

MAGNETIC ORDERING AND SPIN WAVE DYNAMICS IN TRANSITION METAL
ARSENIDES

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BY

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DISSERTATION

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Urbana, Illinois

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Professor Jian-Min Zuo
Research Assistant Professor Gregory MacDougall

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.

Table of Contents

| | |
|---|-----------|
| List of Tables | iv |
| List of Figures | v |
| Chapter 1 Introduction | 1 |
| Chapter 2 Theory of electrical switching in metallic antiferromagnets | 4 |
| Chapter 3 Magnetic structure refinement from neutron diffraction measurements . . | 10 |
| Chapter 4 Materials synthesis and characterization | 16 |
| Chapter 5 Discovery and magnetic frustration of hexagonal Cu_{0.82}Mn_{1.18}As | 18 |
| Chapter 6 Two step magnetic ordering in monoclinic Mn₃As₂ | 27 |
| Chapter 7 Spin canting in tetragonal CuMnAs | 37 |
| Chapter 8 Exchange interactions in Fe₂As probed by inelastic neutron scattering . . | 39 |
| Chapter 9 Conclusions | 46 |
| References | 48 |

List of Tables

List of Figures

| | | |
|-----|---------------------------|----|
| 1.1 | Electronic band structure | 2 |
| 1.2 | Electronic band structure | 2 |
| 1.3 | Electronic band structure | 3 |
| 2.1 | Electronic band structure | 5 |
| 2.2 | Electronic band structure | 5 |
| 2.3 | Electronic band structure | 6 |
| 2.4 | Electronic band structure | 6 |
| 2.5 | Electronic band structure | 7 |
| 2.6 | Electronic band structure | 7 |
| 2.7 | Electronic band structure | 8 |
| 2.8 | Electronic band structure | 8 |
| 3.1 | Electronic band structure | 11 |
| 3.2 | Electronic band structure | 11 |
| 3.3 | Electronic band structure | 12 |
| 3.4 | Electronic band structure | 12 |
| 3.5 | Electronic band structure | 13 |
| 3.6 | Electronic band structure | 14 |
| 3.7 | Electronic band structure | 14 |
| 4.1 | Electronic band structure | 17 |
| 5.1 | Electronic band structure | 19 |
| 5.2 | Electronic band structure | 20 |
| 5.3 | Electronic band structure | 21 |
| 5.4 | Electronic band structure | 22 |
| 5.5 | Electronic band structure | 23 |
| 5.6 | Electronic band structure | 23 |
| 5.7 | Electronic band structure | 24 |
| 5.8 | Electronic band structure | 24 |
| 5.9 | Electronic band structure | 25 |
| 6.1 | Electronic band structure | 28 |
| 6.2 | Electronic band structure | 29 |
| 6.3 | Electronic band structure | 30 |
| 6.4 | Electronic band structure | 31 |

| | | |
|------|---------------------------|----|
| 6.5 | Electronic band structure | 32 |
| 6.6 | Electronic band structure | 33 |
| 6.7 | Electronic band structure | 34 |
| 6.8 | Electronic band structure | 35 |
| 6.9 | Electronic band structure | 36 |
| 8.1 | Electronic band structure | 40 |
| 8.2 | Electronic band structure | 40 |
| 8.3 | Electronic band structure | 41 |
| 8.4 | Electronic band structure | 41 |
| 8.5 | Electronic band structure | 42 |
| 8.6 | Electronic band structure | 43 |
| 8.7 | Electronic band structure | 43 |
| 8.8 | Electronic band structure | 44 |
| 8.9 | Electronic band structure | 44 |
| 8.10 | Electronic band structure | 45 |
| 8.11 | Electronic band structure | 45 |

Chapter 1

Introduction

¹ Here is the first image.

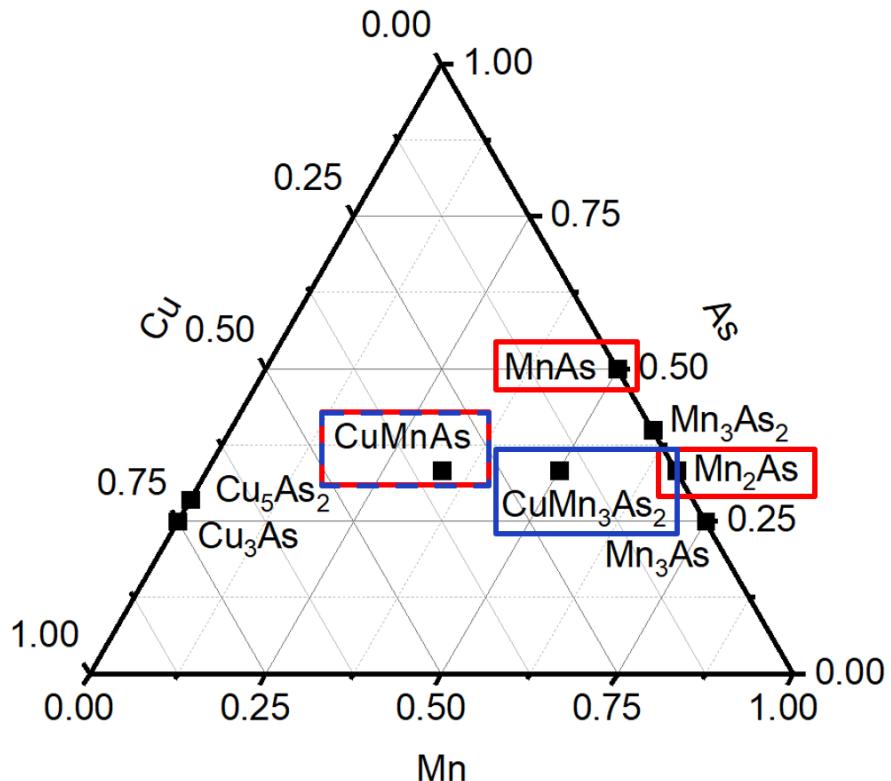


Figure 1.1: Electronic band structure

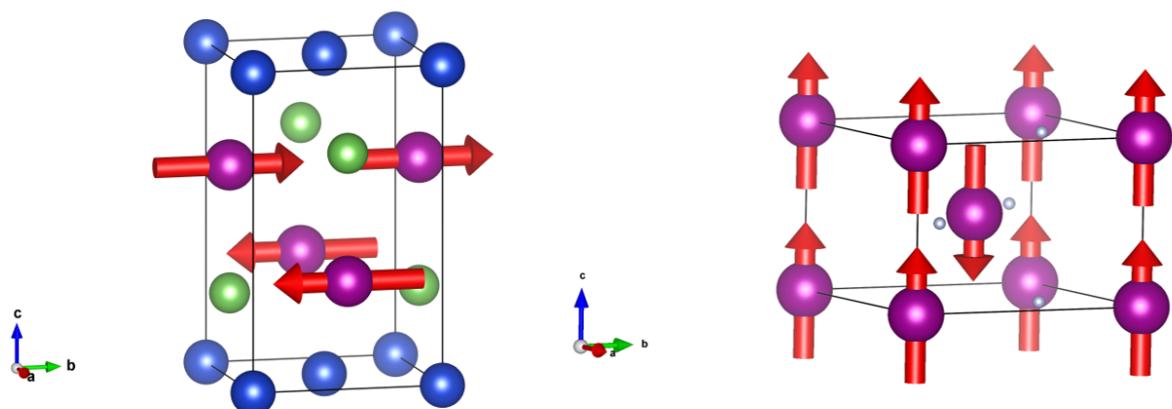


Figure 1.2: Electronic band structure

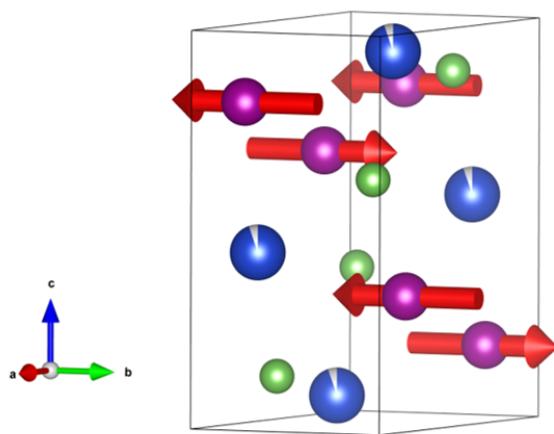


Figure 1.3: Electronic band structure

Chapter 2

Theory of electrical switching in metallic antiferromagnets

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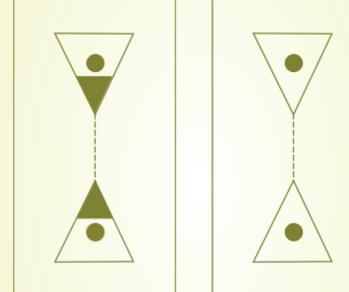
| | | | |
|---|--|---|---|
| Bulk symmetry: Site symmetry: Symmetry schematic: Effect/consequence: Name: | a Centrosymmetric Inversion symmetry  Absence of spin splitting and spin polarization | b Non-centrosymmetric (bulk inversion asymmetry) Dipole field  Site dipole field induced net spin polarization | c Centrosymmetric Inversion asymmetry  Site inversion asymmetry induced net spin polarization |
| | R-1 | D-1 | R-2 |

