

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.

Acknowledgments

This project would not be possible without many people. Firstly, thanks to my advisor, Prof. Daniel P. Shoemaker.

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Chapter 1

Introduction

1.1 Magnetic information storage

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

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
22 the electronic spin degree of freedom to store memory. MRAM devices consist of cells with
23 magnetic tunnel junctions (MTJ) that have two ferromagnet (FM) layers separated by an
24 insulating layer. One of the layer is pinned where the magnetization orientation is fixed
25 and acts as a reference layer. Depending on the orientation of the free layer, the tunneling
26 magnetoresistance (TMR) is high or low and hence, memory can be read using electrical
27 currents. Early MRAMs were written by induced fields from heavy currents passed on the
28 adjacent layer. With recent developments in spin transfer torque in ferromagnets, it has
29 become possible to write using electrical currents. This has reduced the power consumption

30 significantly and made commercialization of MRAM devices possible.

31 **1.2 Antiferromagnets for potential applications as a memory unit**

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

47 Unlike previously discussed STT MRAM devices, spin orbit torque based electrical switch-
48 ing in FM does not require the presence of a pinned FM layer at all. Since the fieldlike torque
49 experienced by the moments are quadratic to the magnetization of the FM, the concept is
50 also equally applicable to AFM. In 2016, Wadley *et al.* showed that in AFM with certain
51 symmetries, the current induced spin polarization of charge carriers is staggered across the
52 two magnetic sublattices resulting in a fieldlike torque that is in the same direction for the
53 two sublattices. This could allow the rotation of the Néel vector orientation with every
54 current pulse. This is possible in materials which are globally centrosymmetric but locally
55 non-centrosymmetric and the two sublattices are related to each other by a center of inversion.
56 It was initially demonstrated in the case of epitaxially grown tetragonal CuMnAs thin films
57 on GaP substrate and since then, it has also been shown in Mn₂Au. It requires the presence
58 of degenerate Néel vectors like in CuMnAs as shown in Fig. 1.1(a) as opposed to compounds
59 like MnF₂ where the Mn moments point along *c* in Fig. 1.1(b).

60 **1.3 Exploration of Cu-Mn-As phase space**

61 Cu-Mn-As phase space has become very popular in recent times primarily due to tetragonal
62 and orthorhombic CuMnAs. As mentioned earlier, tetragonal CuMnAs was the first antifer-
63 romagnet where electrical switching was supposedly demonstrated. Orthorhombic CuMnAs,

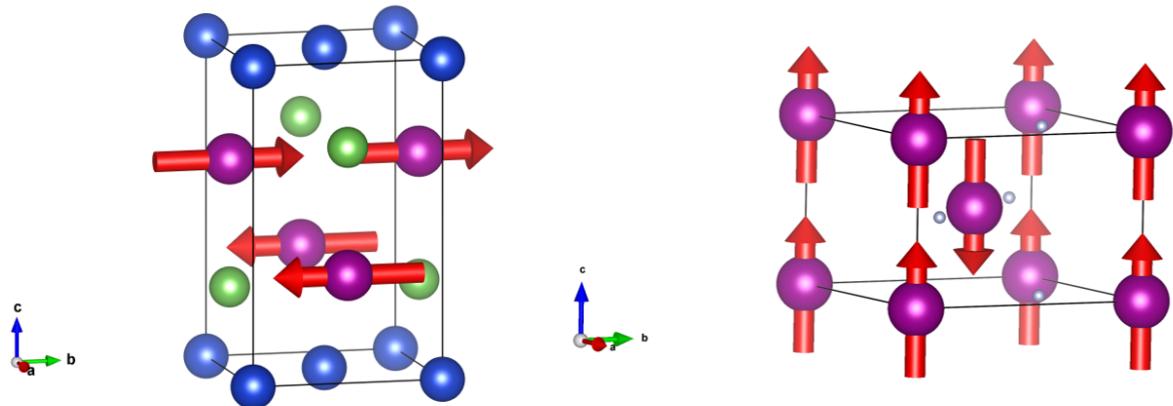


Figure 1.1: The magnetic structures of tetragonal CuMnAs and MnF₂ are shown in (a) and (b), respectively.

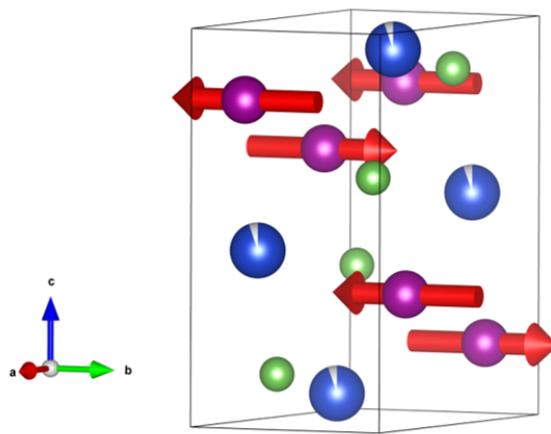


Figure 1.2: Magnetic structure of orthorhombic CuMnAs

64 shown in Fig. 1.2, was the first magnetic compound to be proposed as a Dirac semimetal.
 65 Based on the orientation of the Néel vector, the compound changes from conducting to
 66 insulating and hence, it can be used for voltage based switching applications.

67 Despite the growing importance of the compounds in Cu-Mn-As system, the Cu-Mn-
 68 As ternary phase space has not been explored properly. There are four known ternary
 69 compounds including both the polymorphs of CuMnAs, orthorhombic CuMn₃As₂ and
 70 Cu₂Mn₄As₃ as shown in Fig. 1.3. Bulk orthorhombic CuMnAs can be grown using tra-
 71 ditional solid state synthesis routes by Cu, Mn and As powders in stoichiometric ratio and
 72 heating the powders to 1000°C. In order to synthesize pure bulk tetragonal CuMnAs, we
 73 have to go off-stoichiometry and either substitute Mn with Cu or As. Hence, it is important
 74 to explore different regions in the Cu-Mn-As system and verify the stability of different

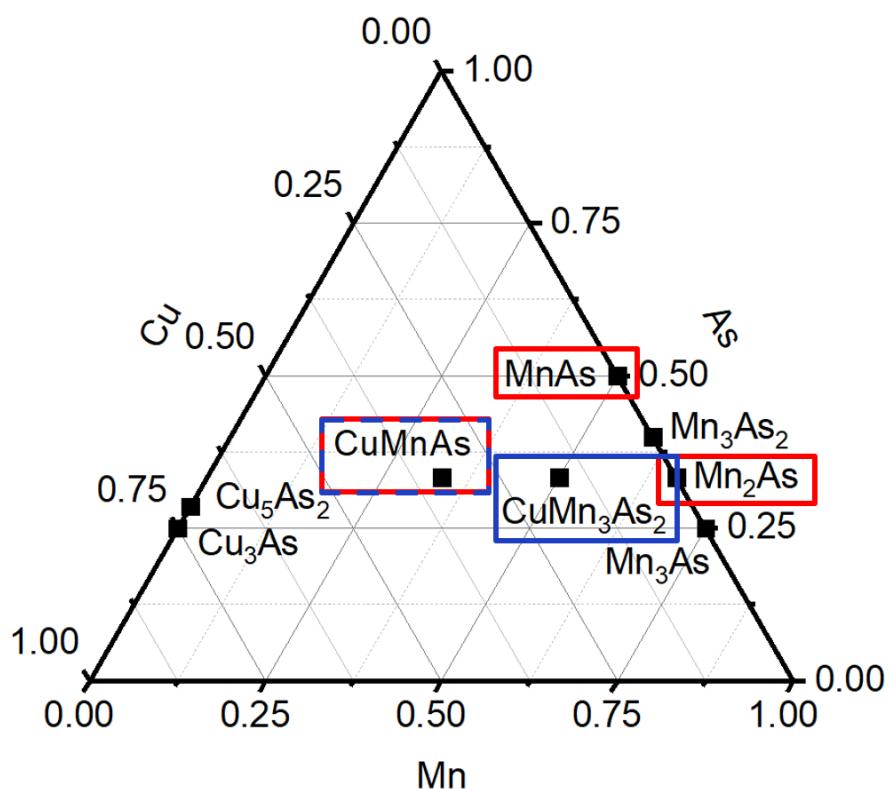


Figure 1.3: Cu-Mn-As ternary phase diagram highlighting the known ternary compounds in blue and known magnetic structures in red.

75 ternary compounds. The magnetic structures in the Cu-Mn-As system have also not been
76 identified for most of the compounds. Apart from the four Cu-Mn-As ternary compounds,
77 there are more than ten Mn-As binary compounds. The magnetic structures are known only
78 for the two previously mentioned CuMnAs compounds, Mn₂As and MnAs as shown in Fig.
79 1.3. Since most, if not all, the binary Mn-As compounds are metallic, there is a need to
80 magnetically characterize the compounds and identify their magnetic structures.

81 **1.4 Exchange interactions in Cu₂Sb type structures**

82 If we want to understand the electrical switching behavior in metallic antiferromagnets, we
83 should be able to quantify the fundamental energies such as magnetocrystalline anisotropy
84 and exchange interactions in materials like CuMnAs. CuMnAs has a Cu₂Sb structure type.
85 Other materials with this structure includes Mn₂As, Cr₂As, Fe₂As, CrMnAs, FeMnAs etc.
86 Althought Mn₂As, Cr₂As and Fe₂As have the same structure, the magnetic ground state is
87 different in all three compounds. The direct exchange interaction between two magnetic
88 atoms is a result of antibonding or non-bonding orbital overlap between the two magnetic
89 atoms. Since these materials are metallic, there are two contributions to indirect exchange
90 interactions. One contribution arises from superexchange interactions mediated by As atoms
91 and the other contribution comes from RKKY interactions that are caused due to exchange
92 interactions with the conduction electrons. It is important that we are able to determine what
93 spin interactions are relevant and how does it affect the magnetic ordering in these materials.
94 It is also crucial that we are able to verify the computational methods and the exchange
95 coupling values obtained from these methods so that we can use these methods for other
96 systems as well.

Chapter 2

Theory of electrical switching in metallic antiferromagnets

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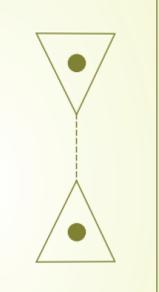
Bulk symmetry: Site symmetry: Symmetry schematic: Effect/consequence: Name:	a Centrosymmetric Inversion symmetry  Absence of spin splitting and spin polarization R-1	b Non-centrosymmetric (bulk inversion asymmetry) Dipole field  Site dipole field induced net spin polarization D-1	c Centrosymmetric Dipole field  Site dipole field induced spin polarization compensated by its inversion counterpart R-2	 Inversion asymmetry  Site inversion asymmetry induced spin polarization compensated by its inversion counterpart D-2
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Figure 2.1: Electronic band structure

Table 1 | Classification of spin polarization in nonmagnetic bulk materials on the basis of bulk space group and site point group.

Site point group \\ Bulk space group	Non-centrosymmetric (at least one site)			Centrosymmetric (all sites) ($C_1, C_2, C_3, C_4, C_6, C_{1v}, C_{2v}, C_{3v}, C_{4v}, C_{6v}$, $D_{4h}, S_6, D_{3d}, D_{6h}, T_h, O_h$)
	Non-polar (all sites) ($D_{2h}, D_{3h}, D_{4h}, D_{6h}, S_{4h}, D_{2d}, C_{3h}, D_{3h}, T, T_d, O$)	Polar (at least one site) ($C_1, C_2, C_3, C_4, C_6, C_{1v}, C_{2v}, C_{3v}, C_{4v}, C_{6v}$)	Dipoles add up to zero	Dipoles add up to non-zero
Non-centrosymmetric (for example, $F\bar{4}3m$)	a D-1 Example: GaAs, ZrCoBi	b D-1 Example: γ -LiAlO ₂	c R-1 & D-1 Example: BiTeI, α -SnTe	<i>Not possible (Site point group cannot be centrosymmetric if space group is non-centrosymmetric)</i>
Centrosymmetric (for example, $R\bar{3}m$)	d D-2 Example: Si, NaCaBi	e R-2 & D-2 Example: MoS ₂ , Bi ₂ Se ₃ , LaOBiS ₂		f Absence of spin polarization Example: β -SnTe

