 518, 1955.
- [23] "Magnetic ordering and metal-atom site preference in tetragonal CrMnAs: Electronic correlation effects," *Journal of Computational Chemistry*, vol. 39, pp. 1585–1593, 2018.
- [24] Y. Zhang, J. Brgoch, and G. J. Miller, "Magnetic ordering in tetragonal 3d metal arsenides M₂As (M = Cr, Mn, Fe): An ab initio investigation," *Inorganic Chemistry*, vol. 52, pp. 3013–3021, 2013.

- [25] Y. Zhang and G. J. Miller, "Competition between direct and indirect exchange couplings in MnFeAs: A first-principles investigation," *Journal of Physical Chemistry C*, vol. 119, pp. 580–589, 2015.
- [26] X. Zhang, Q. Liu, J.-W. Luo, A. J. Freeman, and A. Zunger, "Hidden spin polarization in inversion-symmetric bulk crystals," *Nature Physics*, vol. 10, pp. 387–393, 2014.
- [27] S. Y. Bodnar, M. Filianina, S. P. Bommanaboyena, T. Forrest, F. Maccherozzi, A. A. Sapozhnik, Y. Skourski, M. Kläui, and M. Jourdan, "Imaging of current induced Néel vector switching in antiferromagnetic Mn₂Au," *Physical Review B*, vol. 99, pp. 8–12, 2019.
- [28] M. A. Susner, D. S. Parker, and A. S. Sefat, "Importance of doping and frustration in itinerant Fe-doped Cr₂Al," *Journal of Magnetism and Magnetic Materials*, vol. 392, pp. 68–73, 2015.
- [29] M. Atoji, "Antiferromagnetic structure of AlCr₂," *The Journal of Chemical Physics*, vol. 43, pp. 222–225, 1965.
- [30] A. Kallel and F. D. Bergevin, "ANTIFERROMAGNETISME DE LA SOLUTION SOLIDE DE L'ALUMINTUM DANS LE CHROME," *Solid State Communications*, vol. 5, pp. 955–958, 1967.
- [31] G. Venturini, R. Welter, and B. Malaman, "Crystallographic data and magnetic properties of RT₆Ge₆ compounds (R Sc, Y, Nd, Sm, GdLu; TMn, Fe)," *Journal of Alloys and Compounds*, vol. 185, pp. 99–107, 1992.
- [32] T. Mazet, O. Isnard, and B. Malaman, "Neutron diffraction and 57Fe Mössbauer study of the HfFe₆Ge₆-type RFe₆Ge₆ compounds (R = Sc , Ti , Zr , Hf , Nb)," *Solid State Communications*, vol. 114, pp. 91–96, 2000.
- [33] S. Nakatsuji, N. Kiyohara, and T. Higo, "Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature," *Nature*, vol. 527, pp. 212–215, 2015.
- [34] J. Kübler and C. Felser, "Non-collinear antiferromagnets and the anomalous Hall effect," *Epl*, vol. 108, p. 67001, 2014.
- [35] M. Kimata, H. Chen, K. Kondou, S. Sugimoto, P. K. Muduli, M. Ikhlas, Y. Omori, T. Tomita, A. H. MacDonald, S. Nakatsuji, and Y. Otani, "Magnetic and magnetic inverse spin Hall effects in a non-collinear antiferromagnet," *Nature*, vol. 565, pp. 627–630, 2019.
- [36] U. Häussermann, M. Boström, P. Viklund, R. Ö, and T. Björnängen, "FeGa₃ and RuGa₃: Semiconducting intermetallic compounds," *Journal of Solid State Chemistry*, vol. 165, pp. 94–99, 2002.
- [37] P. Viklund, S. Lidin, P. Berastegui, and U. Häussermann, "Variations of the FeGa₃ structure type in the systems CoIn_{3-x}Zn_x and CoGa_{3-x}ZN_x," *Journal of Solid State Chemistry*, vol. 165, pp. 100–110, 2002.
- [38] Y. Zhang, C. Michioka, M. Imai, H. Ueda, and K. Yoshimura, "Effect of Co substitution on the magnetic properties in Fe_{1-x}CoxGa₃," *Journal of Physics: Conference Series*, vol. 868, p. 012025, 2017.

- [39] D. Harker, "The crystal structure of Ni₄Mo," *The Journal of Chemical Physics*, vol. 12, pp. 315–317, 1944.
- [40] A. Taylor and N. J. Doyle, "Further studies on the nickel–aluminium system. I. β -NiAl and δ -Ni₂Al₃ phase fields," *Journal of Applied Crystallography*, vol. 5, pp. 201–209, 1972.