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

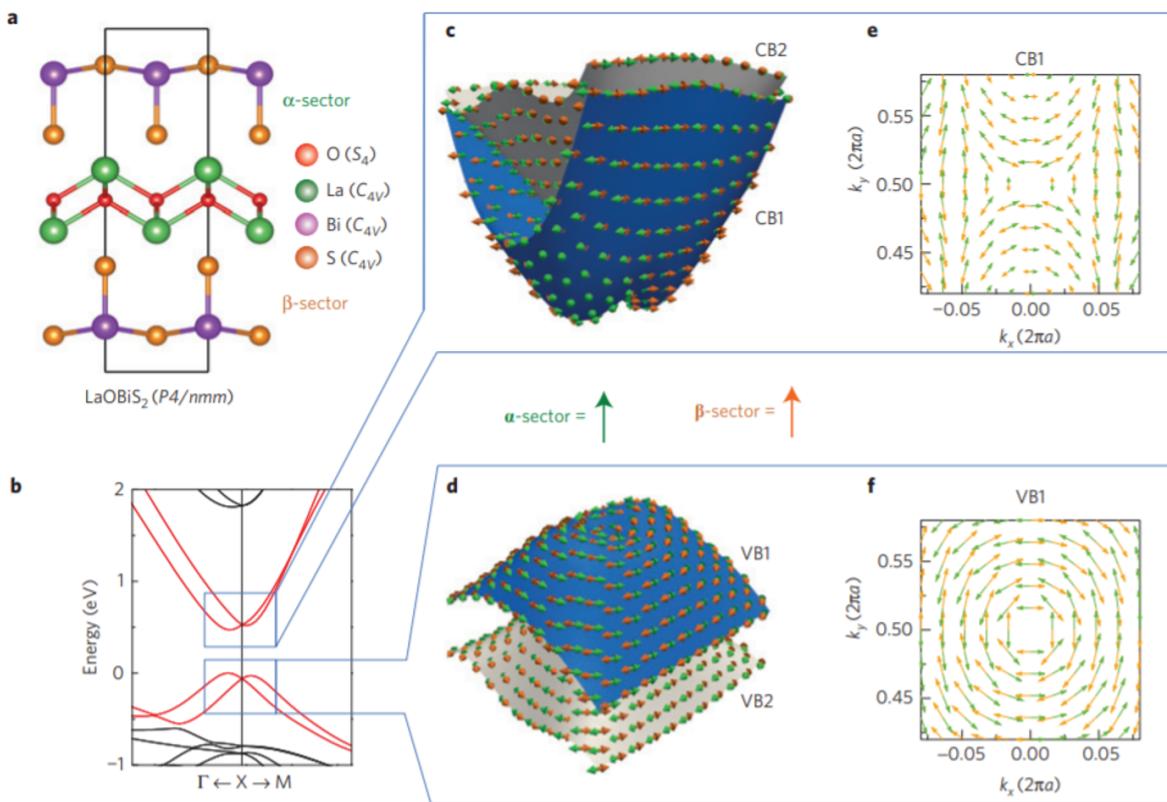


Figure 2.3: Electronic band structure

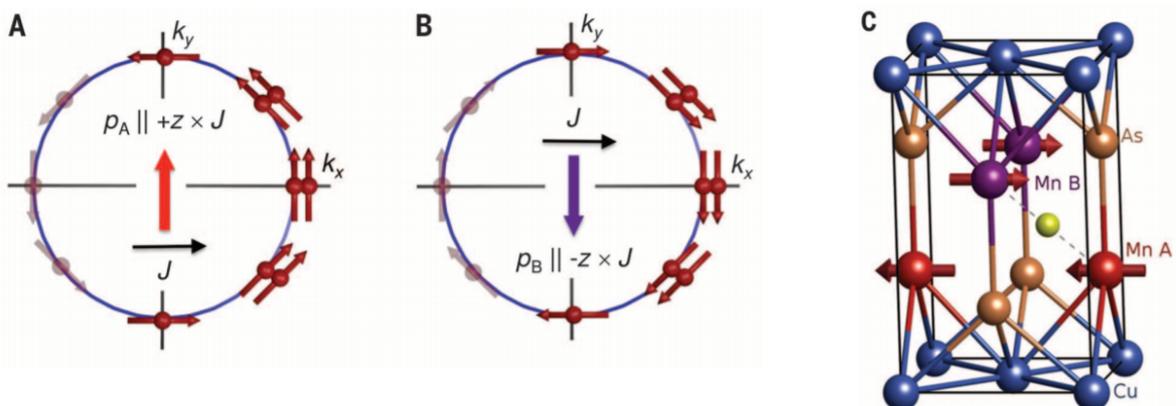


Figure 2.4: Electronic band structure

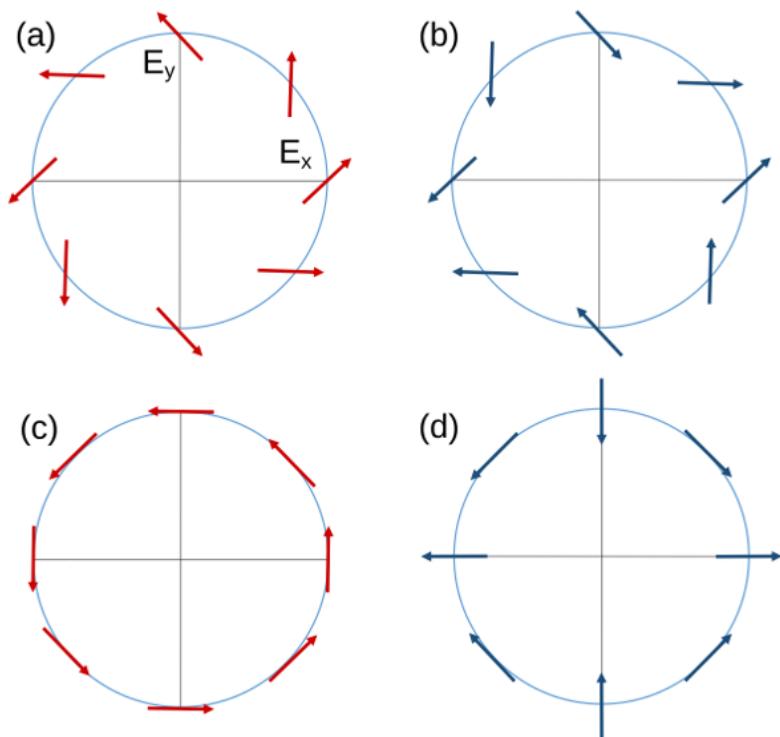


Figure 2.5: Electronic band structure

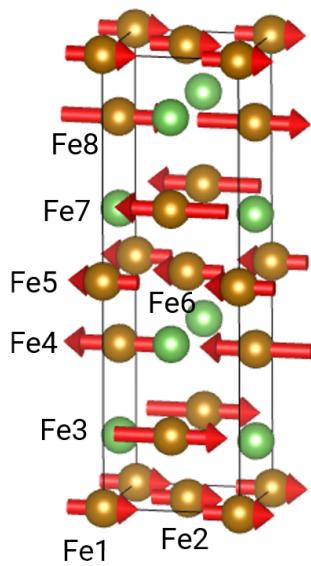


Figure 2.6: Electronic band structure

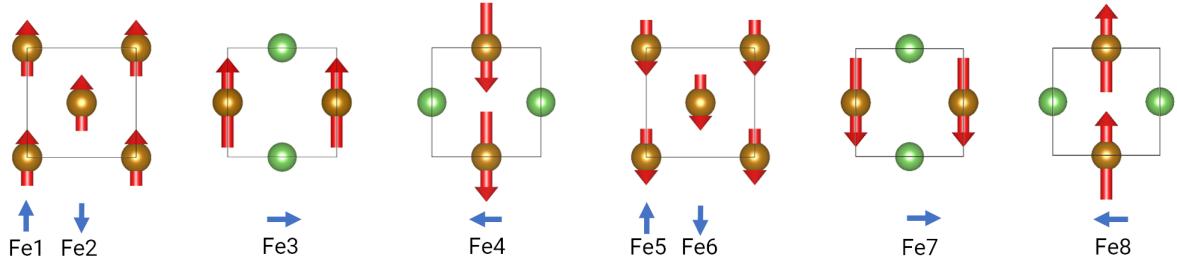


Figure 2.7: Electronic band structure

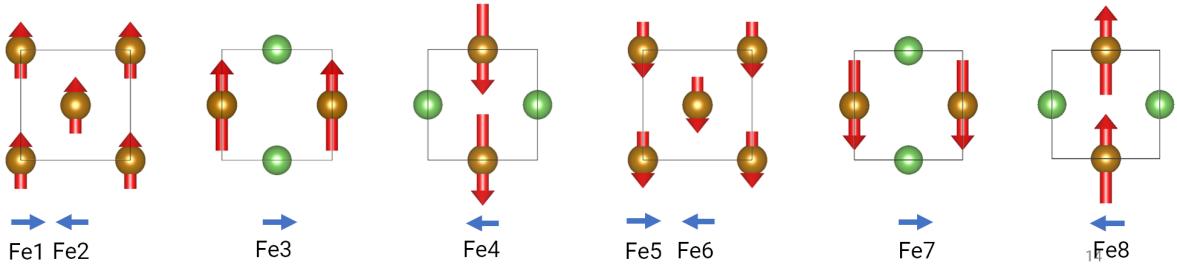


Figure 2.8: Electronic band structure

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Chapter 3

Magnetic structure refinement from neutron diffraction measurements

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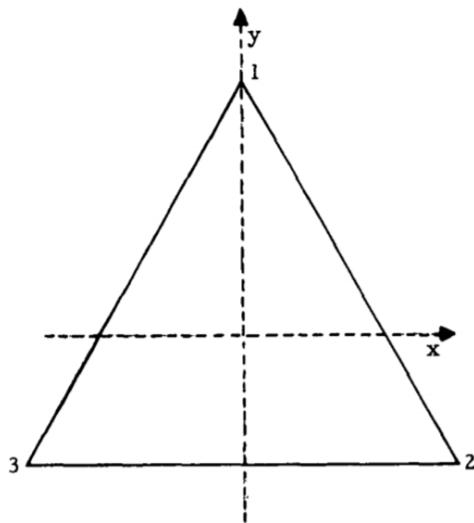