Figure 2.2: Electronic band structure

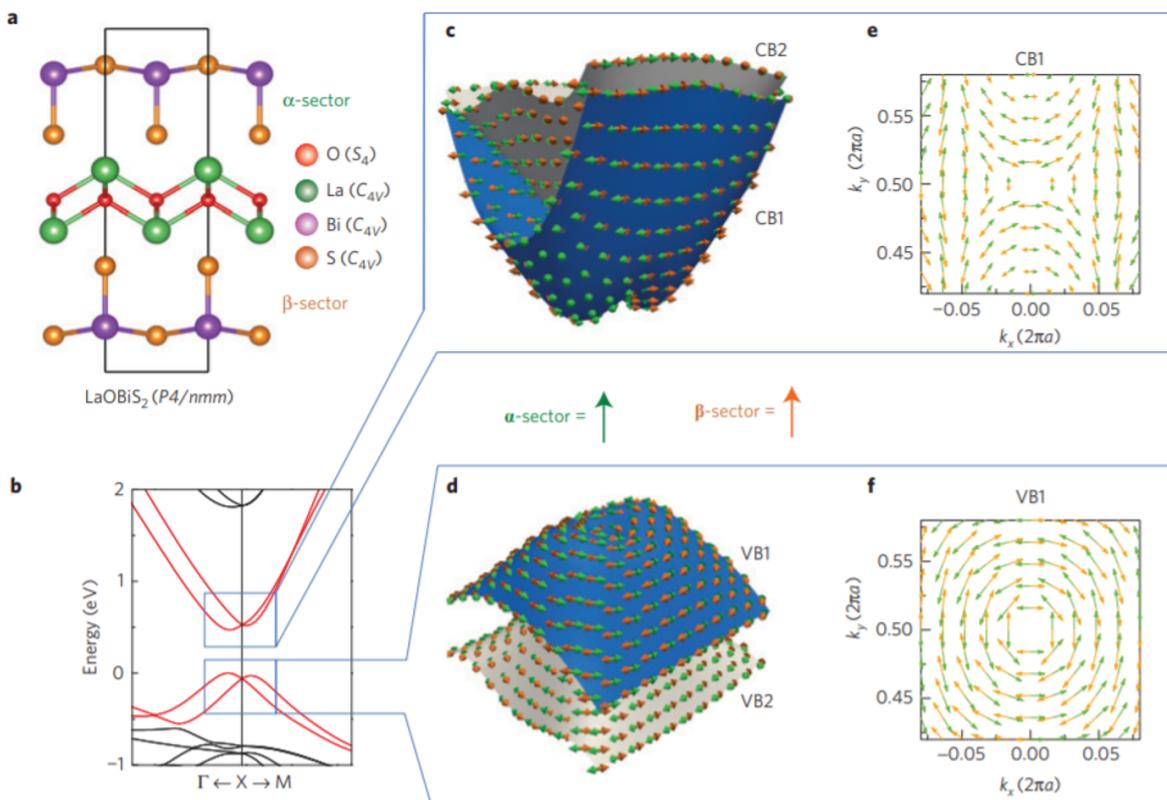


Figure 2.3: Electronic band structure

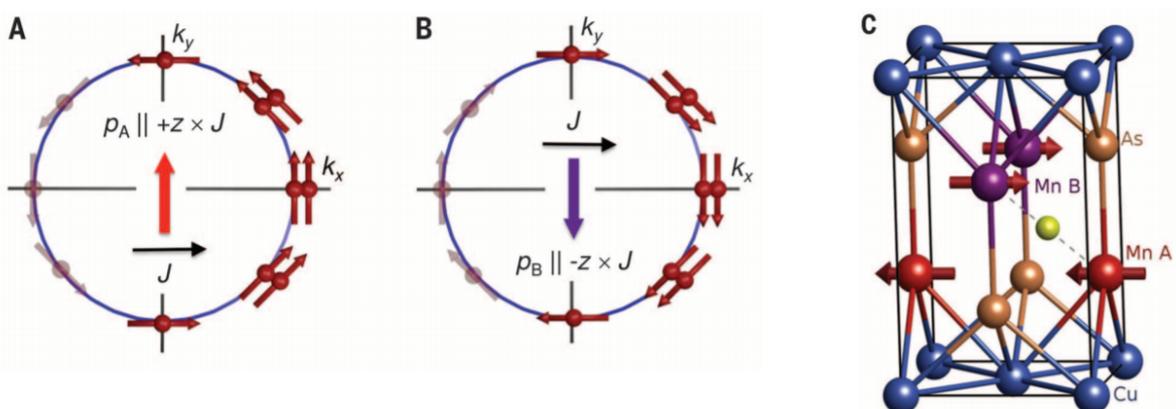


Figure 2.4: Electronic band structure

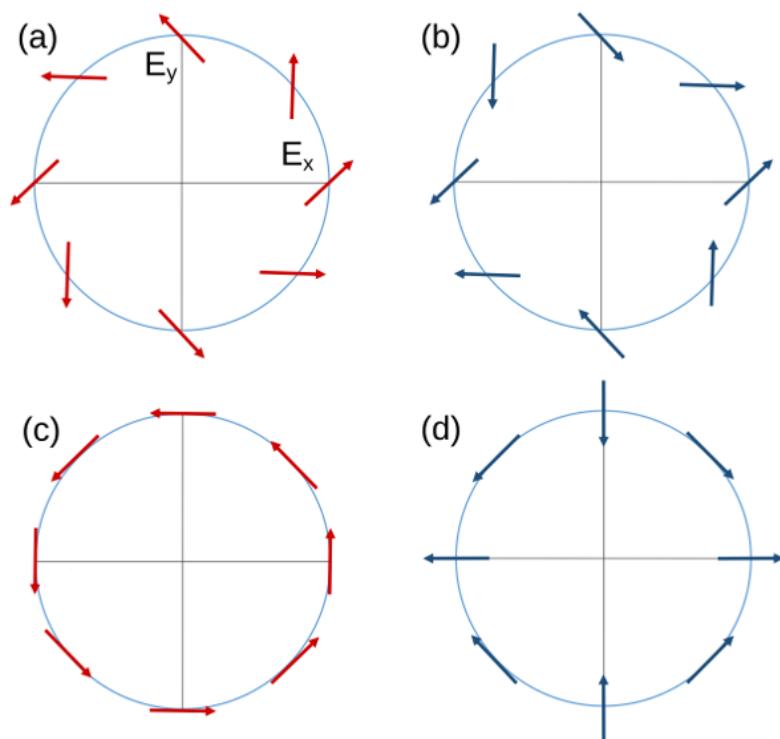


Figure 2.5: Electronic band structure

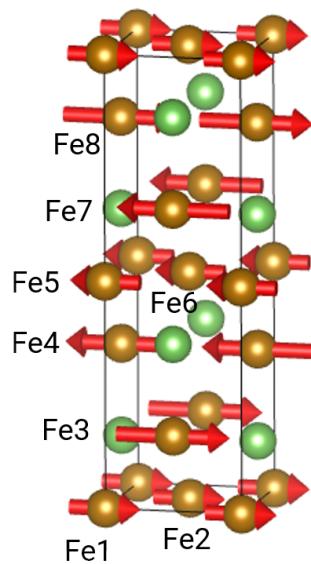


Figure 2.6: Electronic band structure

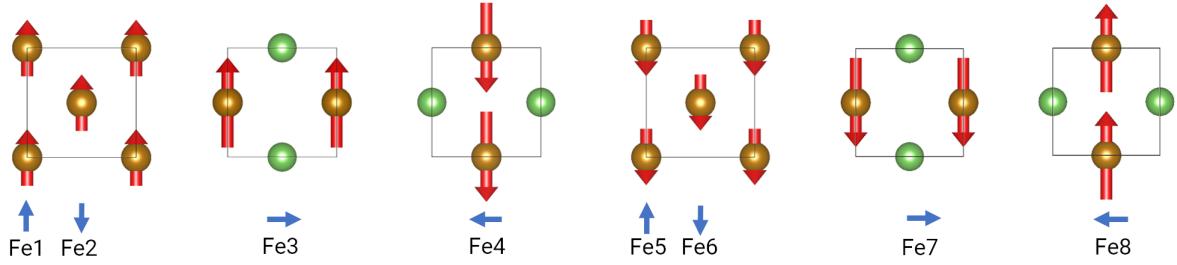


Figure 2.7: Electronic band structure

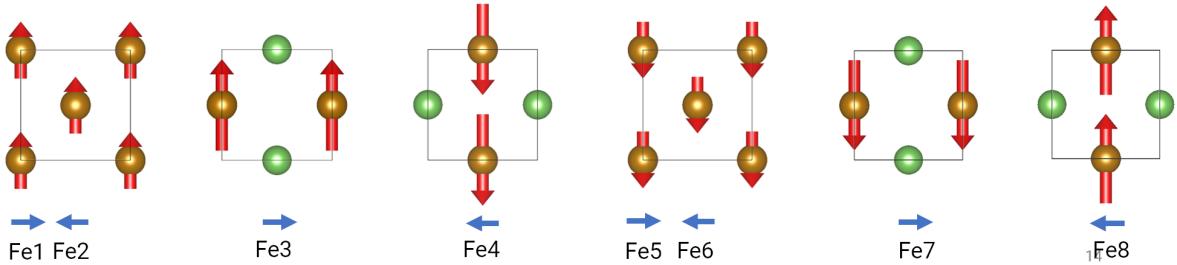


Figure 2.8: Electronic band structure

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Chapter 3

Magnetic structure refinement from neutron diffraction measurements

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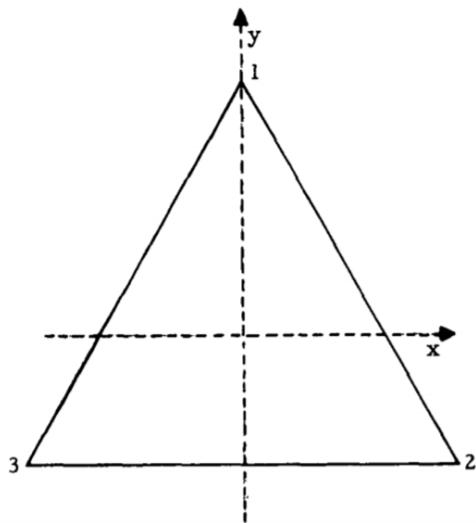


Figure 3.1: Electronic band structure

	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 3.2: Electronic band structure

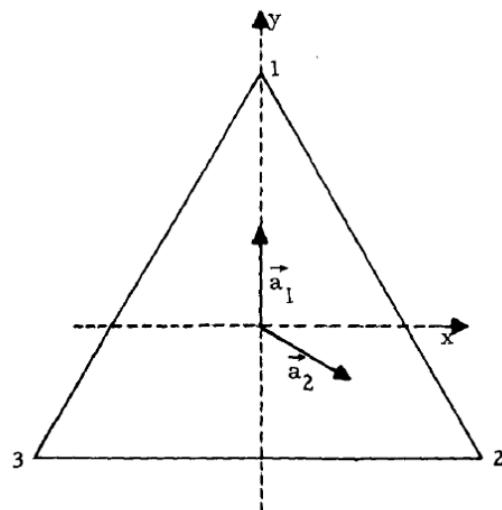


Figure 3.3: Electronic band structure

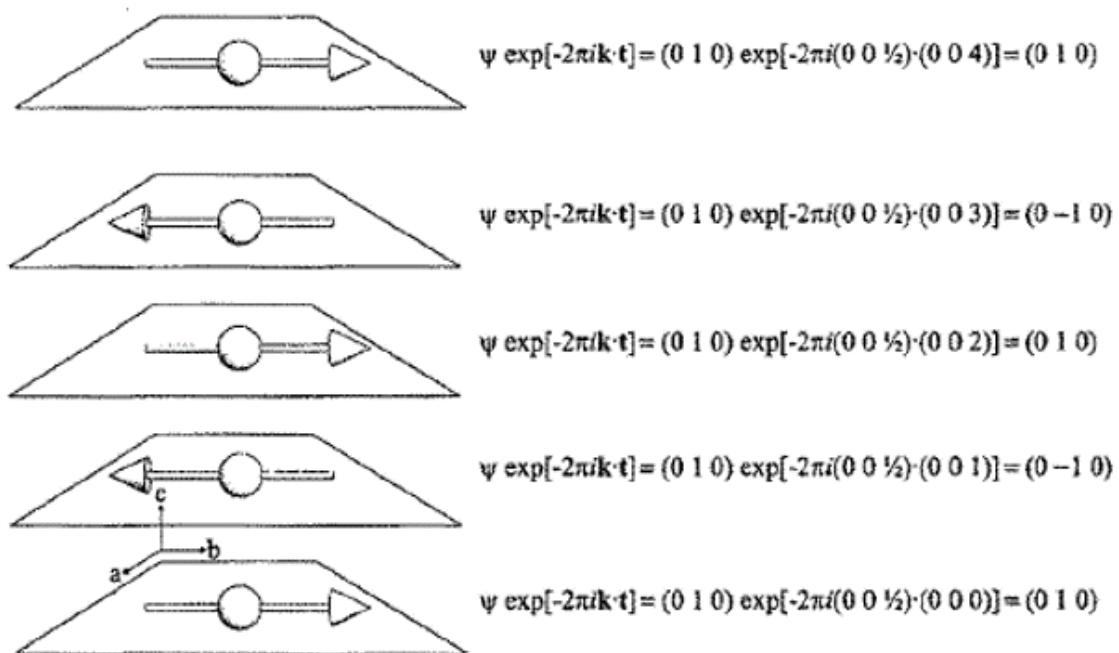


Figure 3.4: Electronic band structure

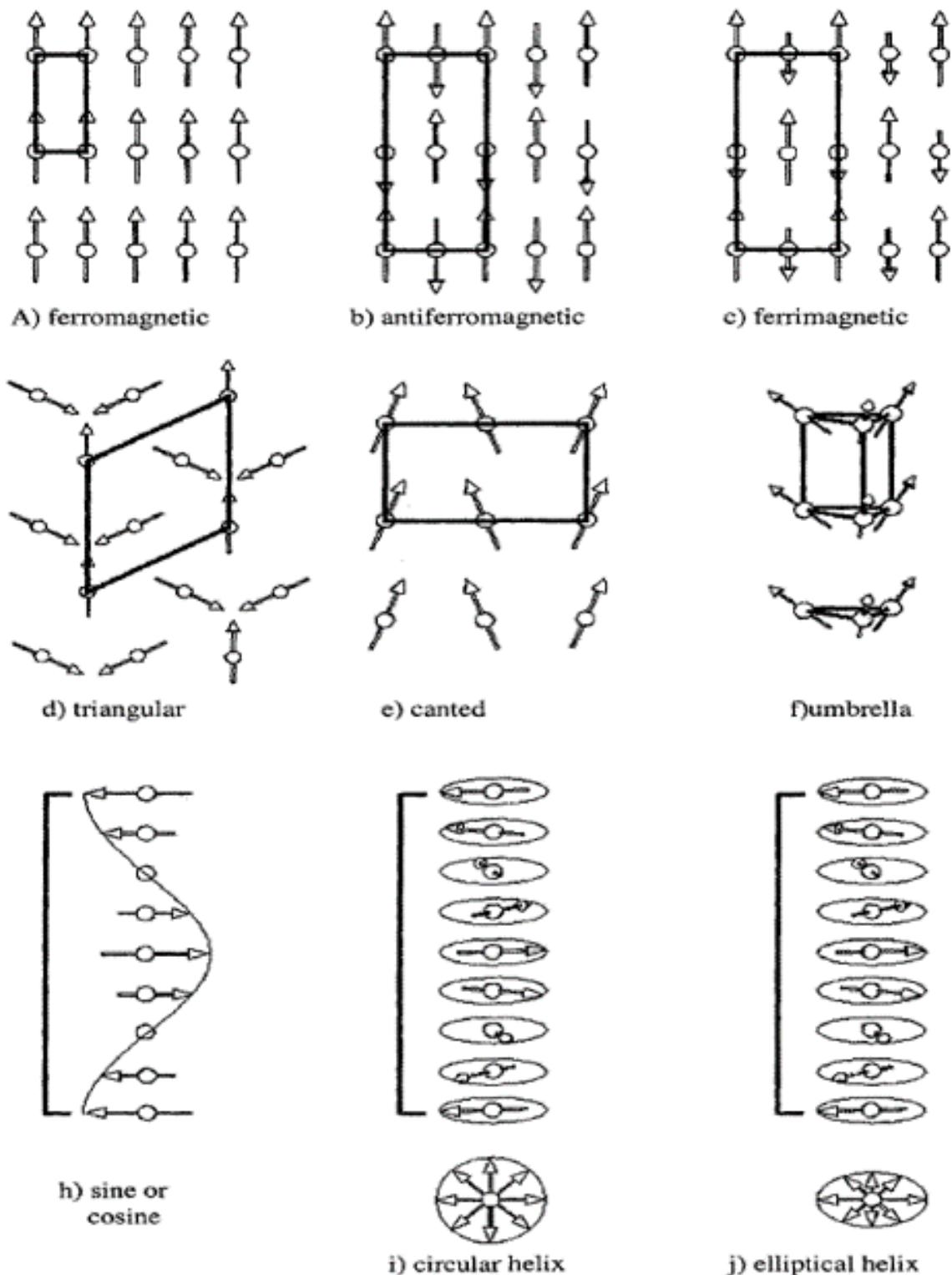


Figure 3.5: Electronic band structure

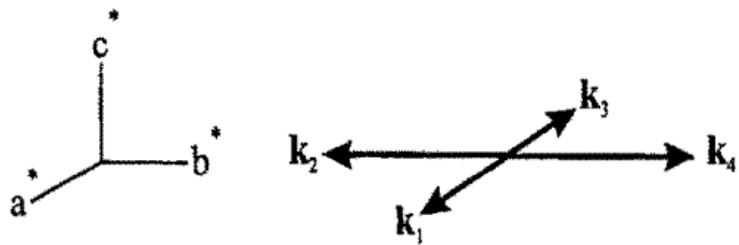


Figure 3.6: Electronic band structure

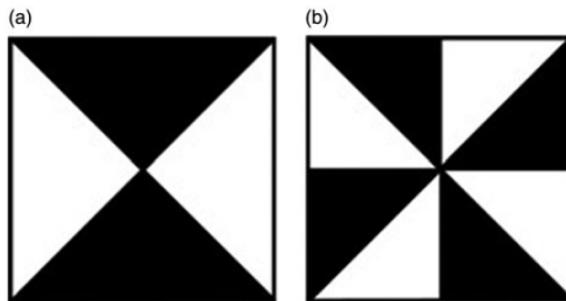


Figure 3.7: Electronic band structure

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Chapter 4

Materials synthesis and characterization