Figure 3.1: Electronic band structure

| | 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

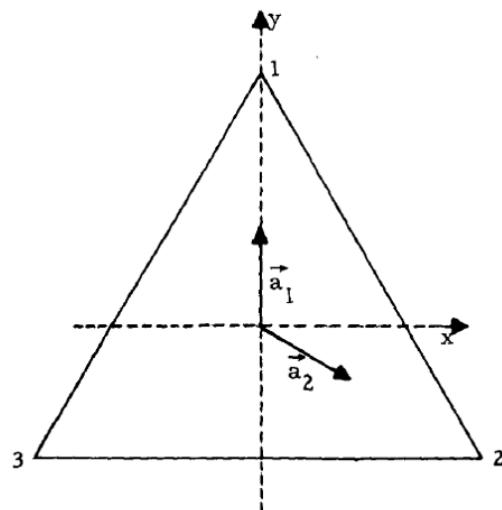


Figure 3.3: Electronic band structure

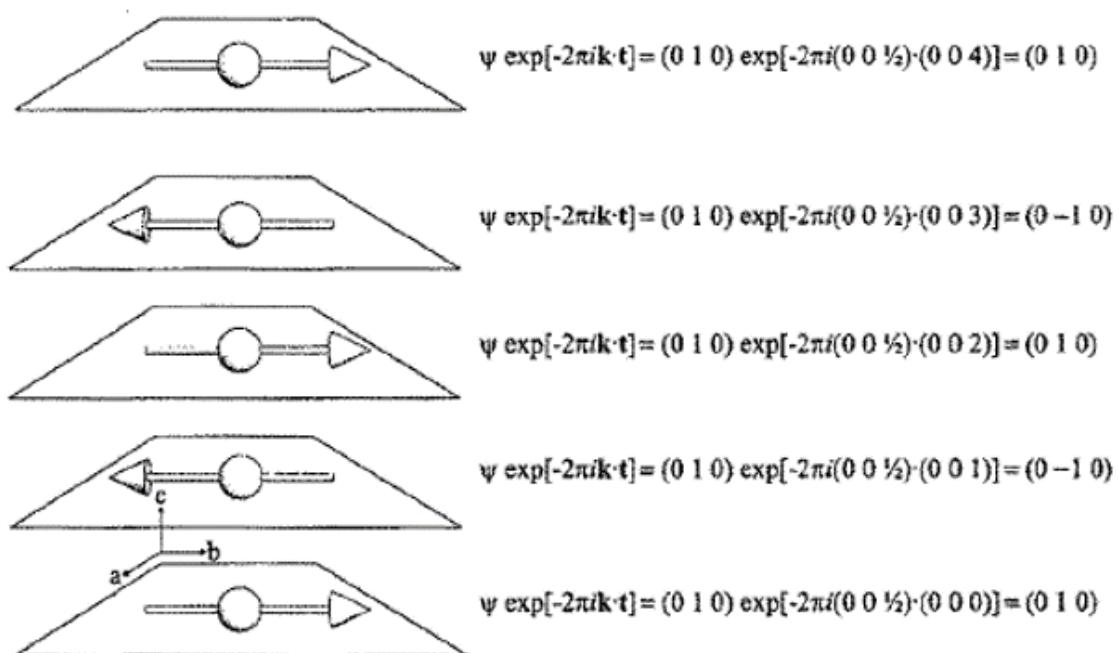


Figure 3.4: Electronic band structure

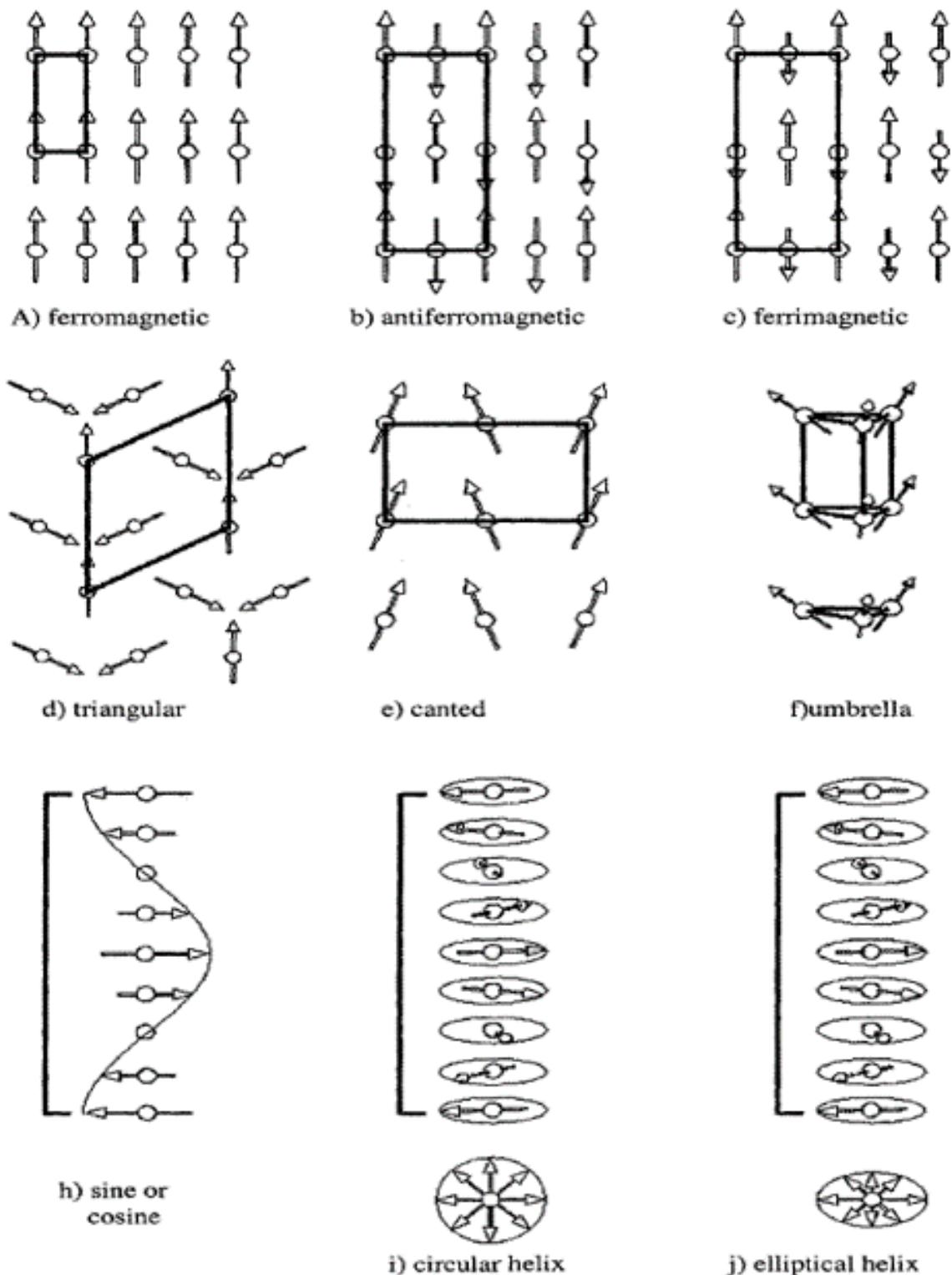


Figure 3.5: Electronic band structure

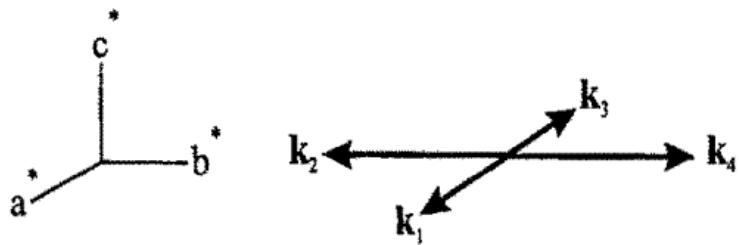


Figure 3.6: Electronic band structure

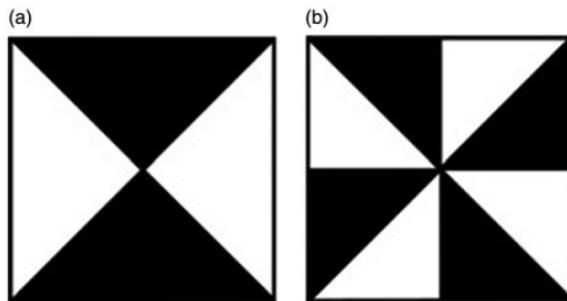


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Chapter 4

Materials synthesis and characterization

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

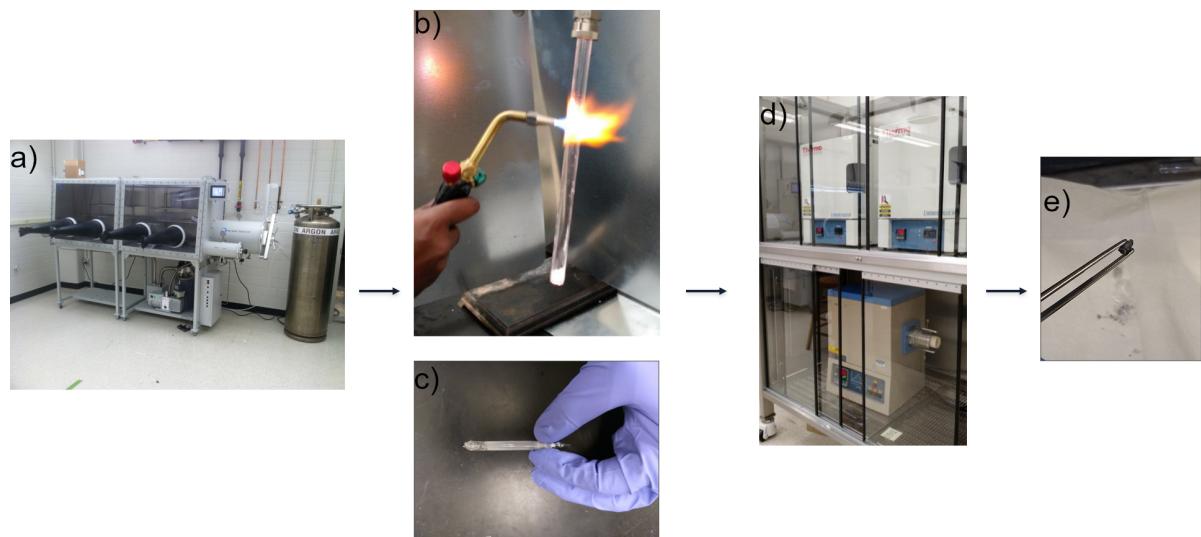


Figure 4.1: Electronic band structure

Chapter 5

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

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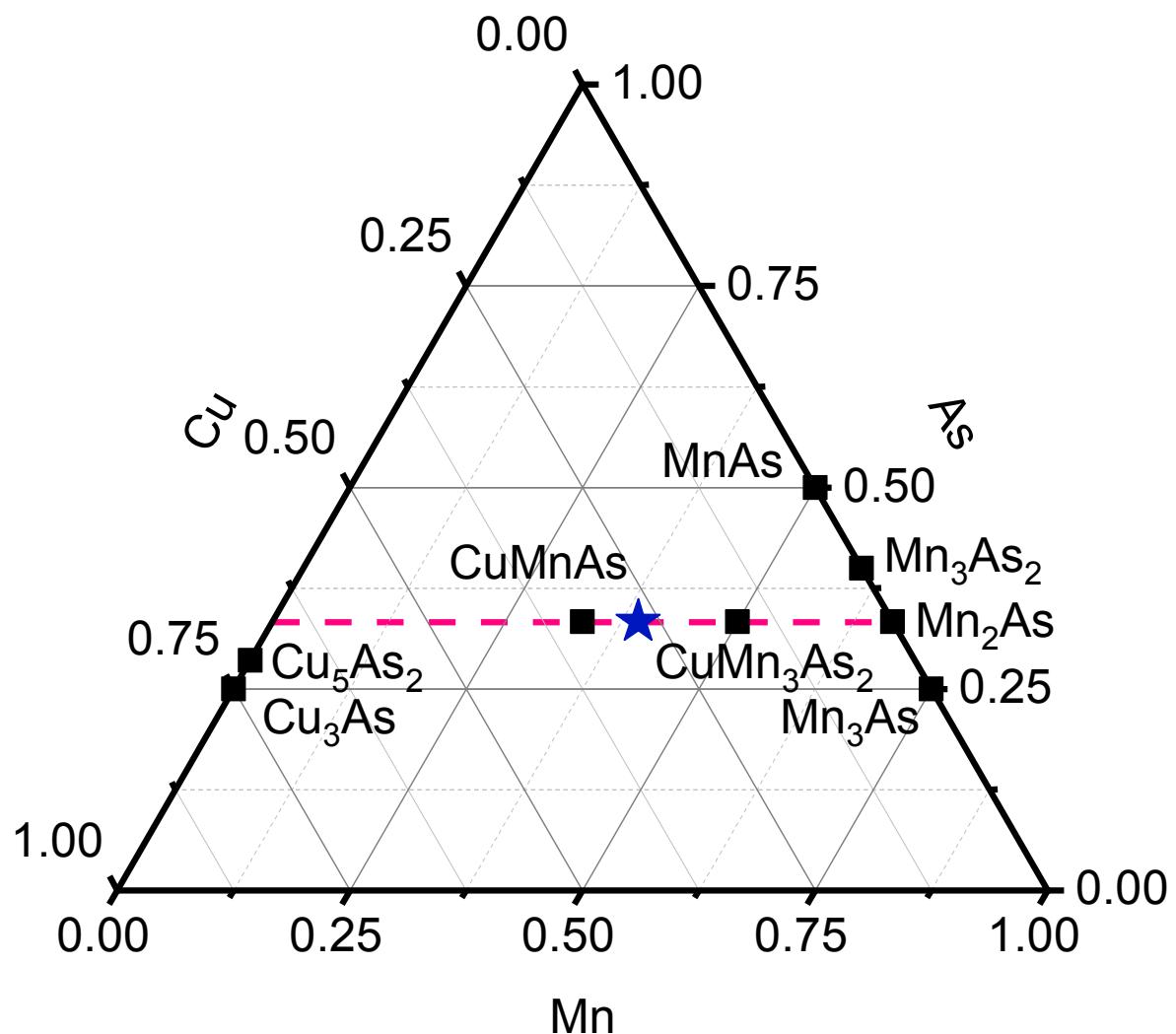


Figure 5.1: Electronic band structure

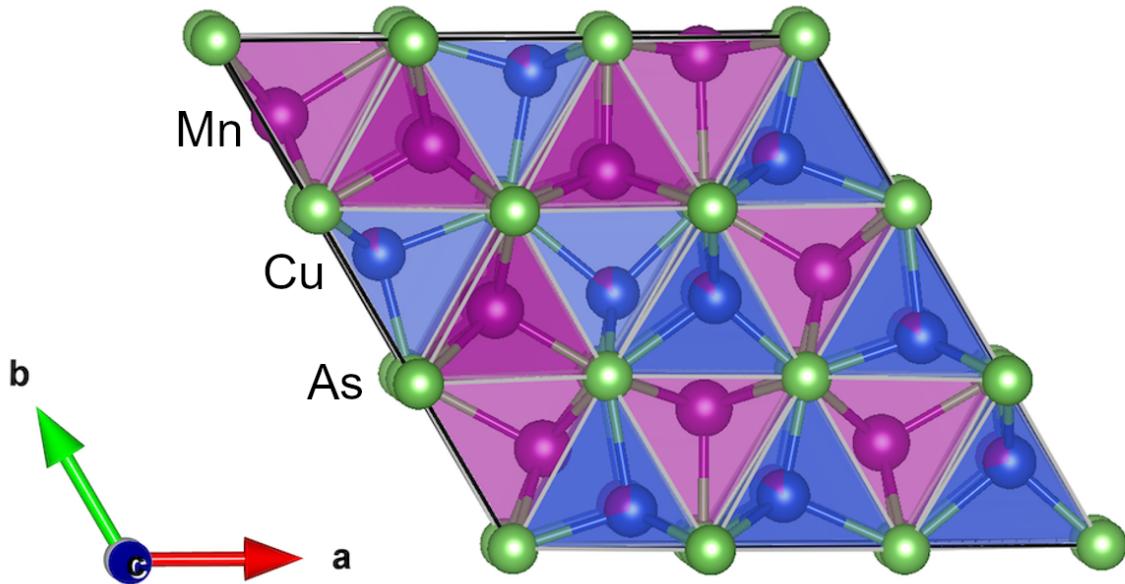


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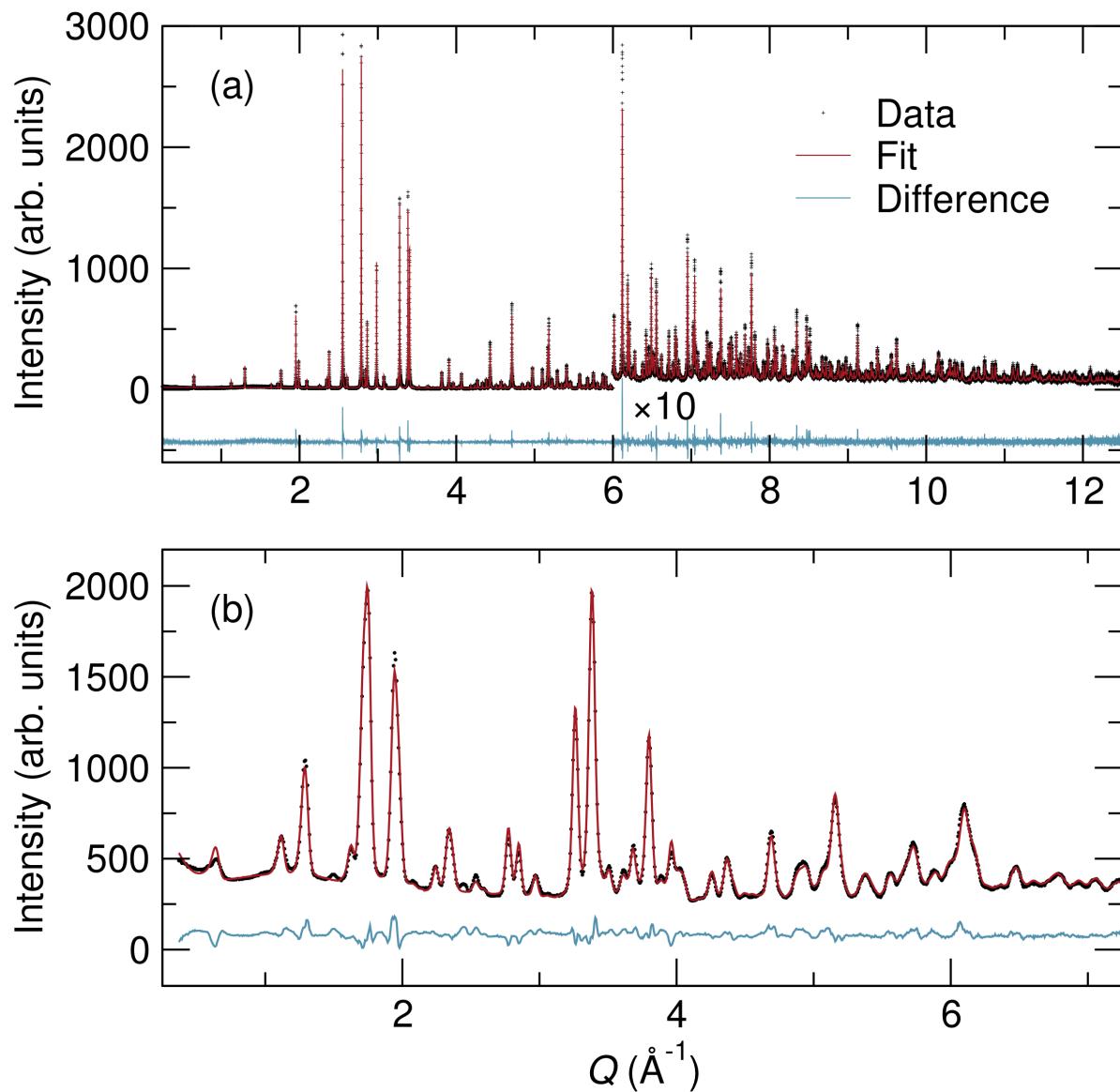


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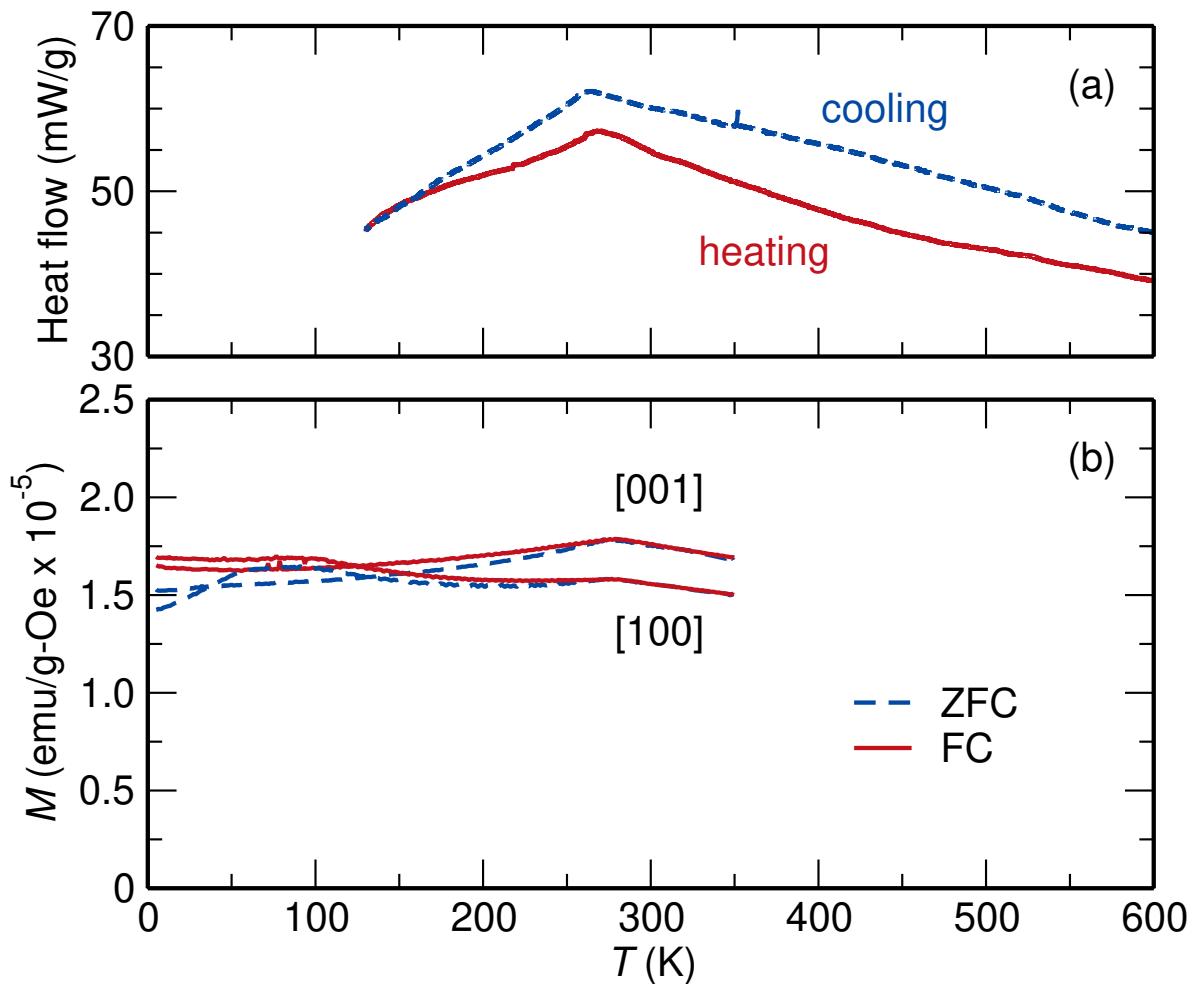


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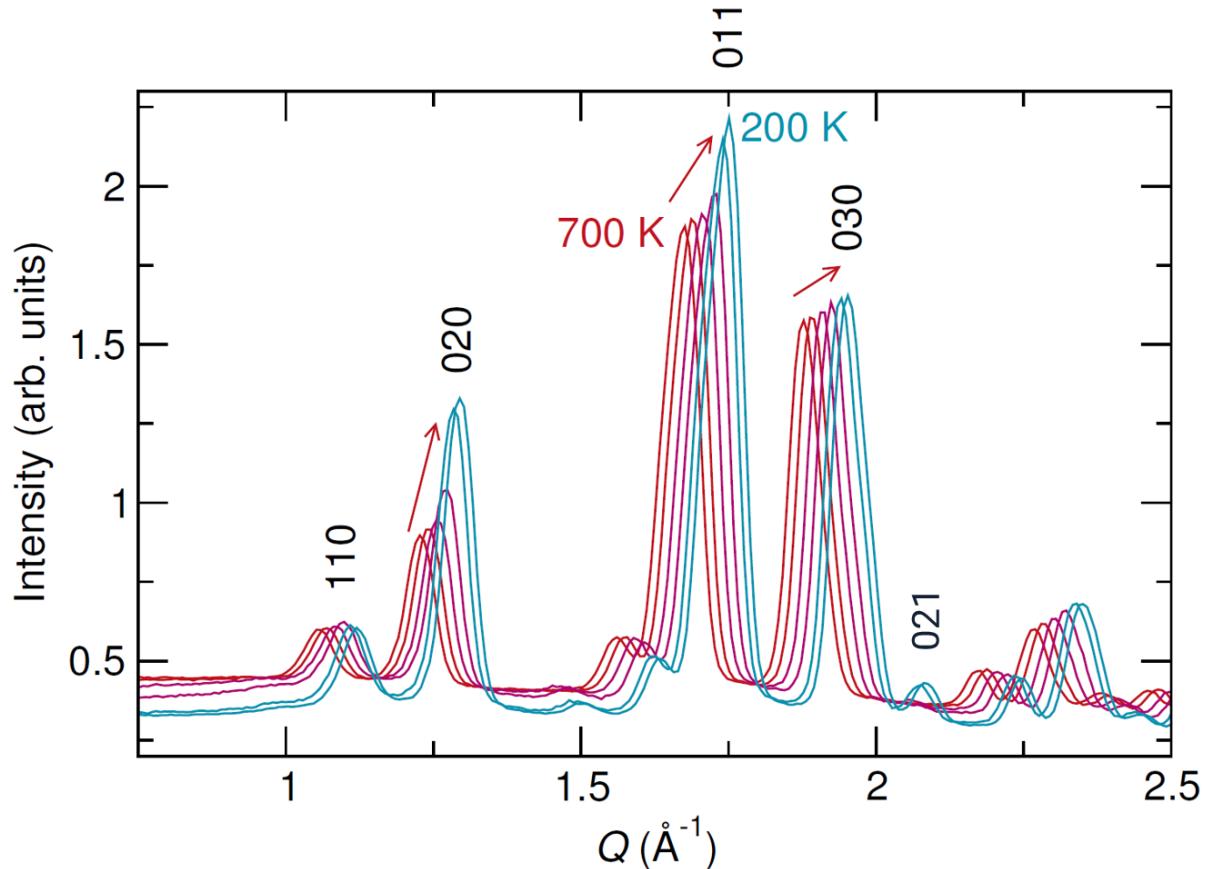


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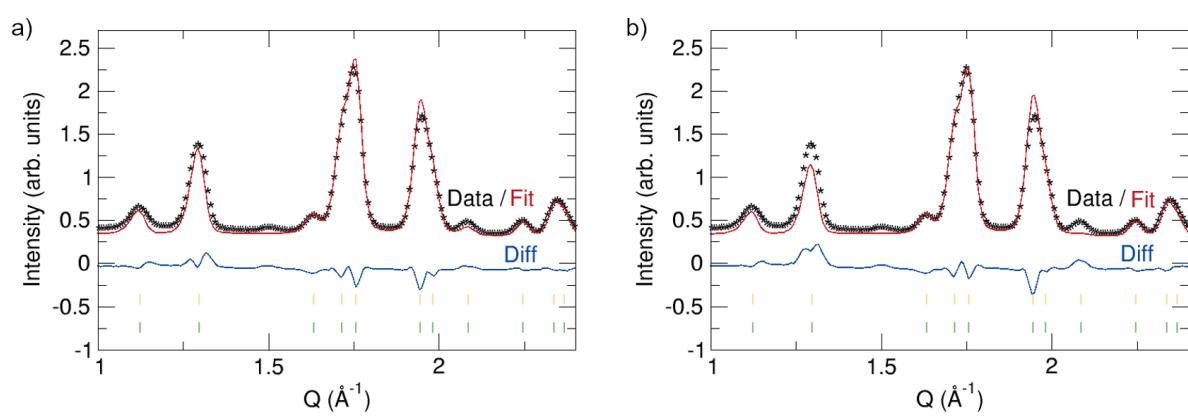