205 This is a citation to [1] and [2].

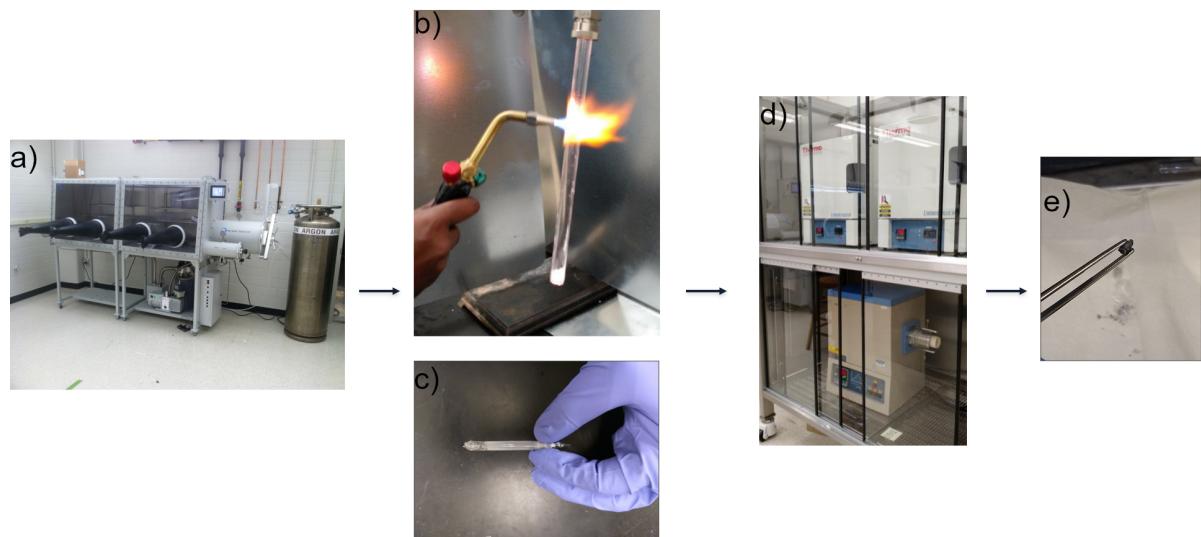


Figure 4.1: Electronic band structure

Chapter 5

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

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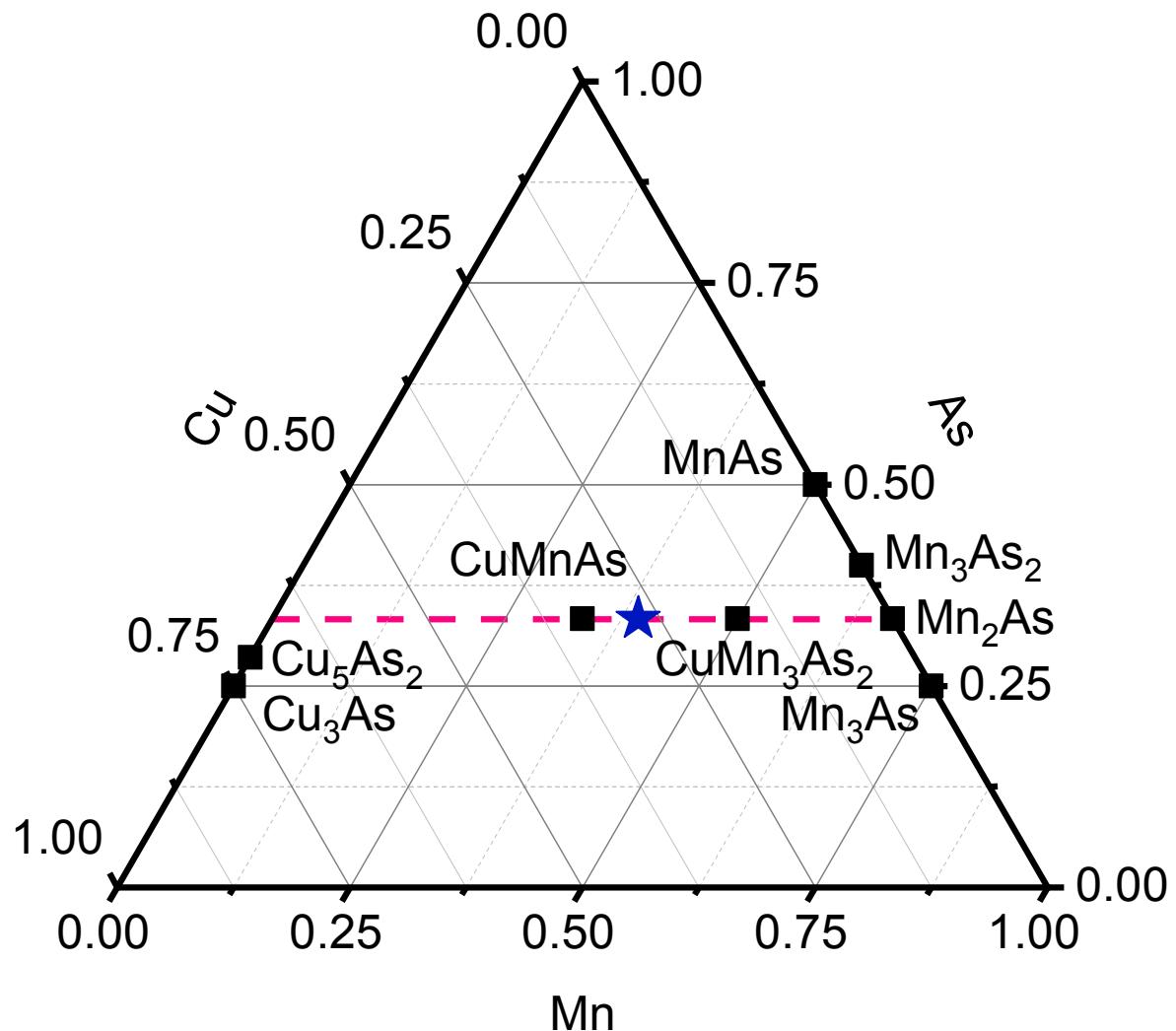


Figure 5.1: Electronic band structure

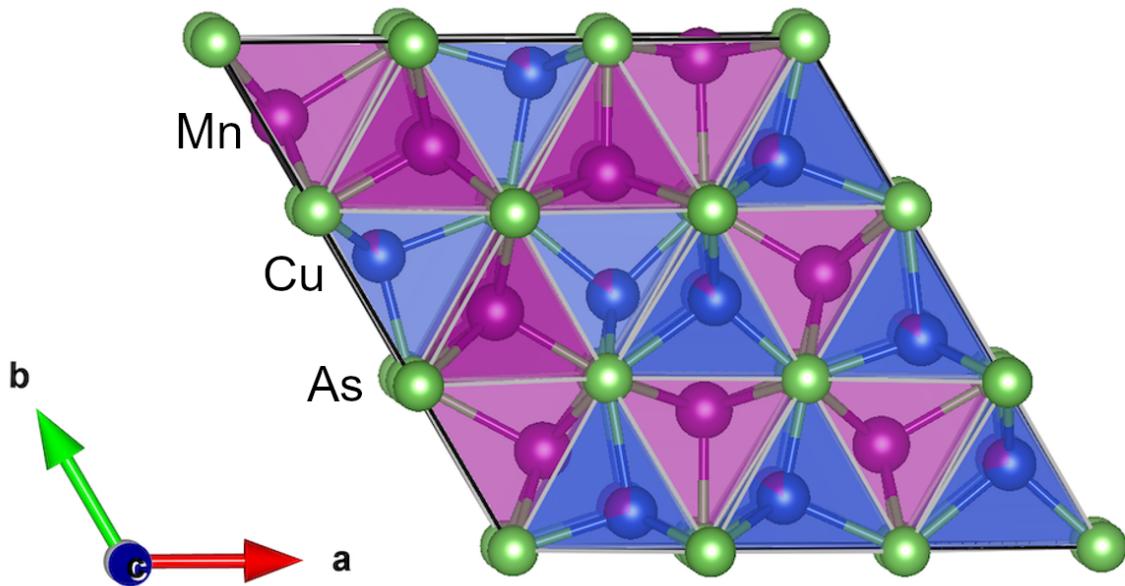


Figure 5.2: Electronic band structure

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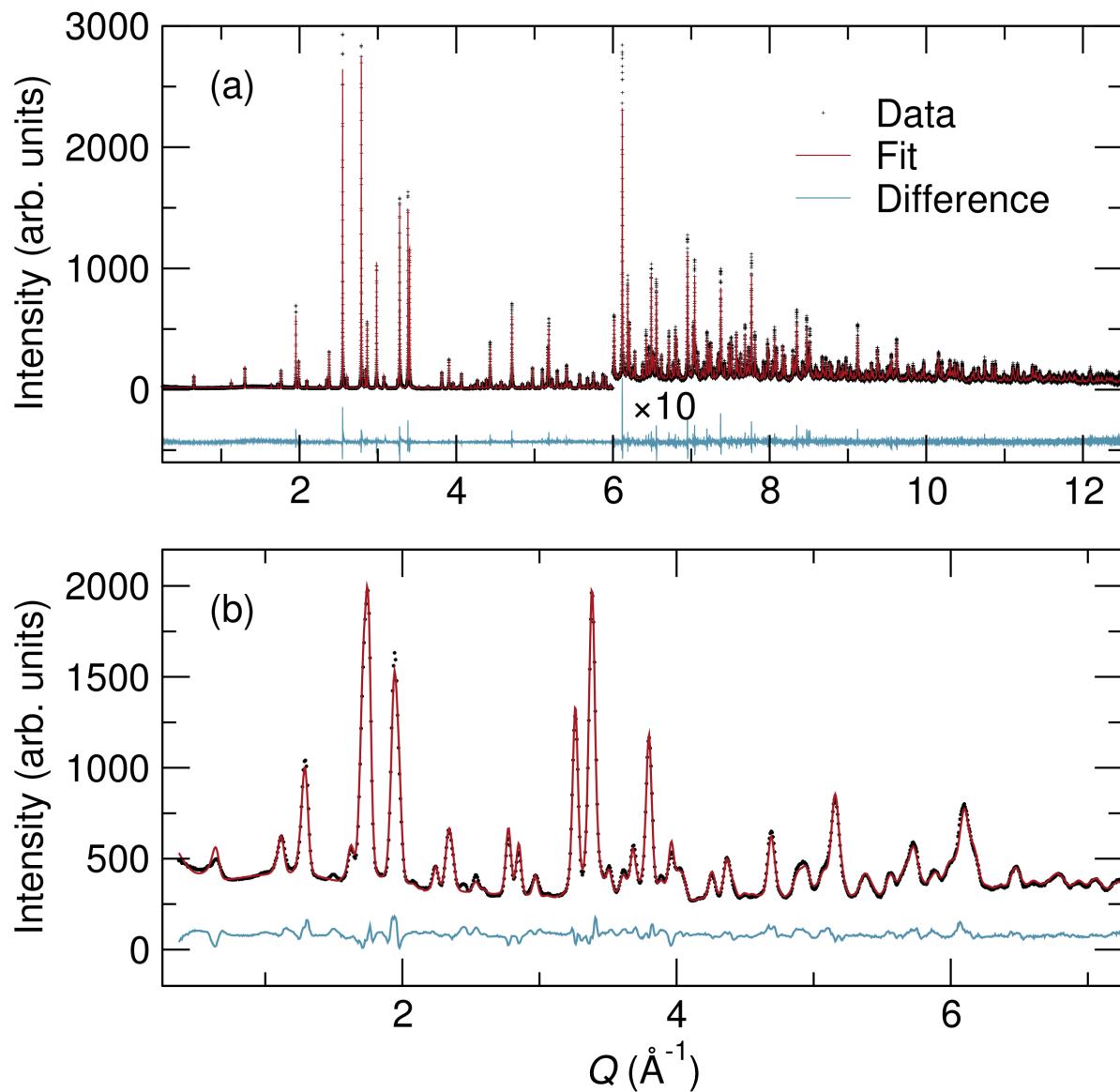