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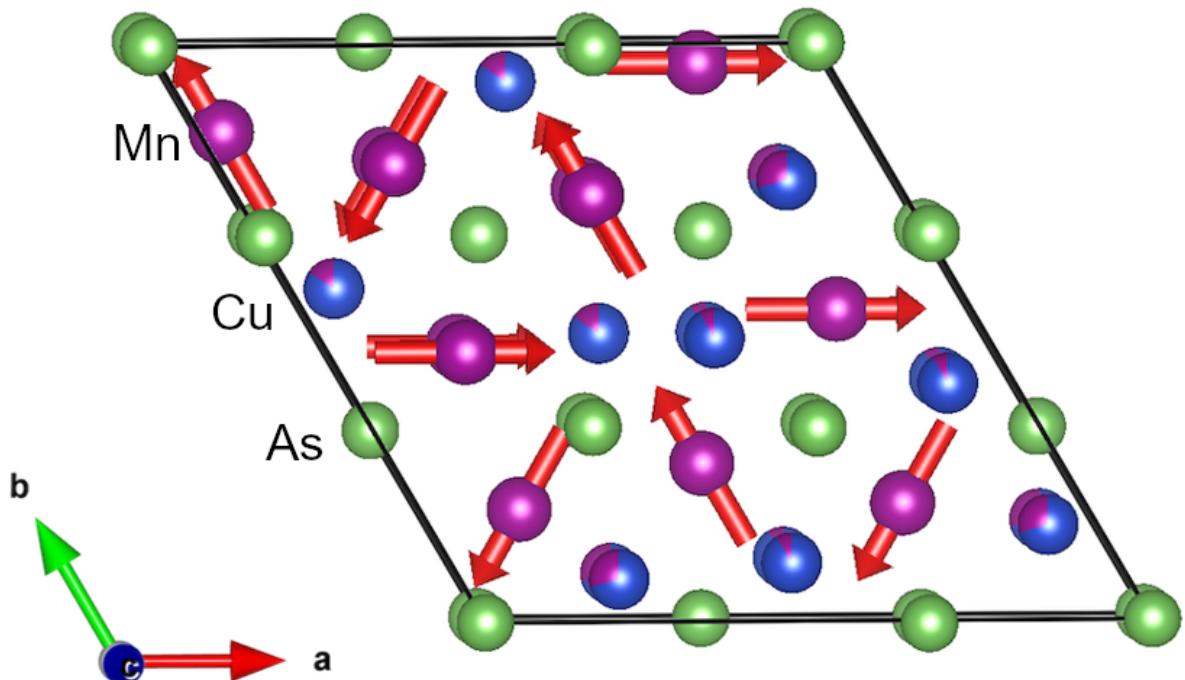


Figure 5.7: Electronic band structure

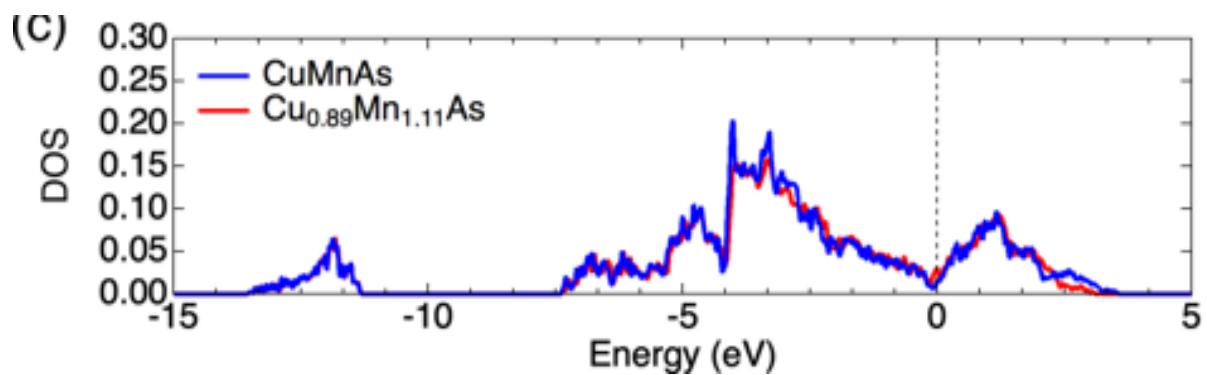


Figure 5.8: Electronic band structure

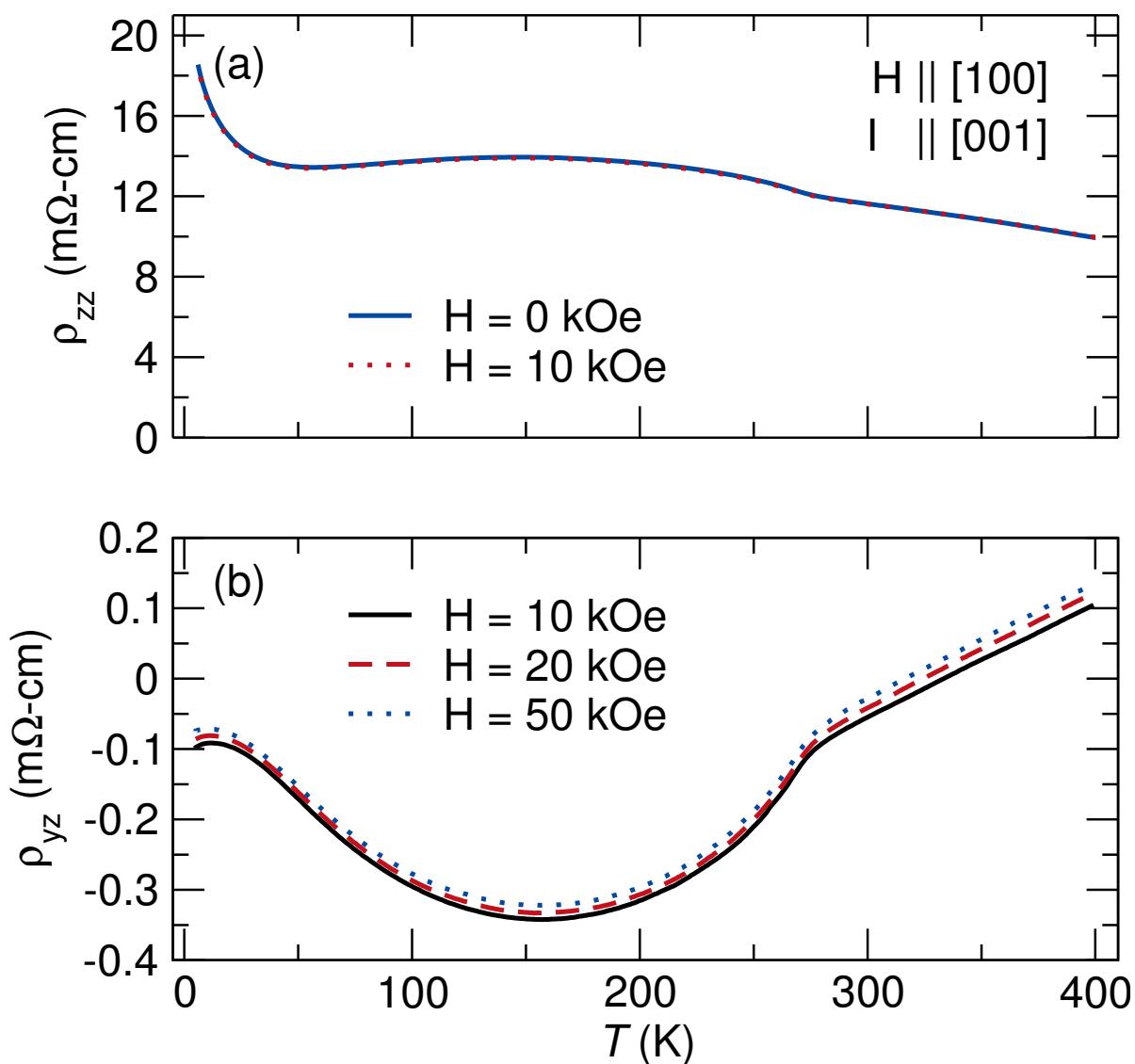


Figure 5.9: Electronic band structure

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Chapter 6

Two step magnetic ordering in monoclinic Mn₃As₂

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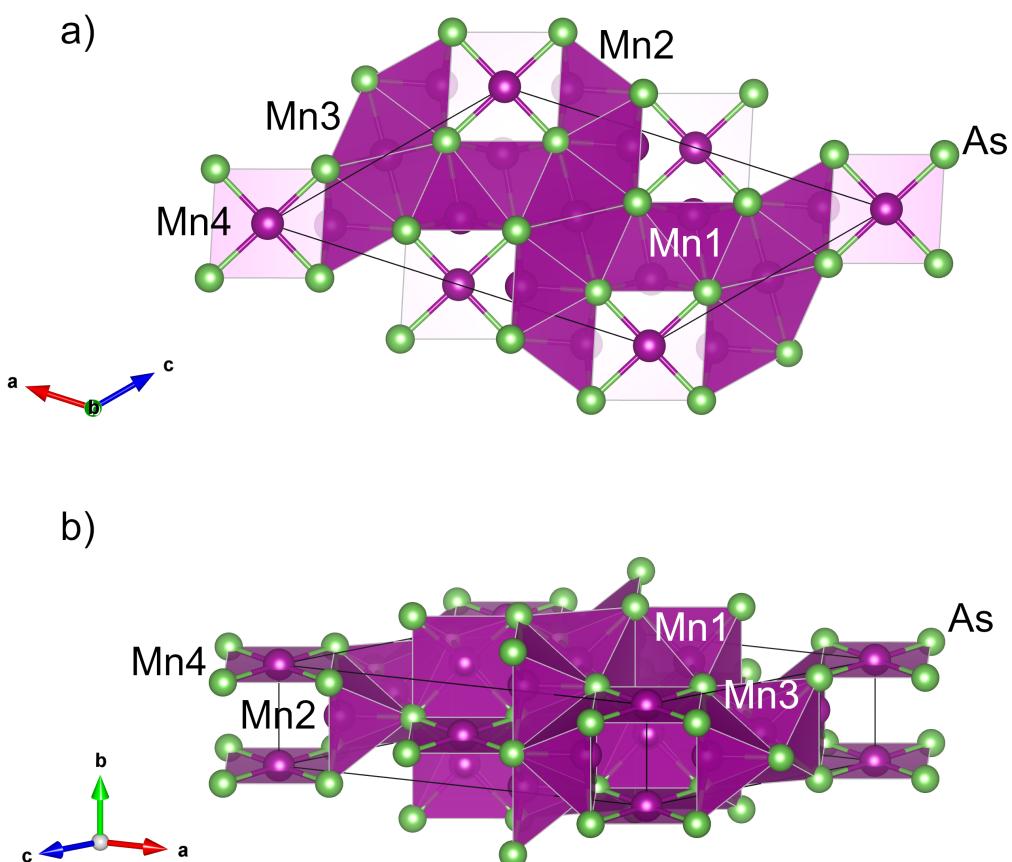


Figure 6.1: Electronic band structure

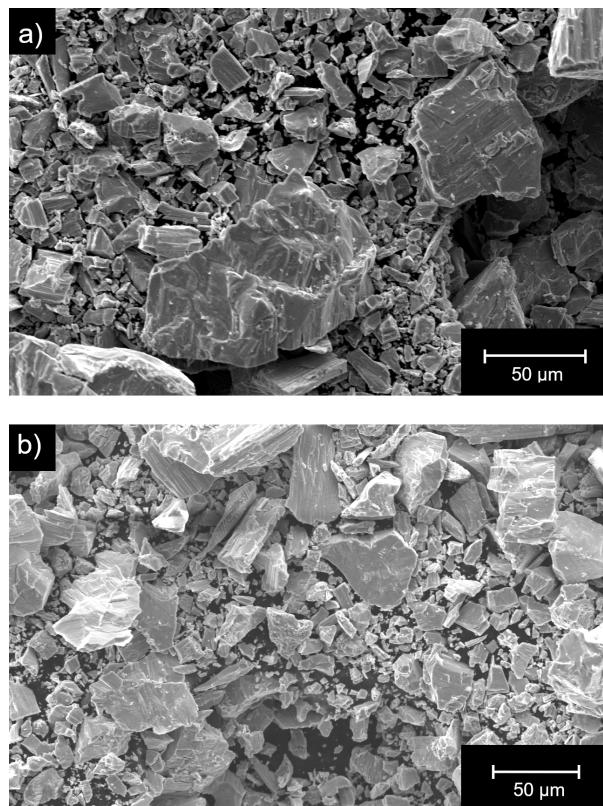


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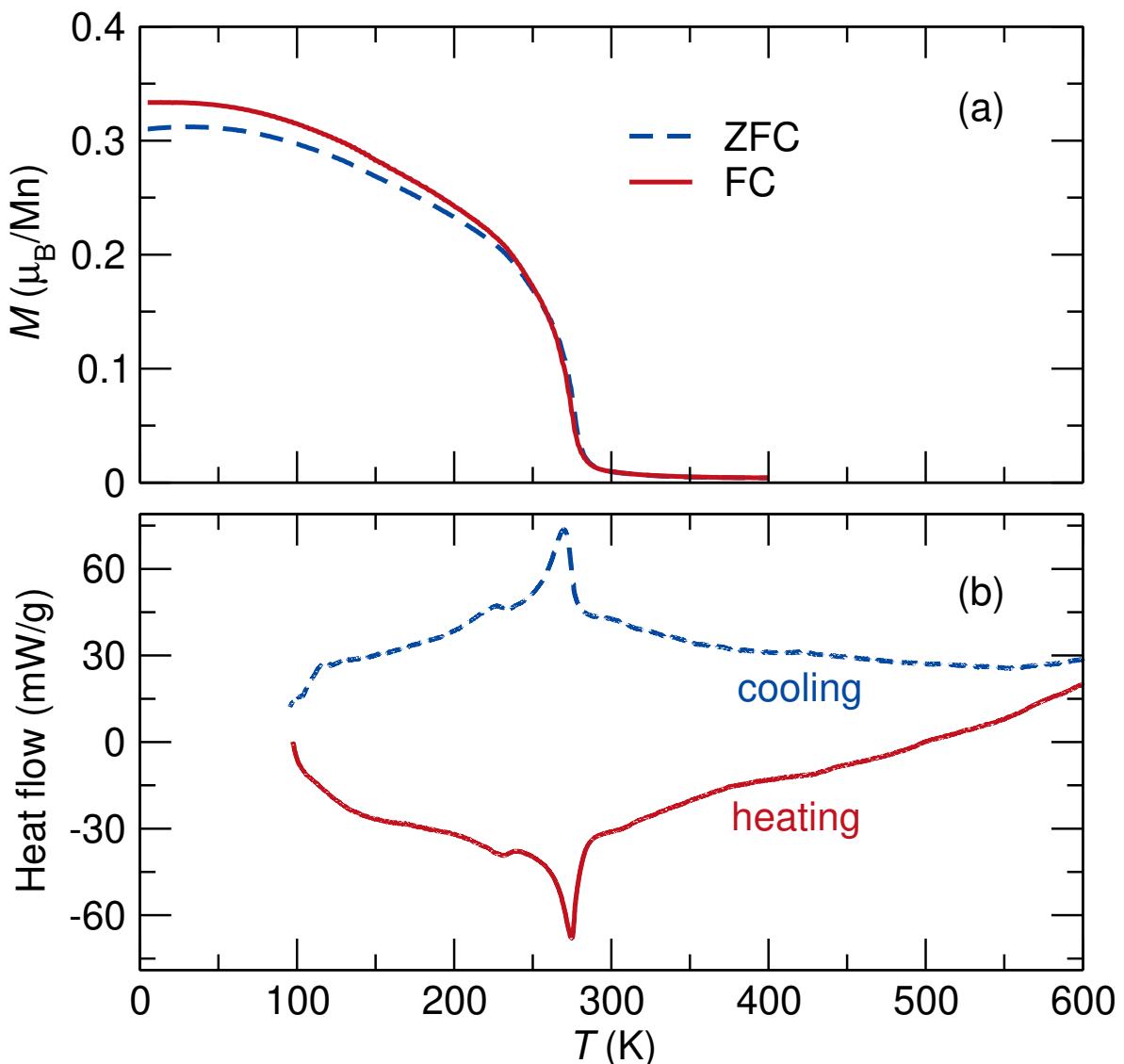


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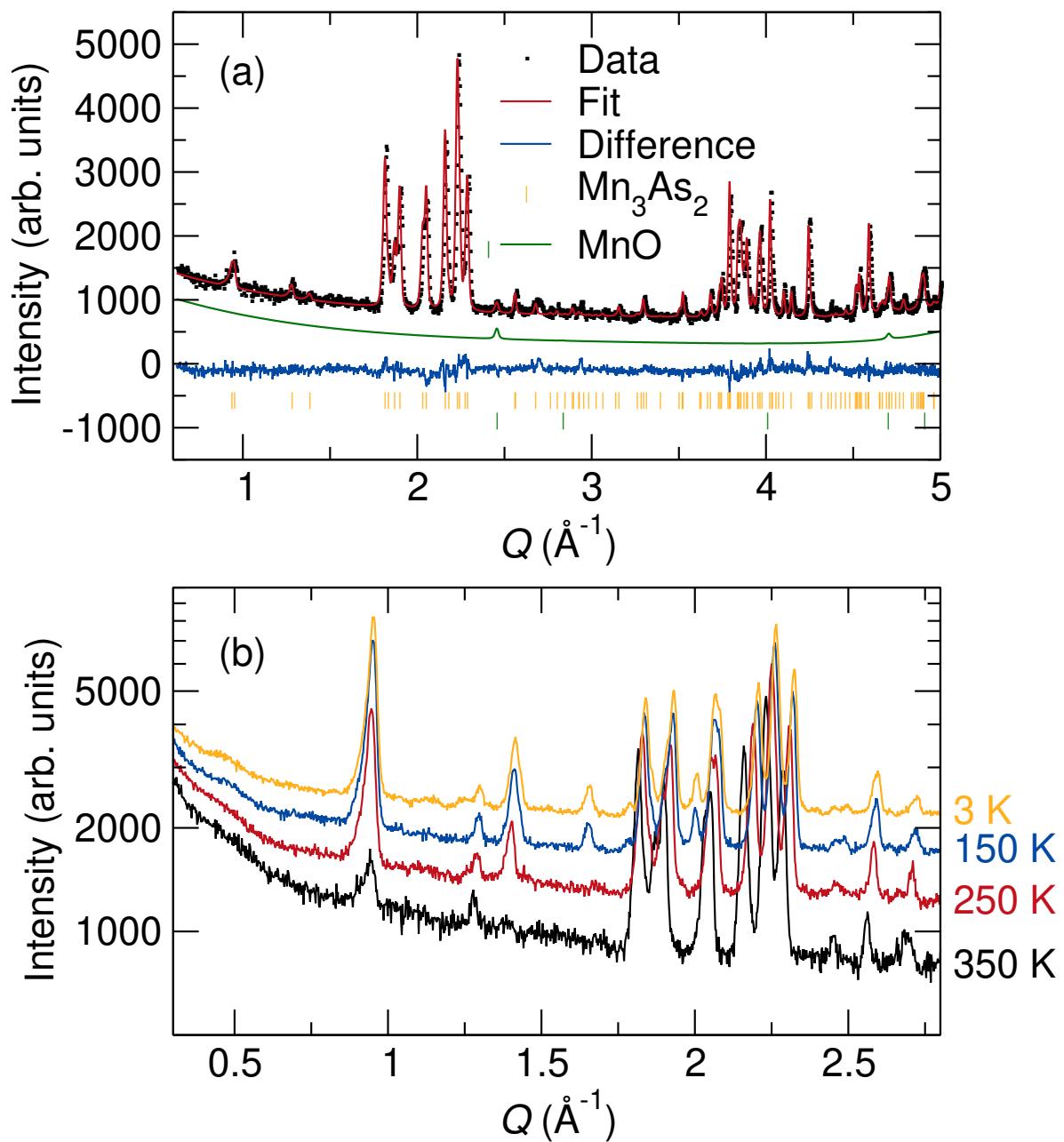


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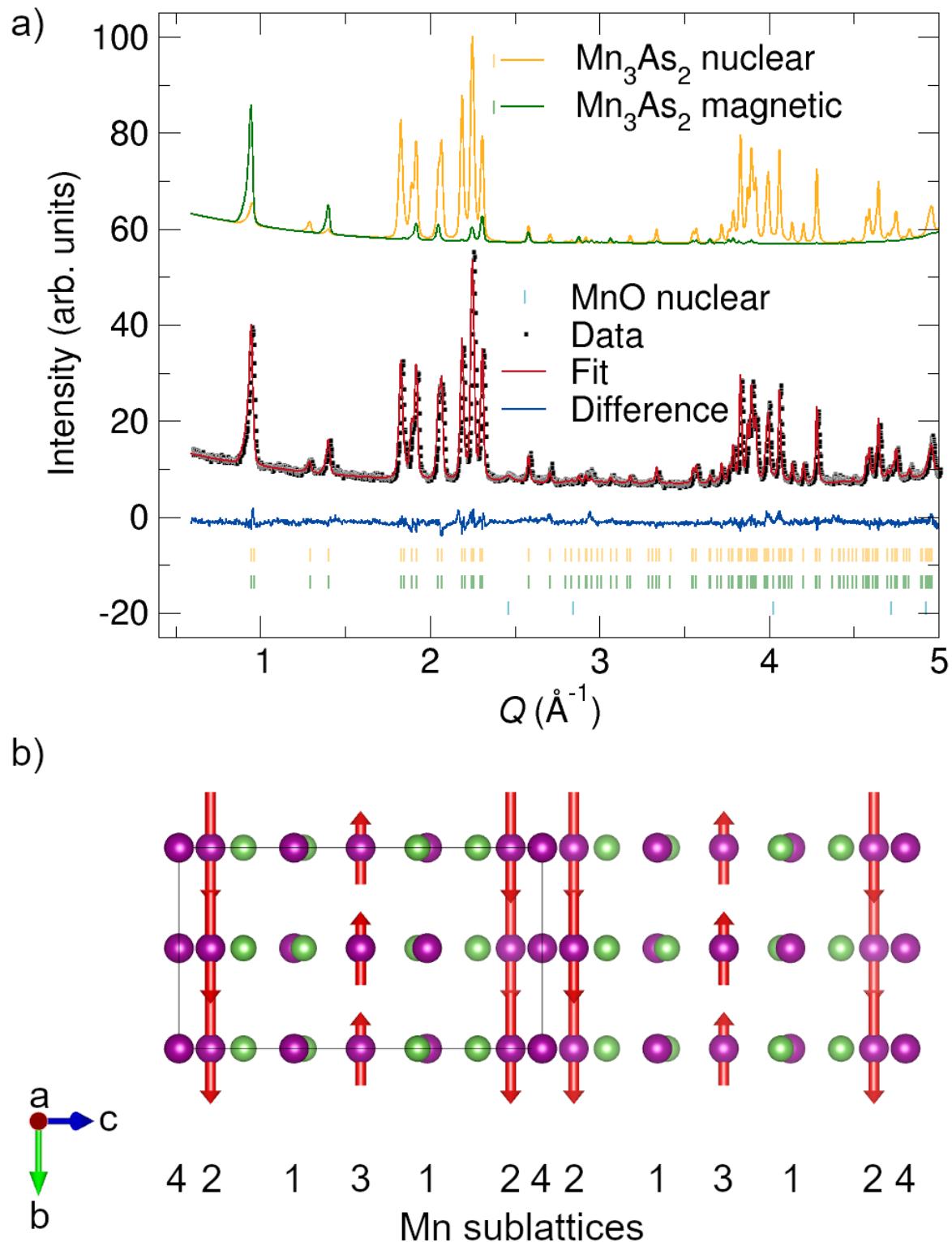