Figure 5.3: Electronic band structure

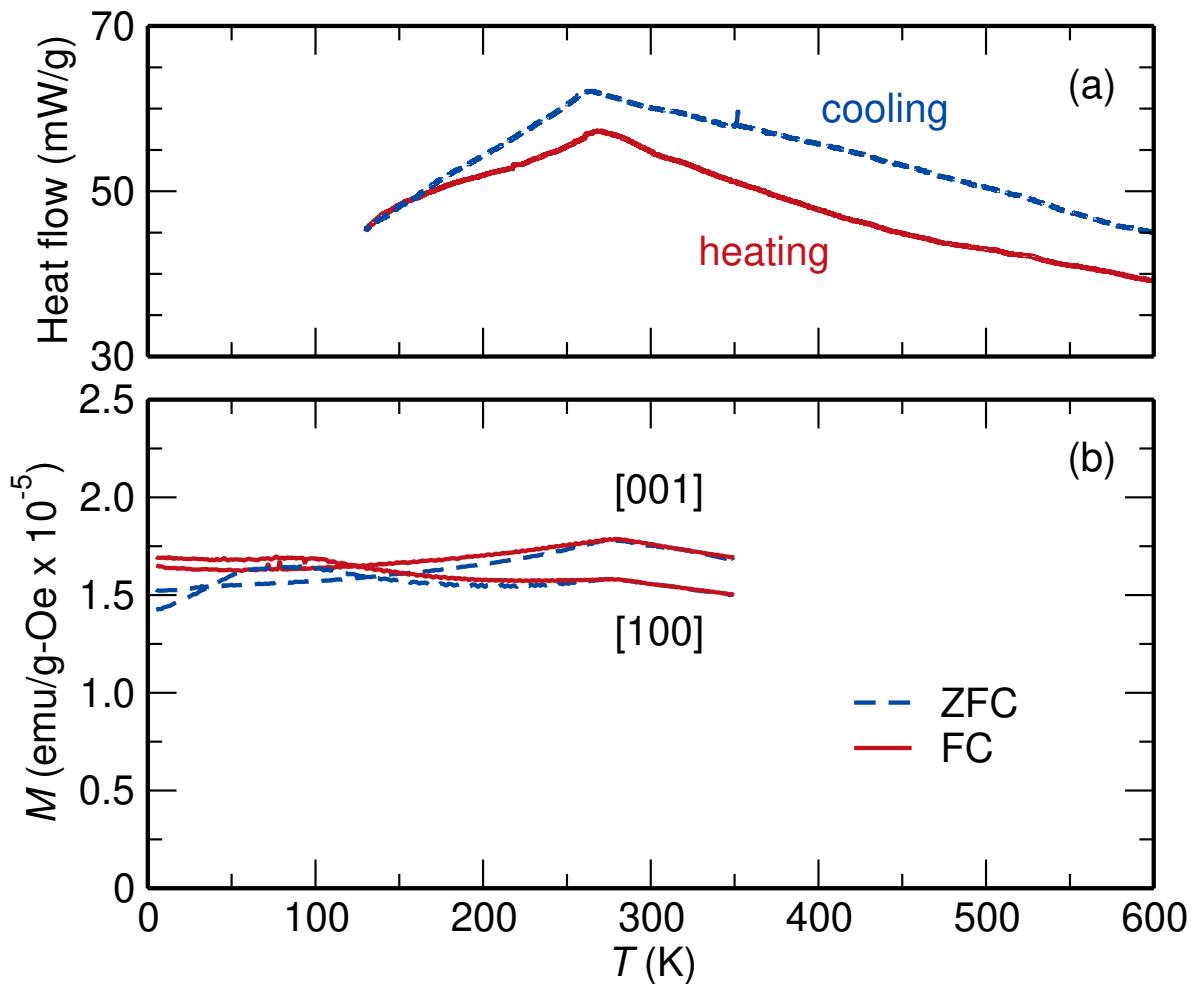


Figure 5.4: Electronic band structure

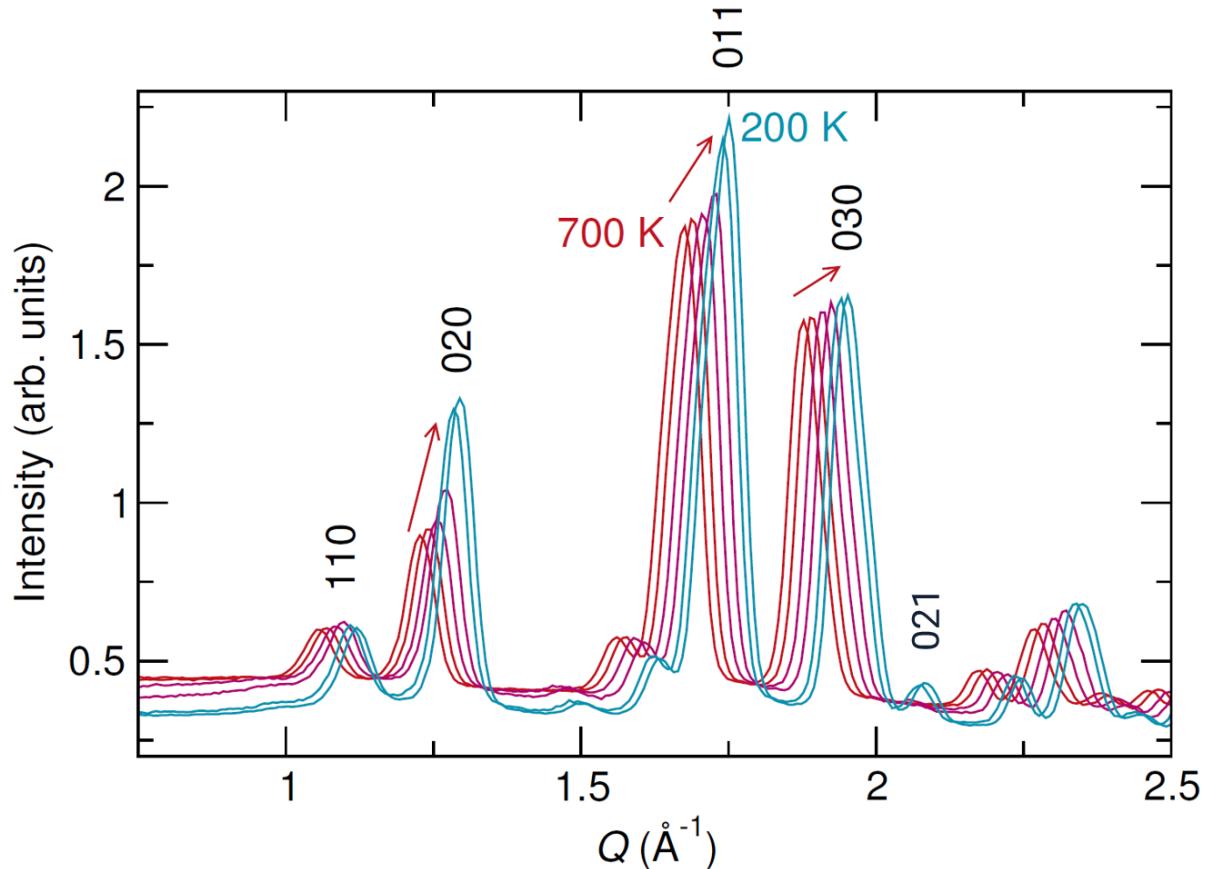


Figure 5.5: Electronic band structure

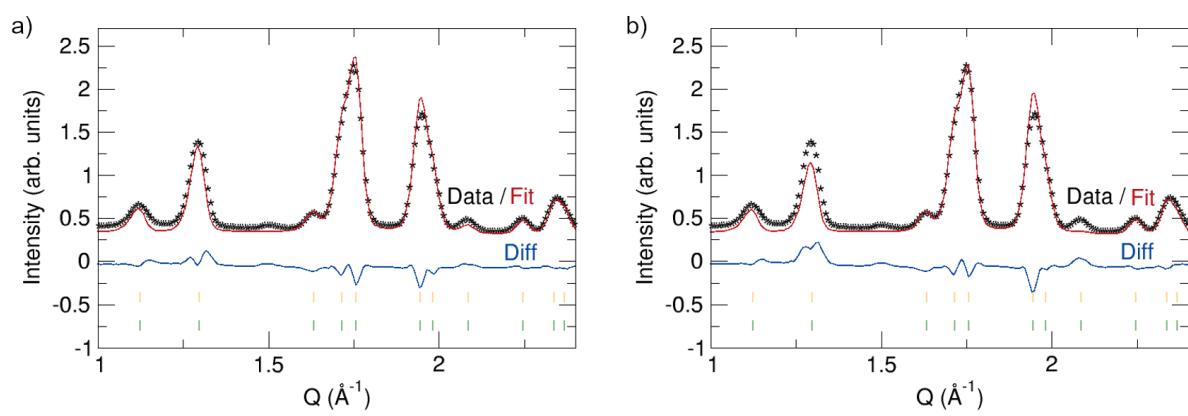


Figure 5.6: Electronic band structure

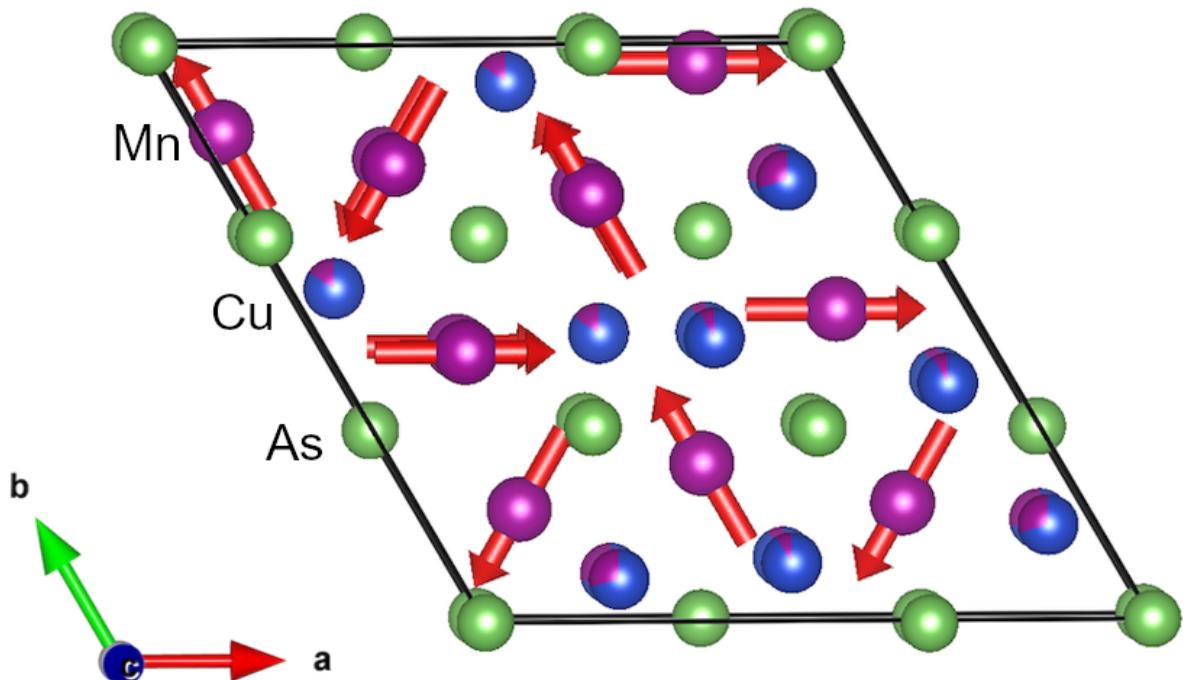


Figure 5.7: Electronic band structure

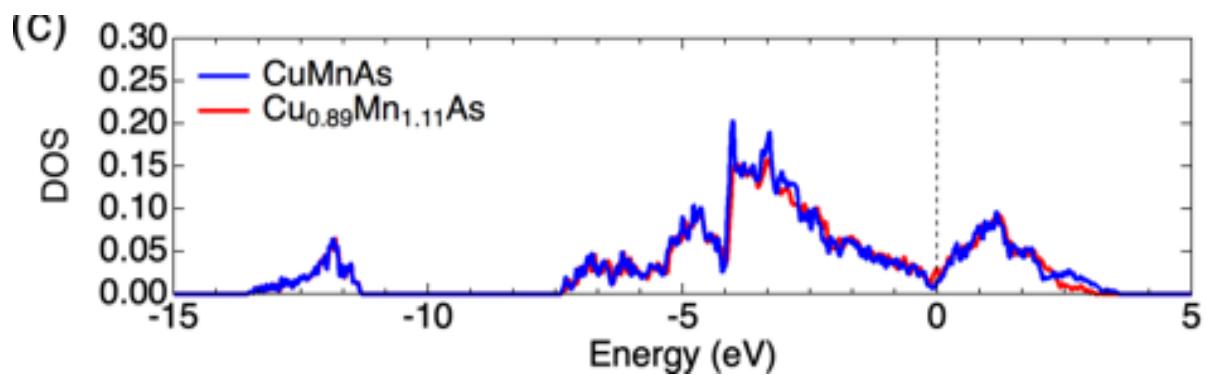


Figure 5.8: Electronic band structure

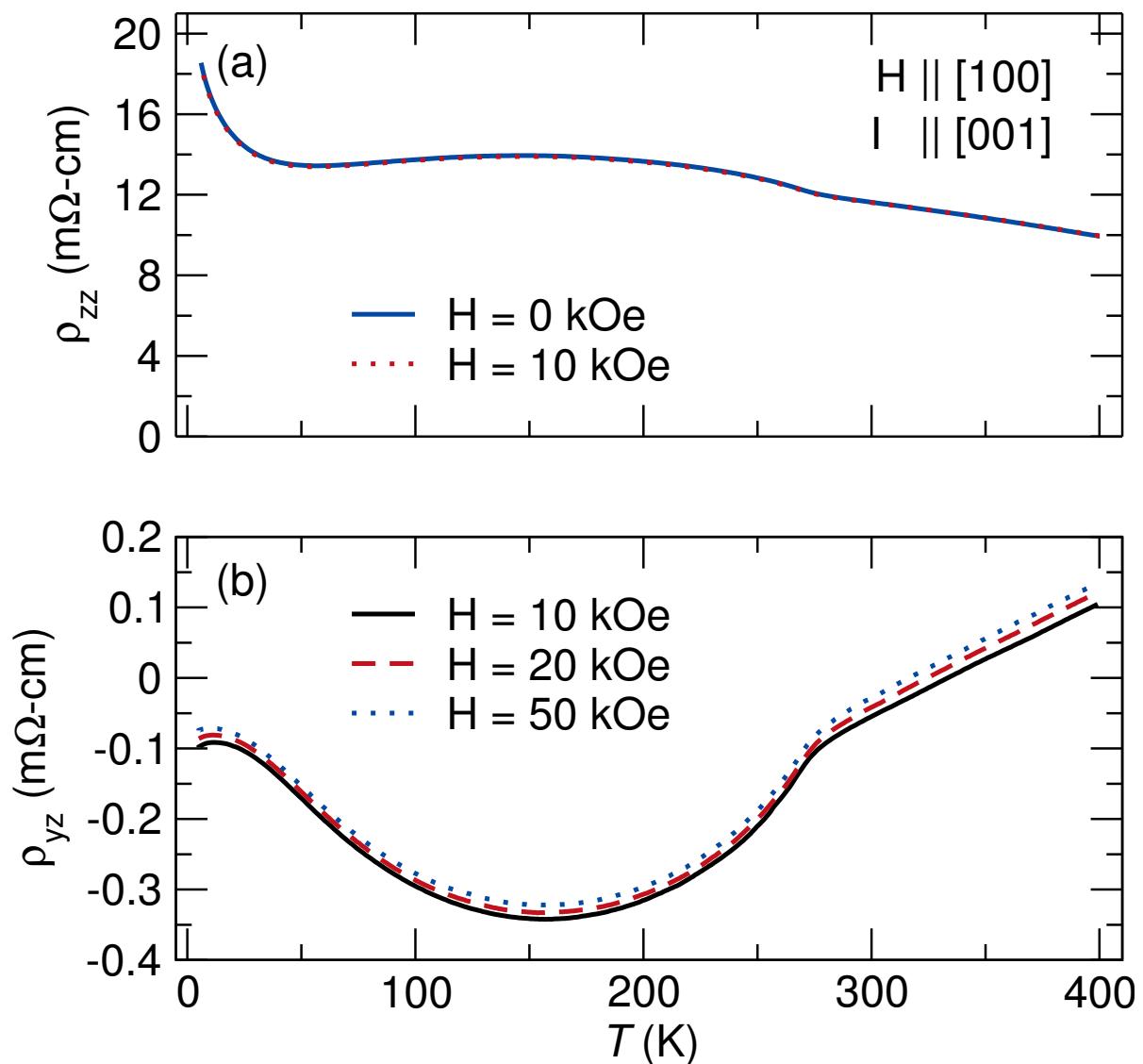


Figure 5.9: Electronic band structure

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Chapter 6

Two step magnetic ordering in monoclinic Mn₃As₂

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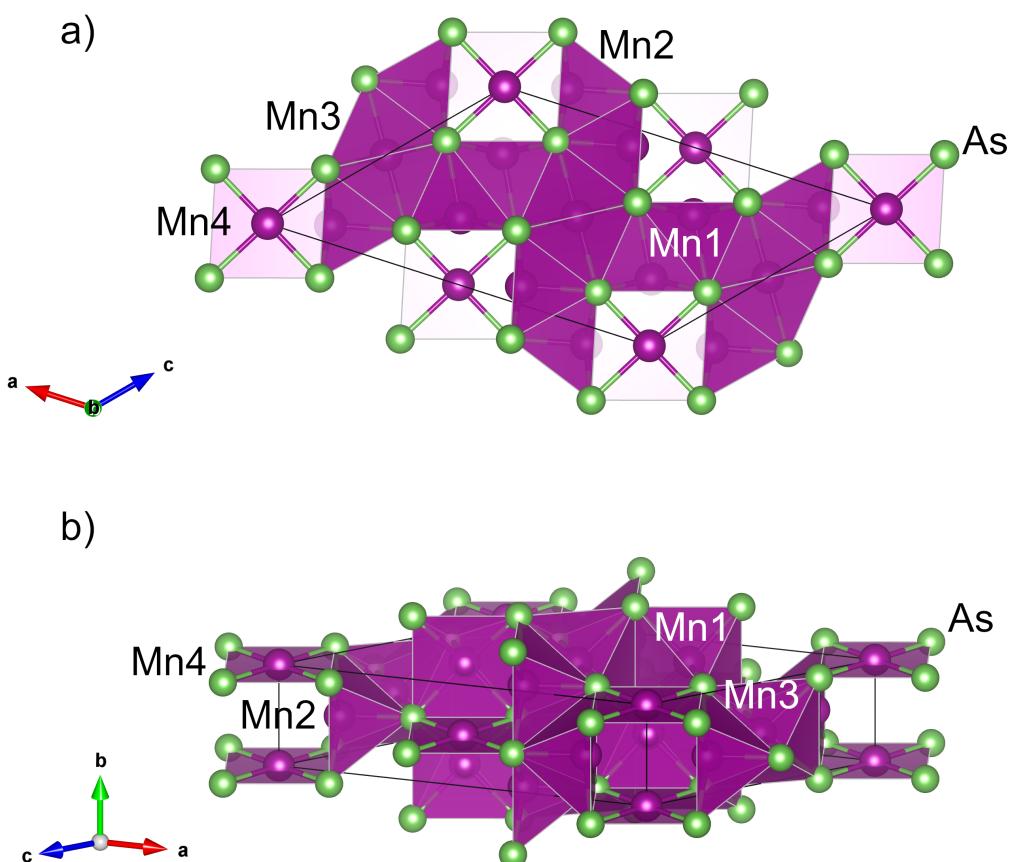