Figure 6.5: Electronic band structure

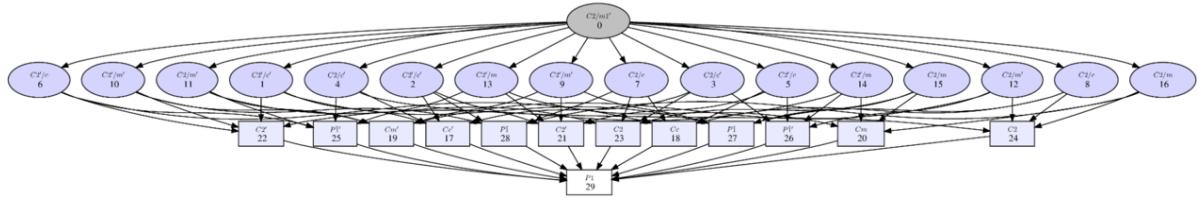


Figure 6.6: Electronic band structure

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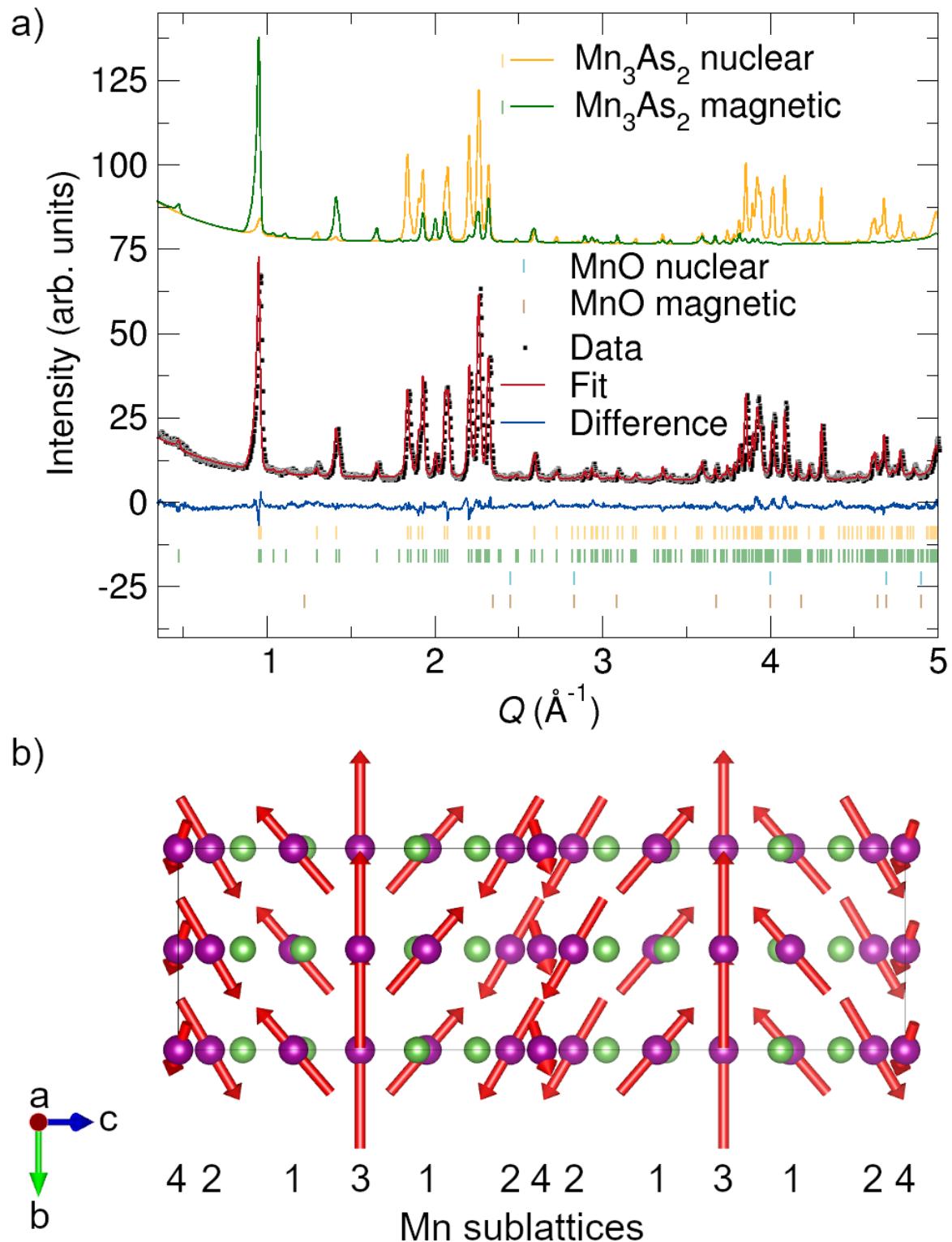


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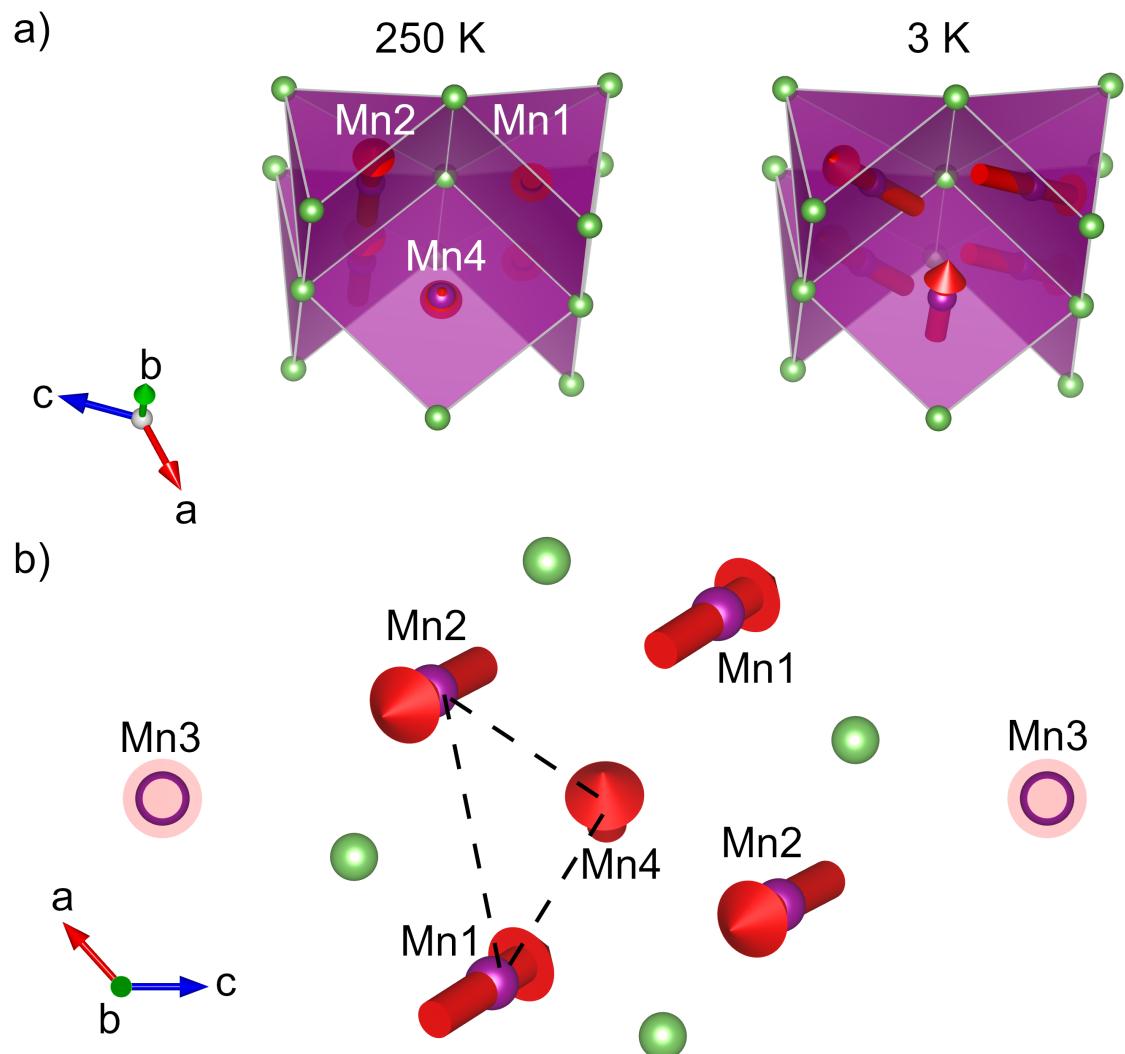


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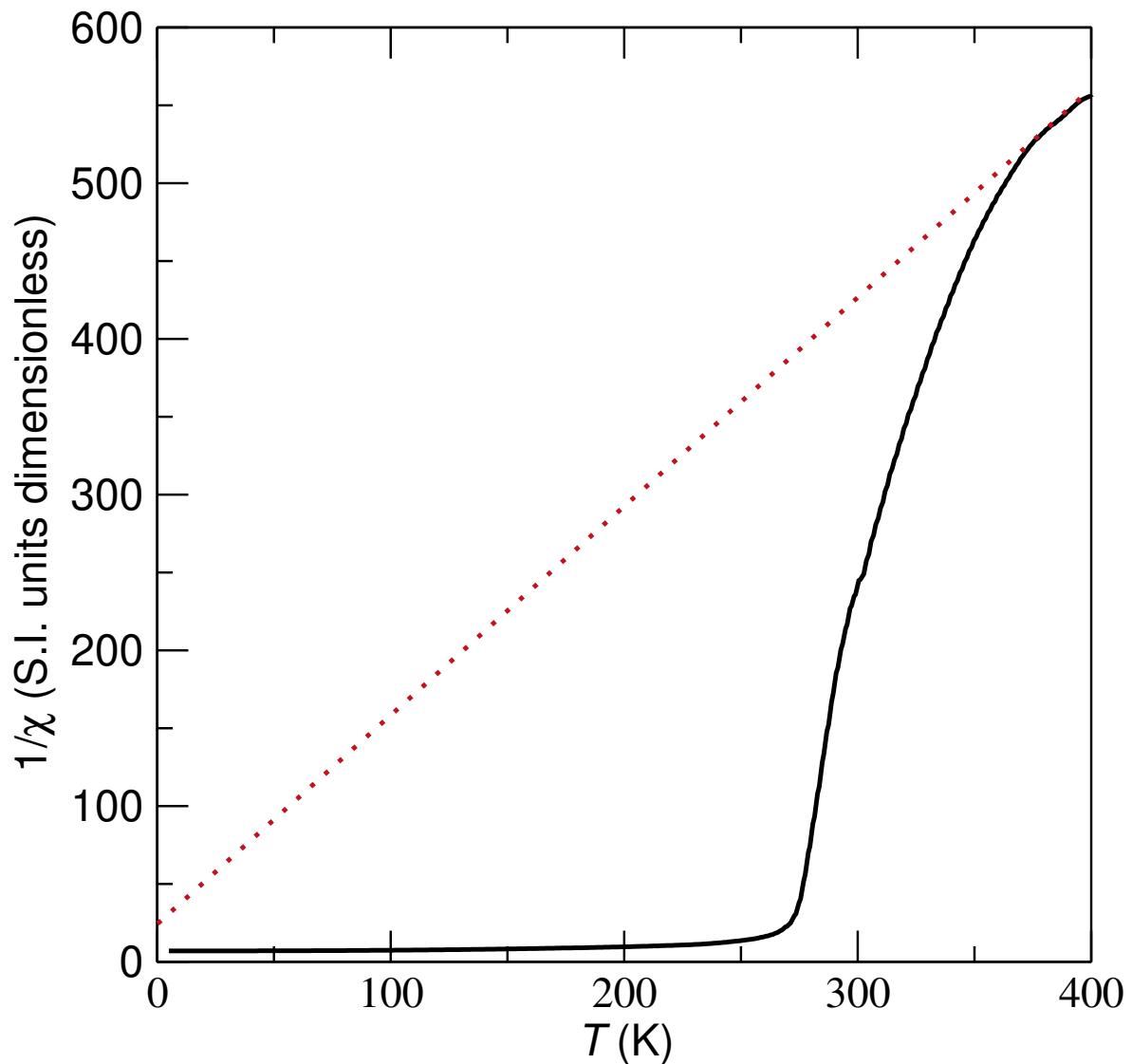