Figure 6.1: Electronic band structure

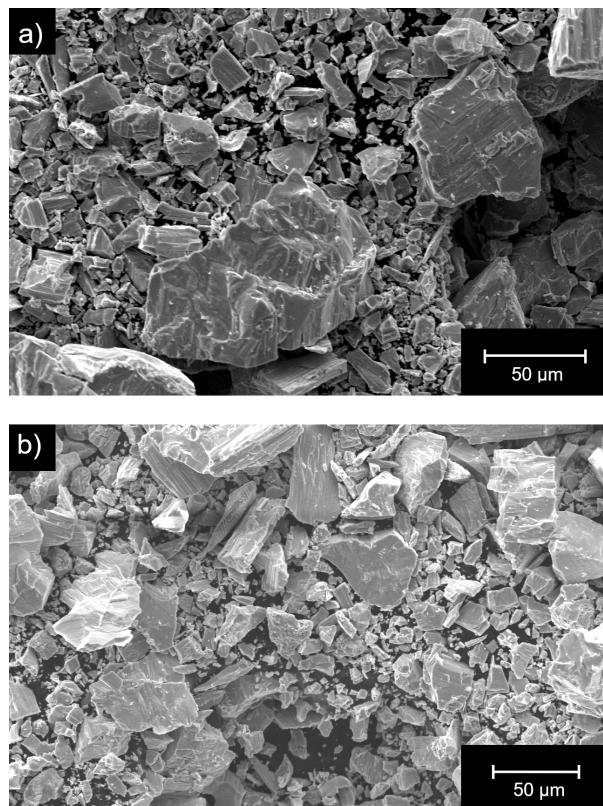


Figure 6.2: Electronic band structure

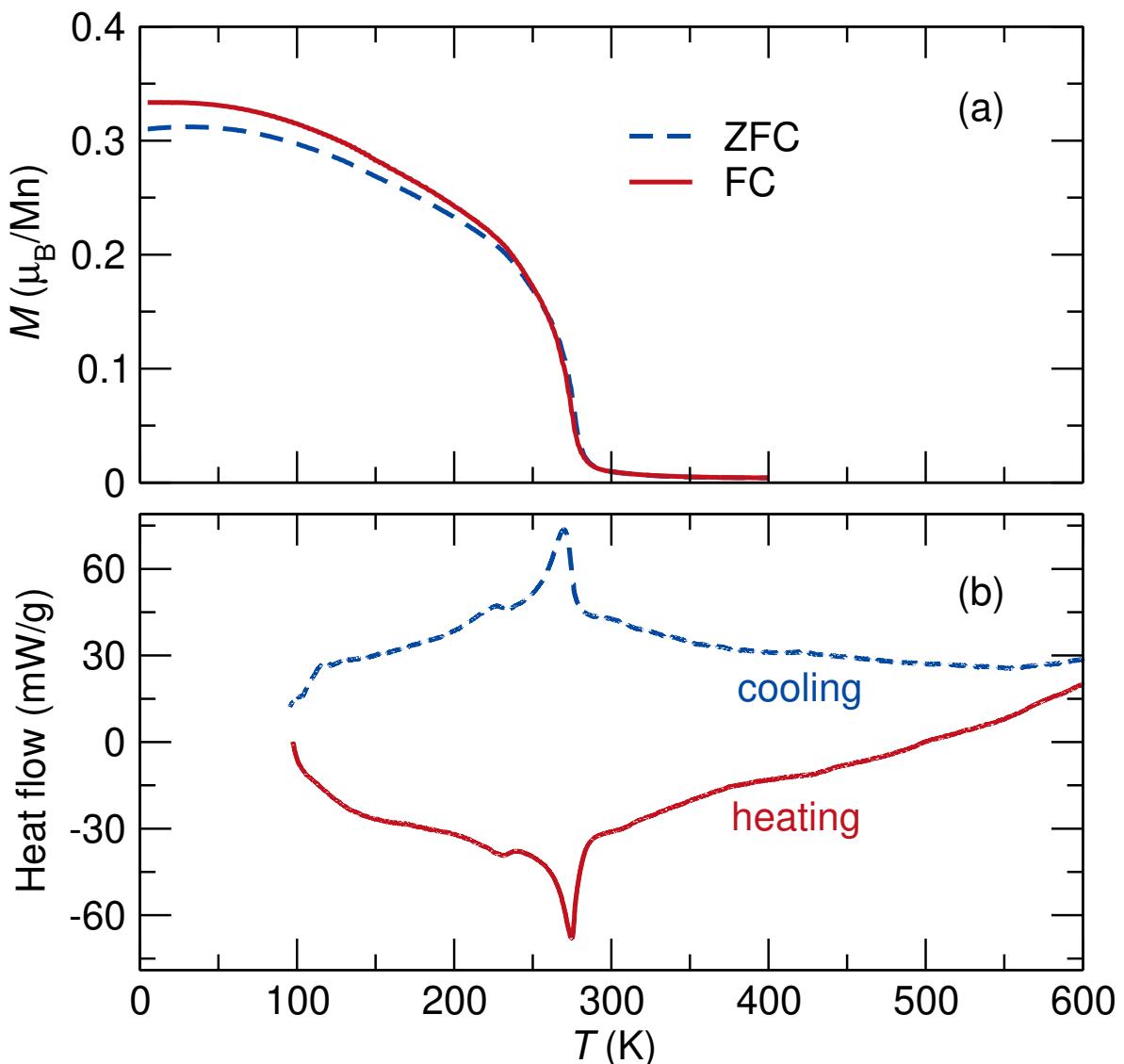


Figure 6.3: Electronic band structure

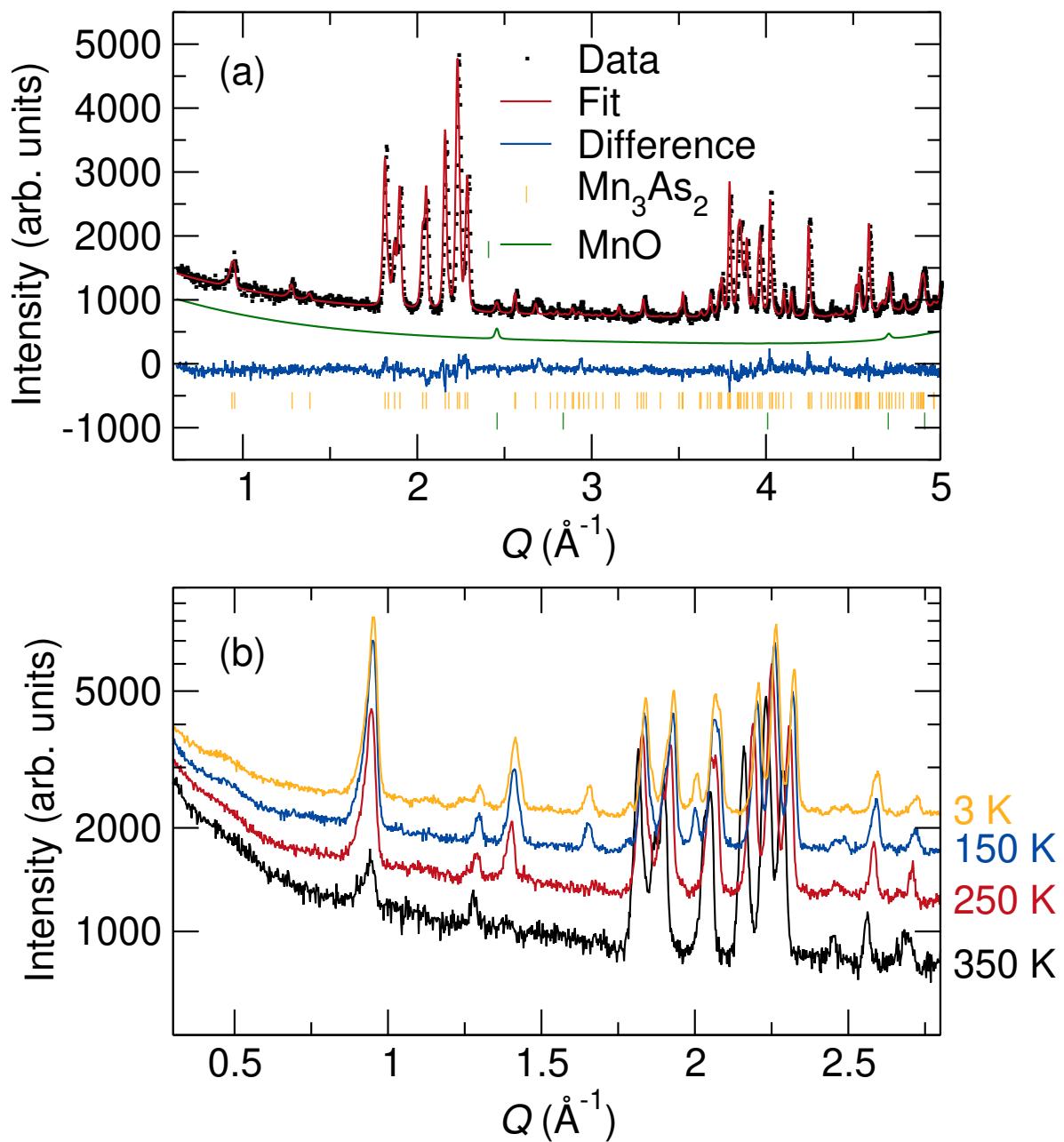


Figure 6.4: Electronic band structure

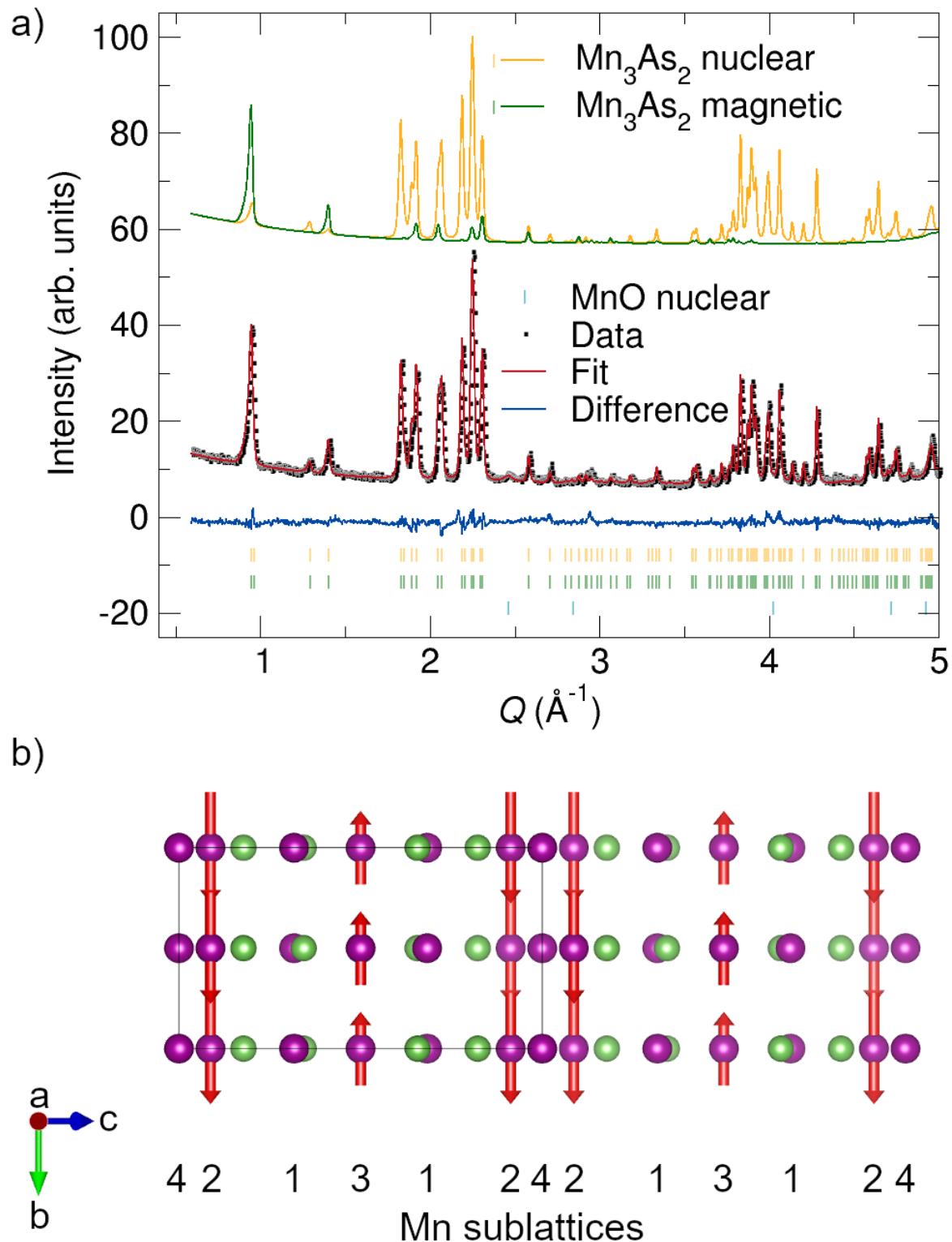


Figure 6.5: Electronic band structure

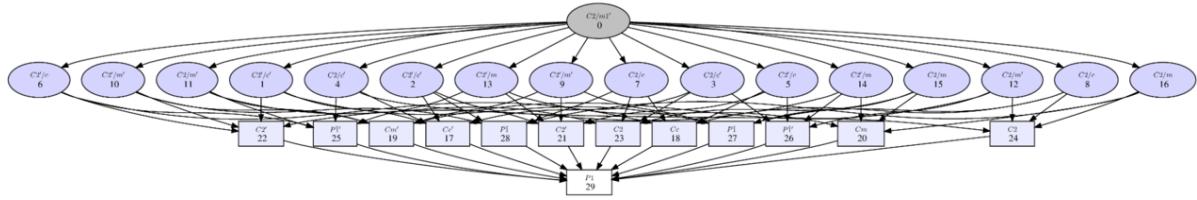


Figure 6.6: Electronic band structure

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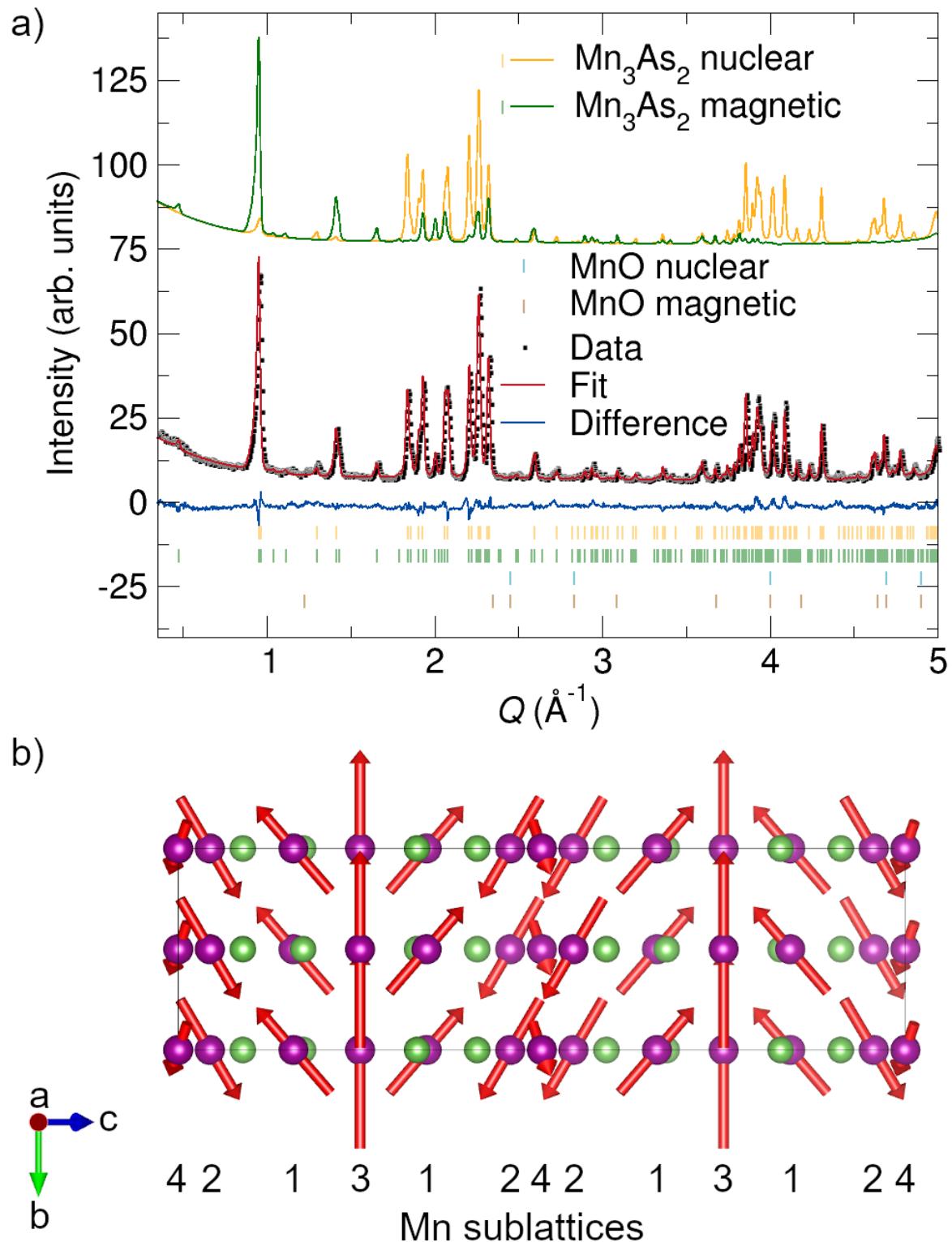


Figure 6.7: Electronic band structure

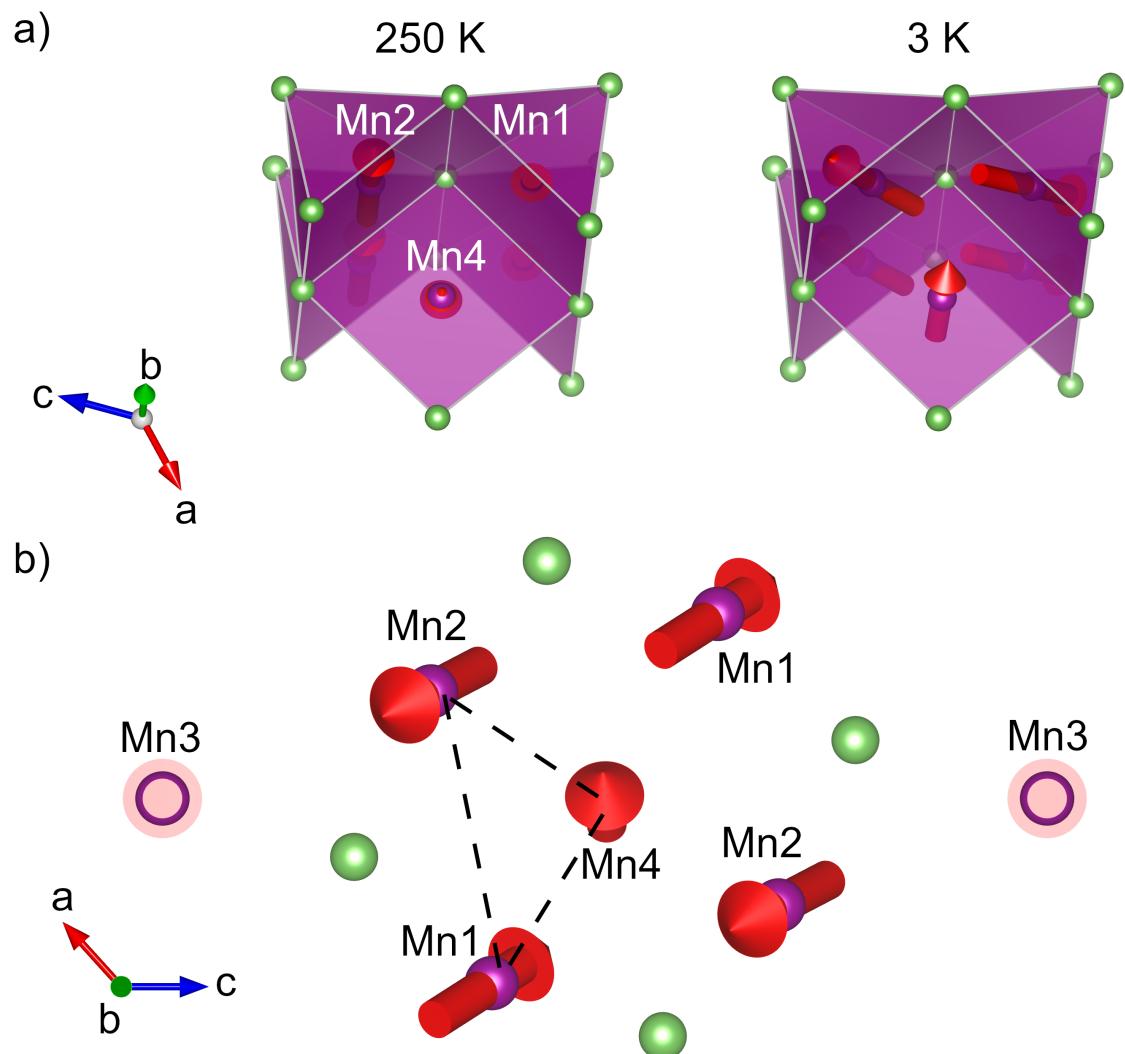


Figure 6.8: Electronic band structure

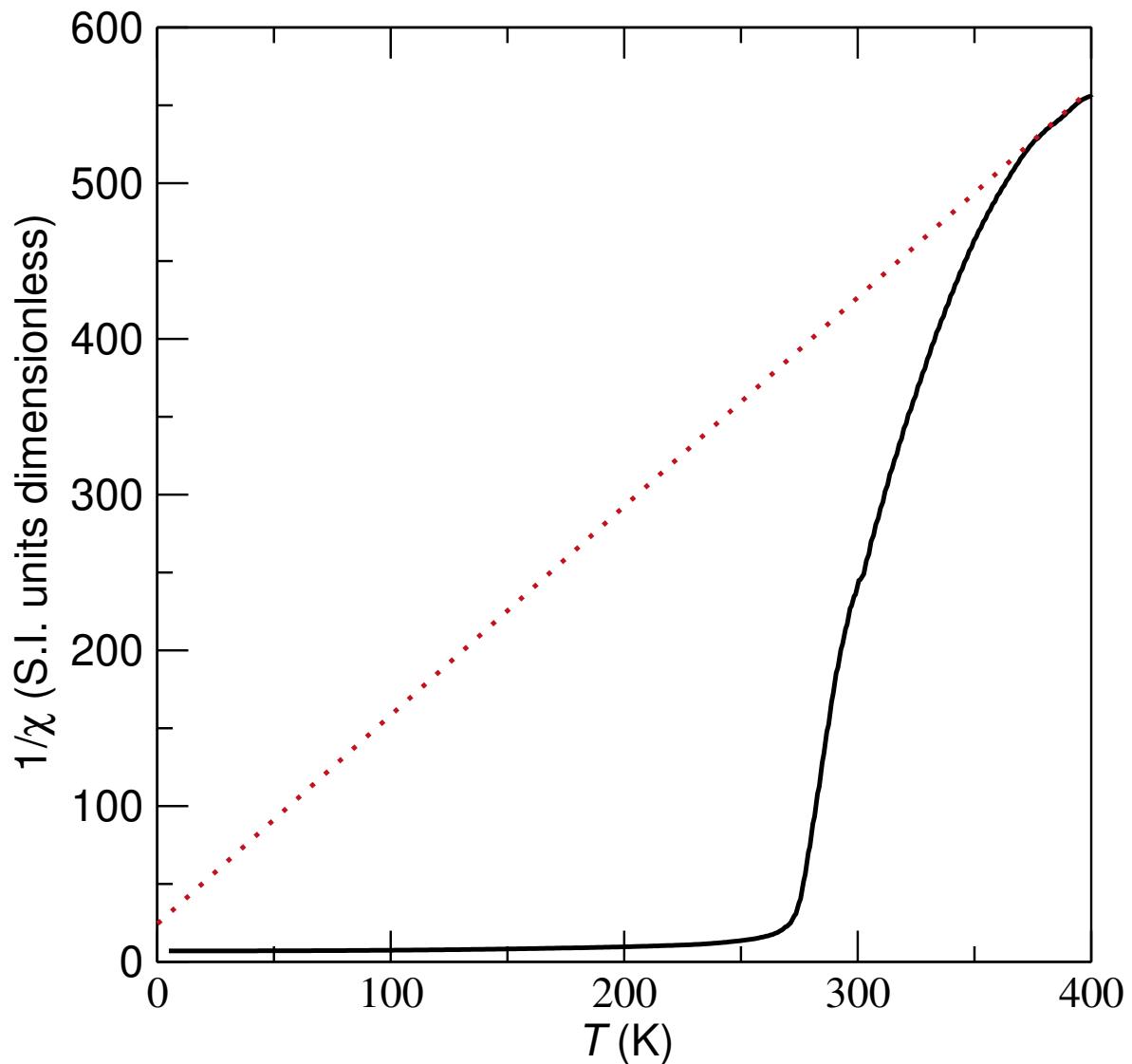


Figure 6.9: Electronic band structure

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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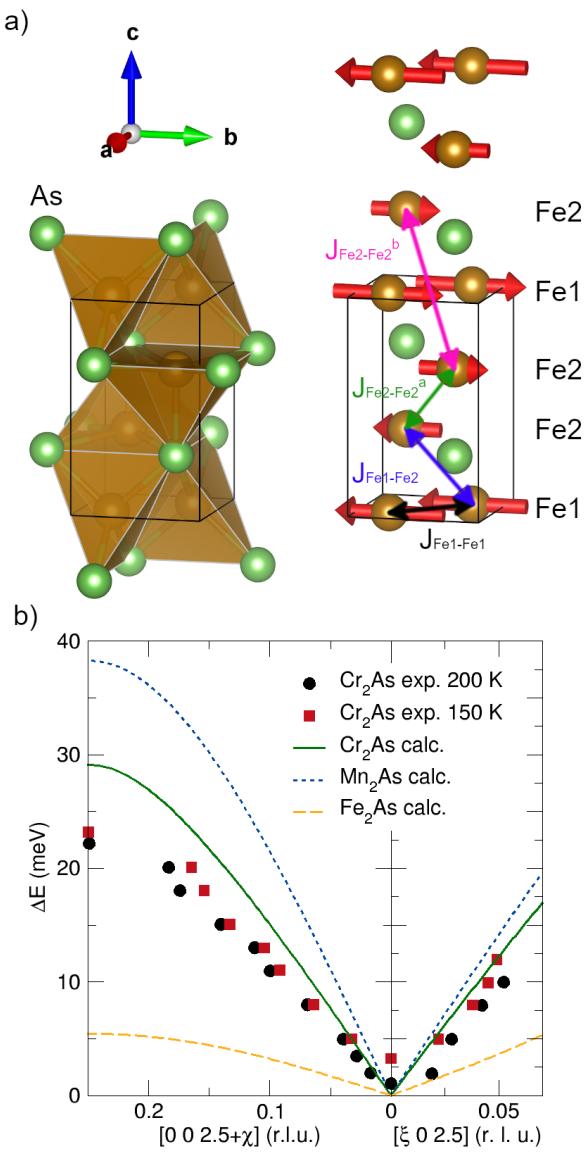


Figure 8.1: Electronic band structure

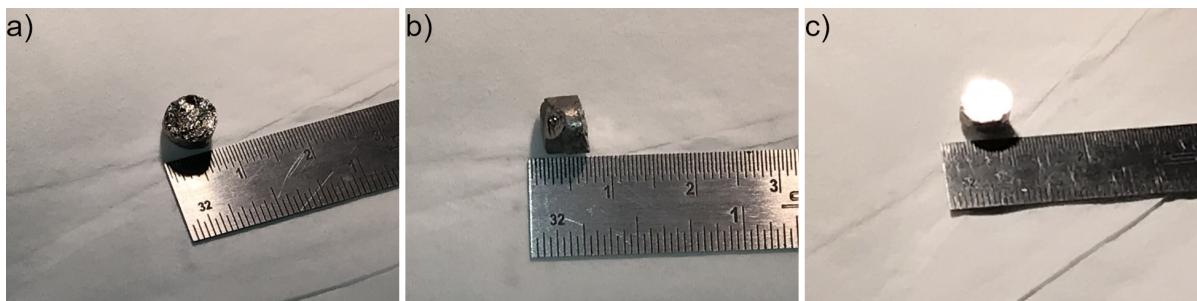


Figure 8.2: Electronic band structure

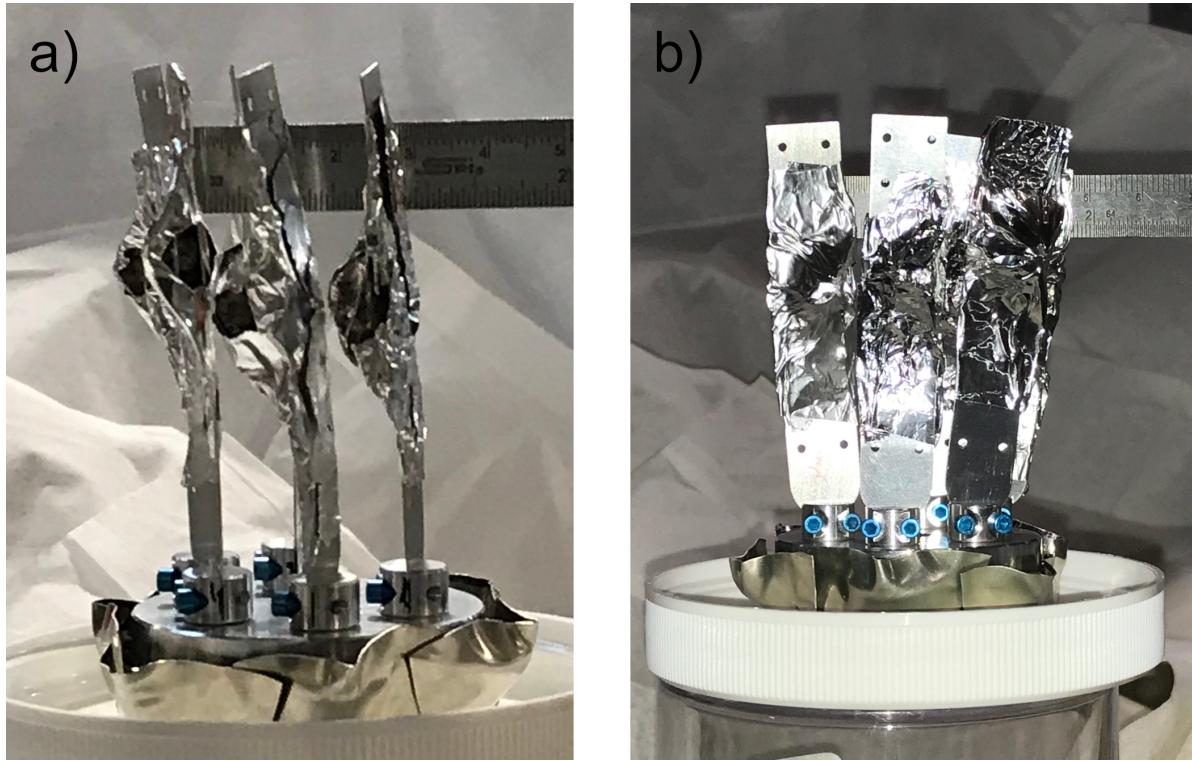


Figure 8.3: Electronic band structure

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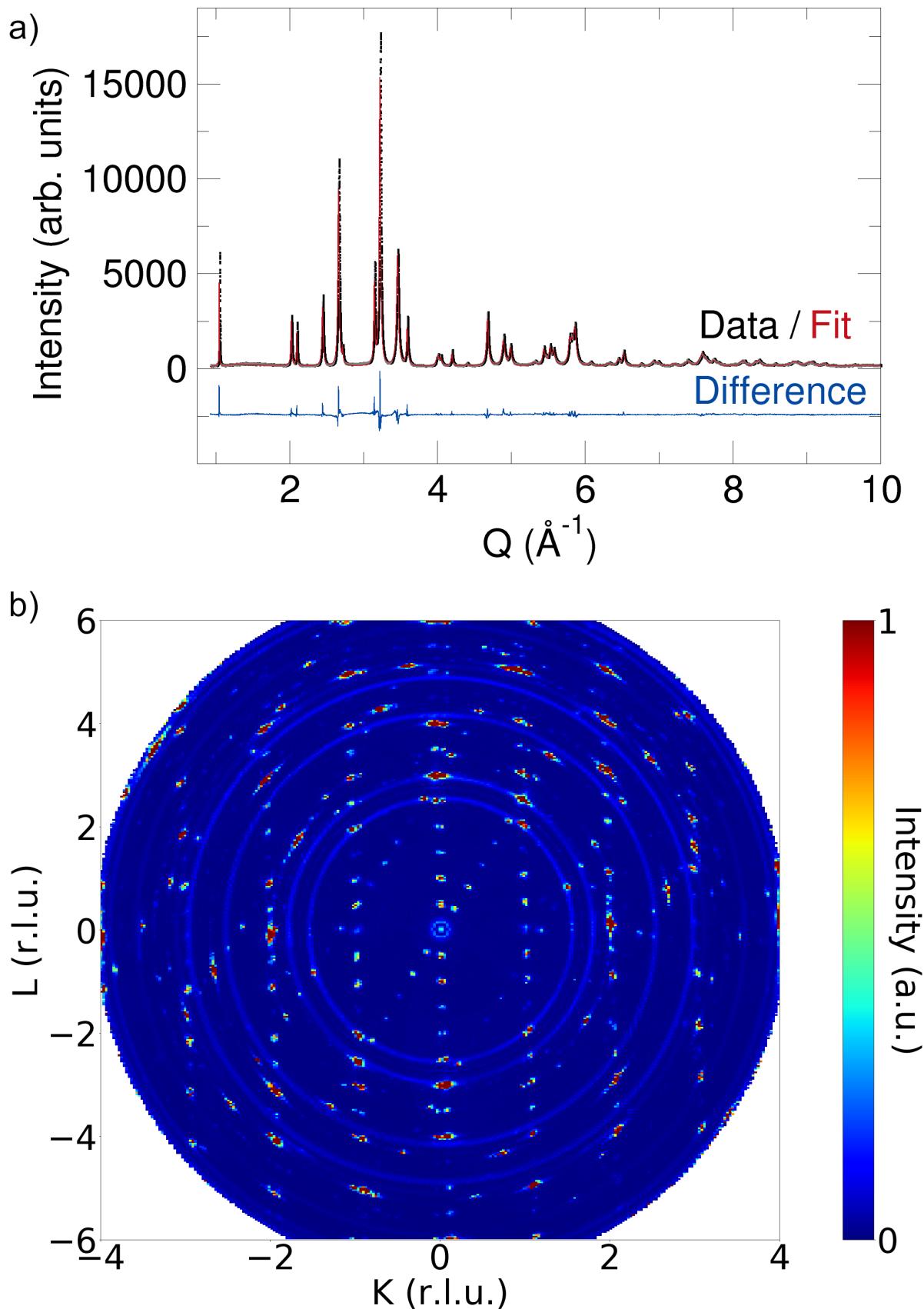


Figure 8.4: Electronic band structure

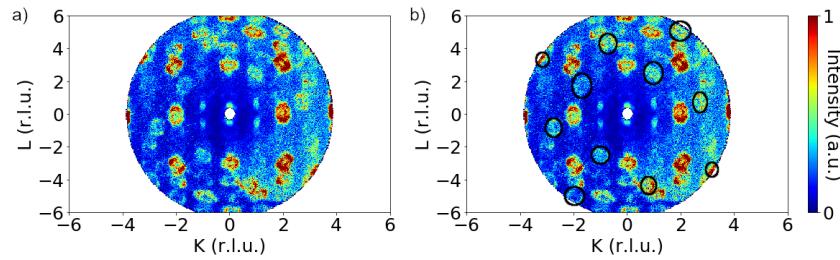


Figure 8.5: Electronic band structure

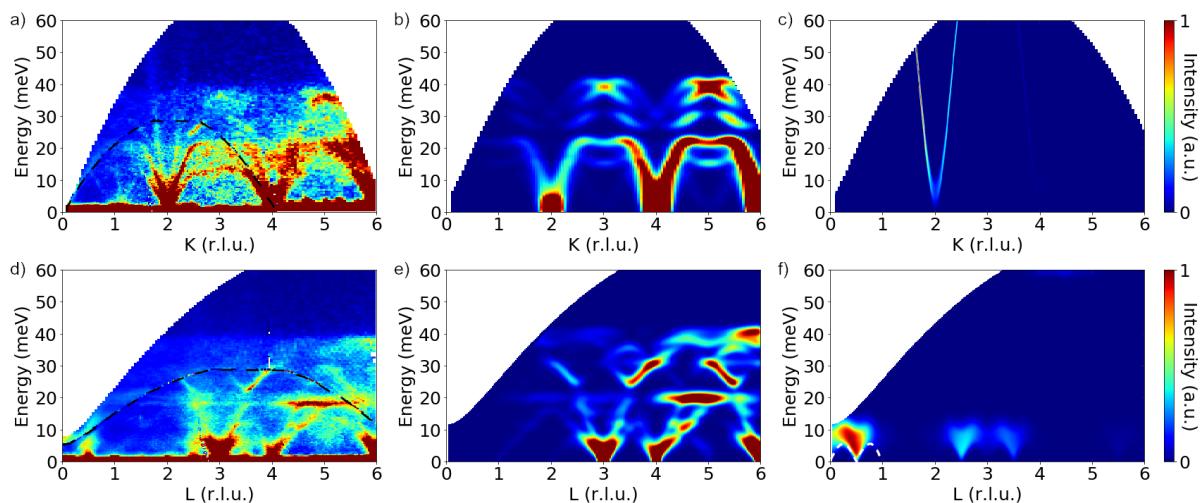


Figure 8.6: Electronic band structure

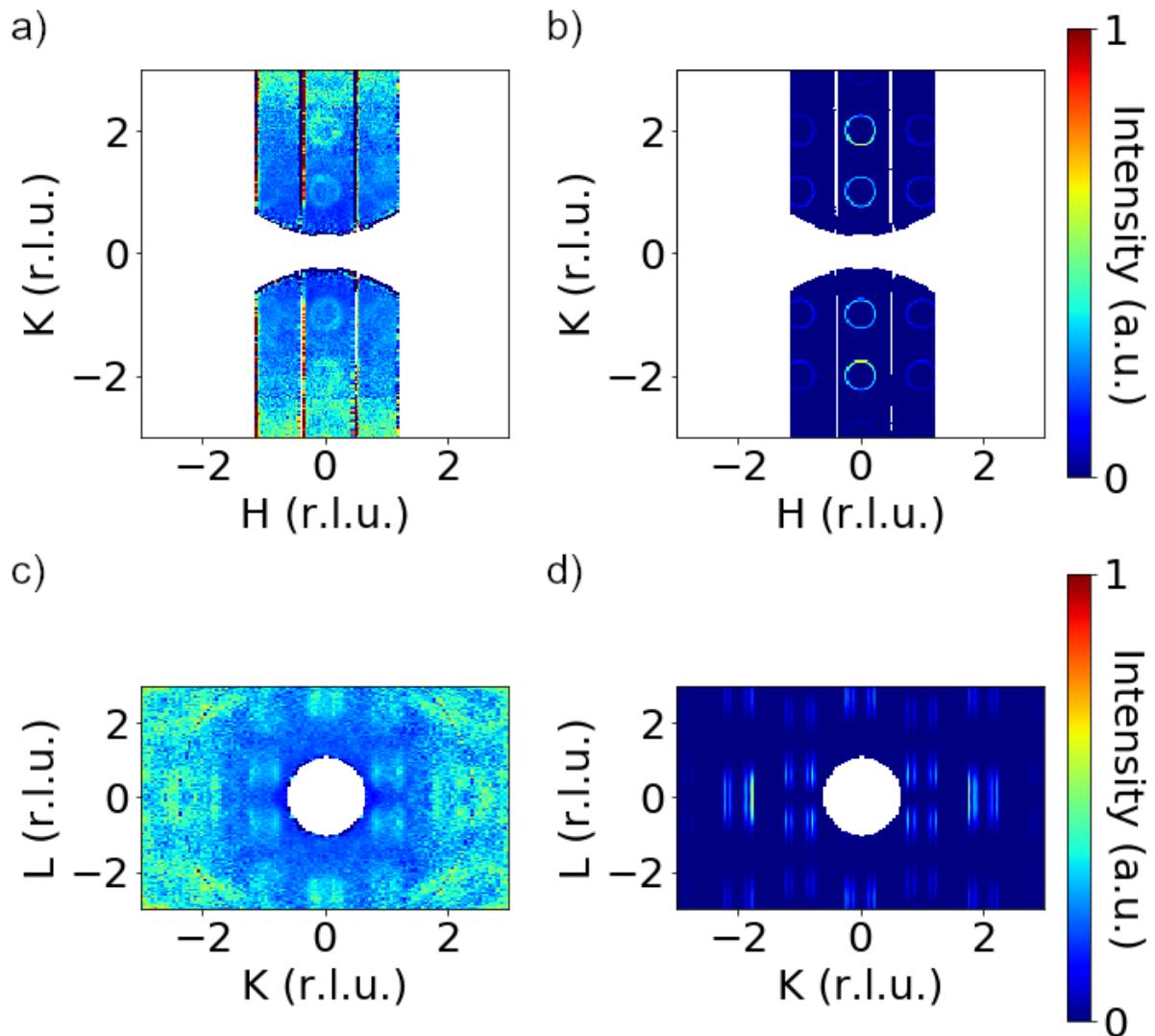


Figure 8.7: Electronic band structure

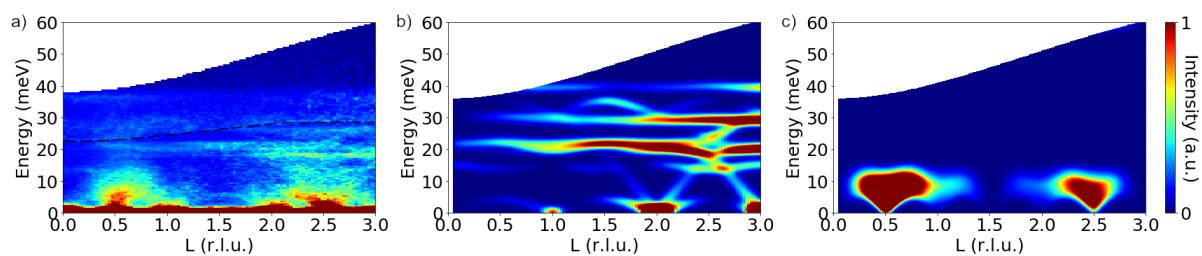


Figure 8.8: Electronic band structure

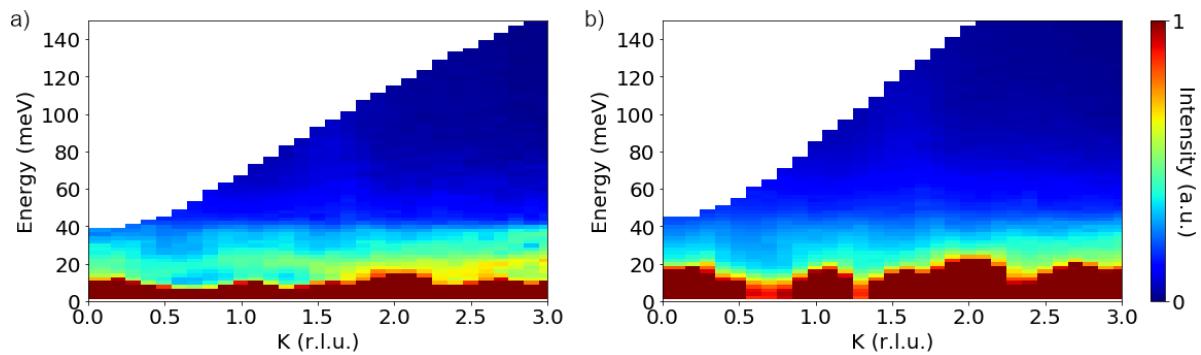


Figure 8.9: Electronic band structure

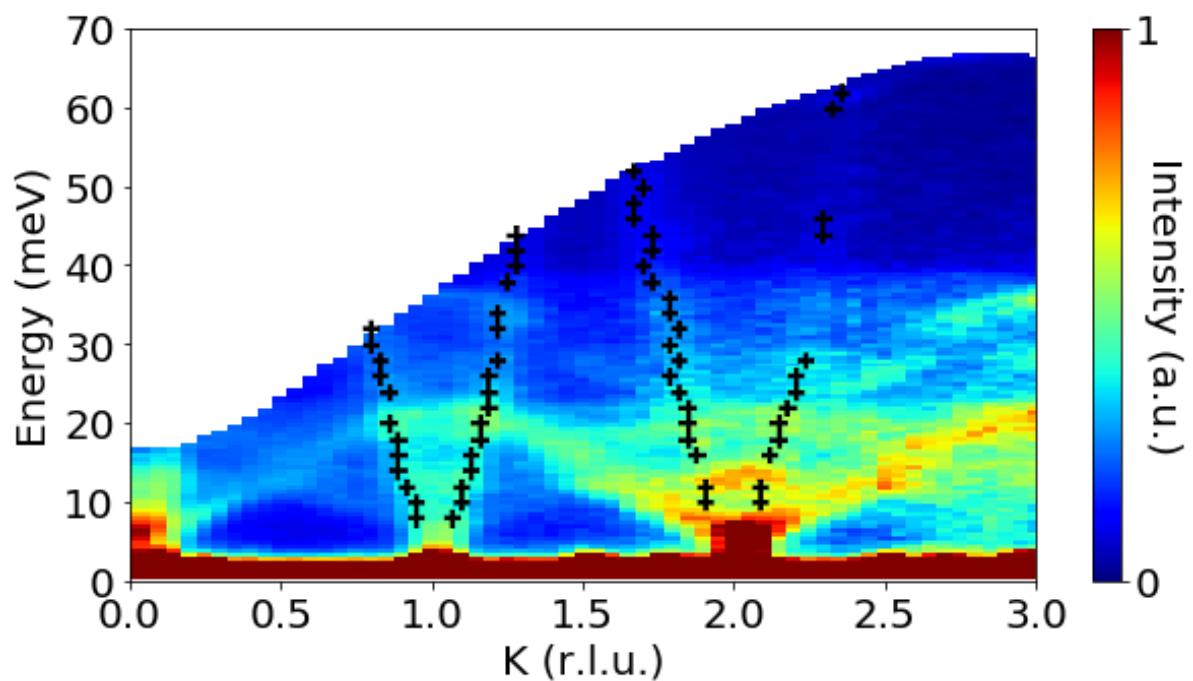


Figure 8.10: Electronic band structure

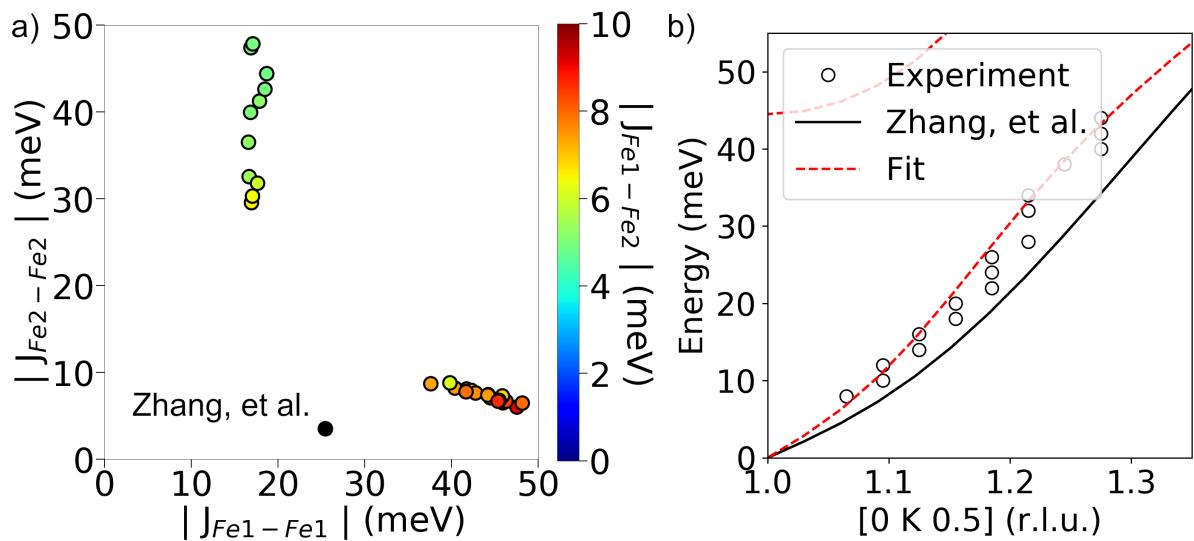


Figure 8.11: Electronic band structure

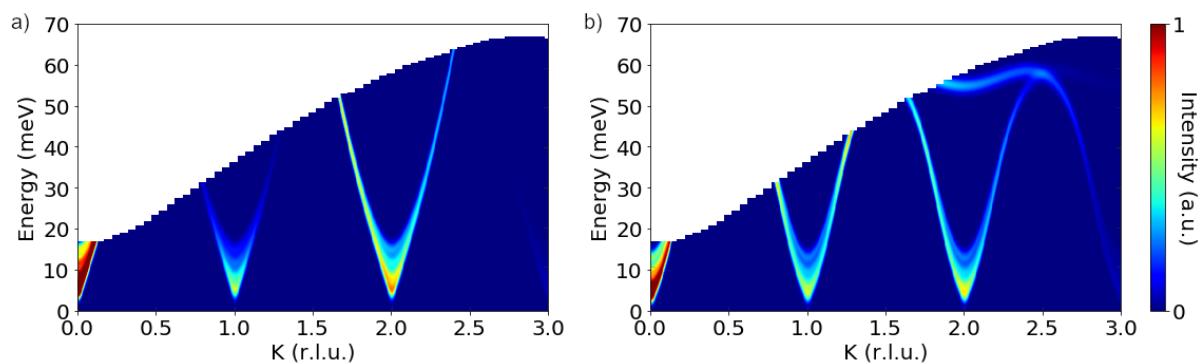


Figure 8.12: Electronic band structure

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Chapter 9

Conclusions

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