Figure 6.9: Electronic band structure

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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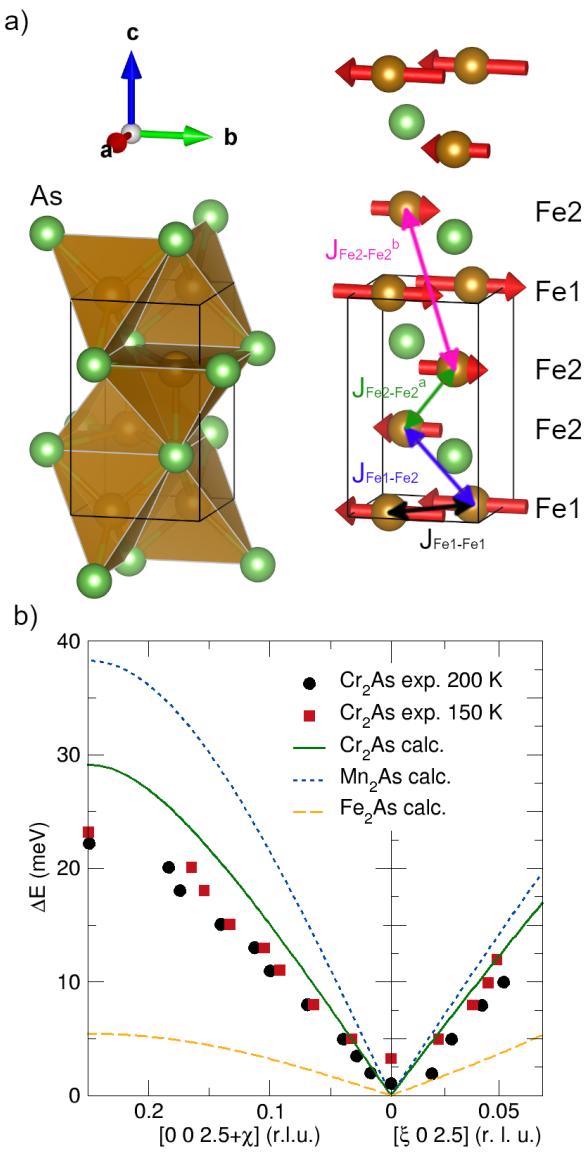


Figure 8.1: Electronic band structure



Figure 8.2: Electronic band structure

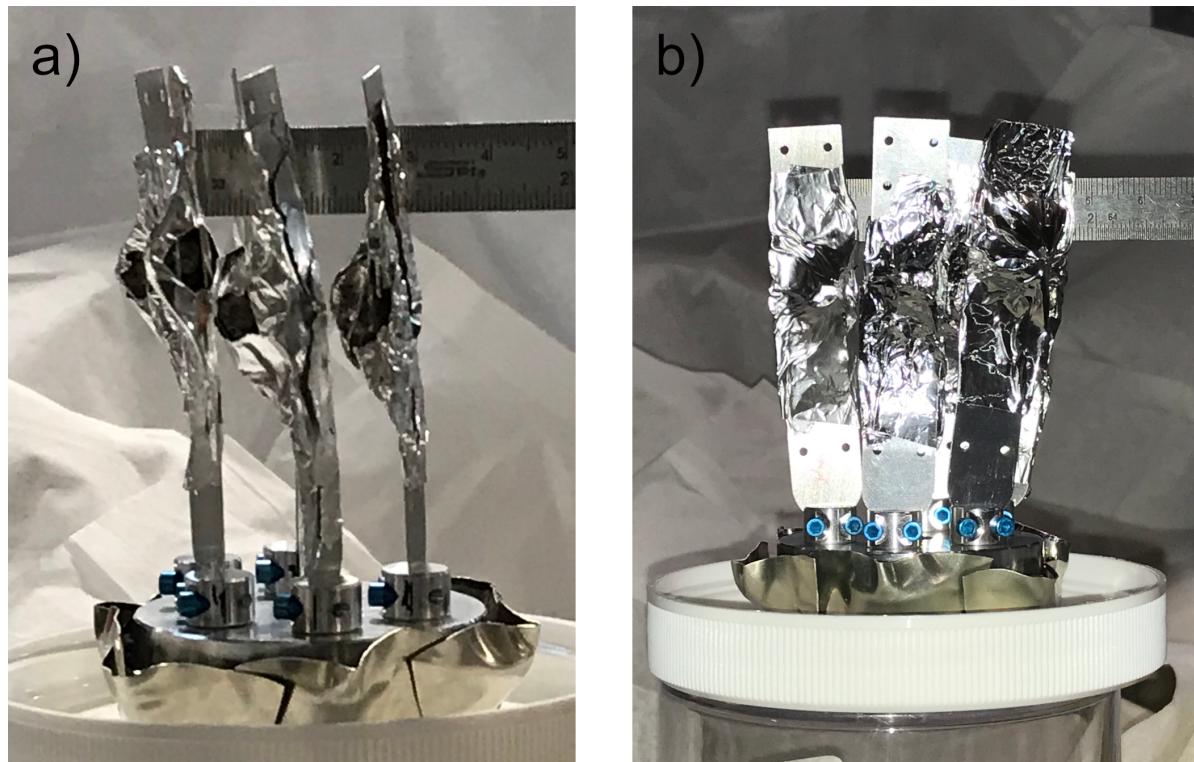


Figure 8.3: Electronic band structure

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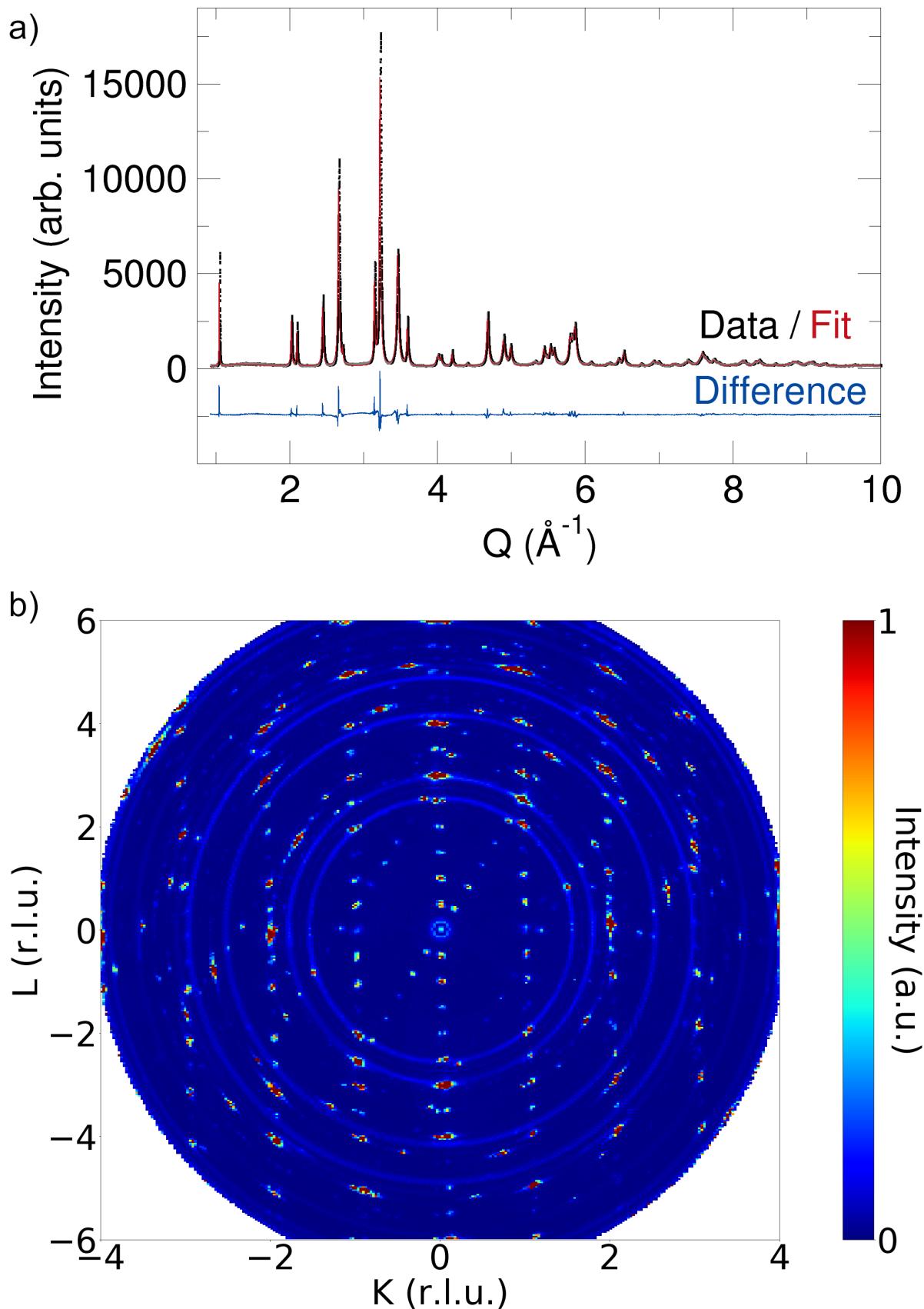


Figure 8.4: Electronic band structure

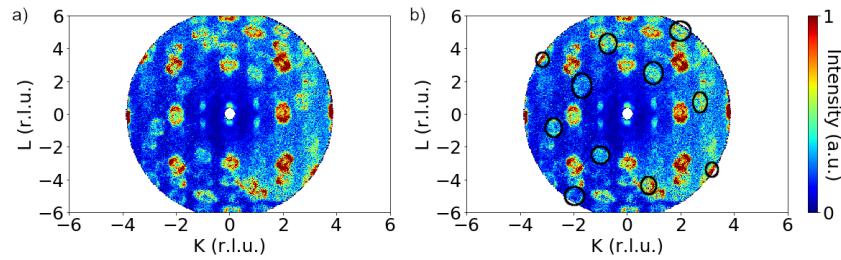


Figure 8.5: Electronic band structure

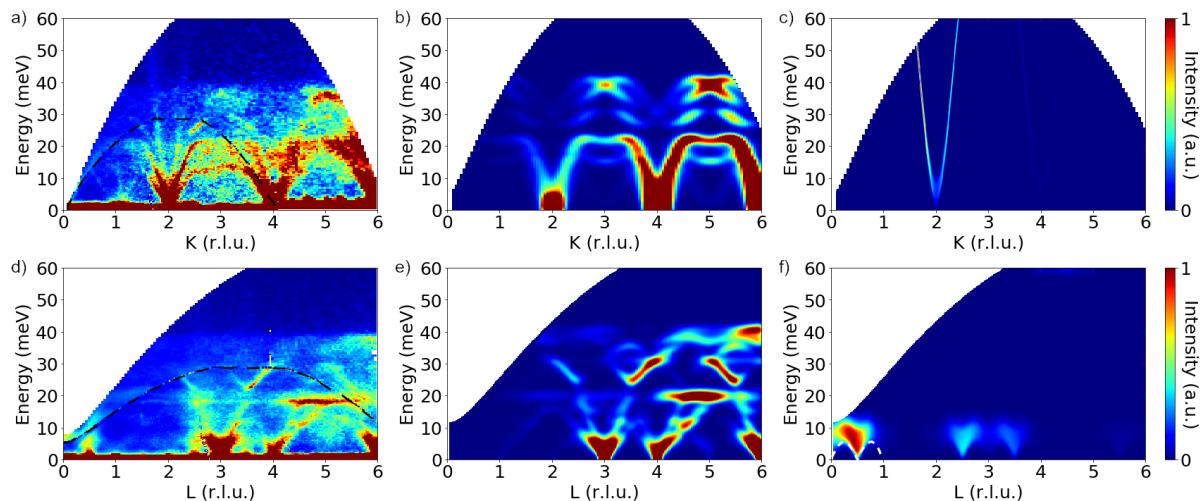


Figure 8.6: Electronic band structure

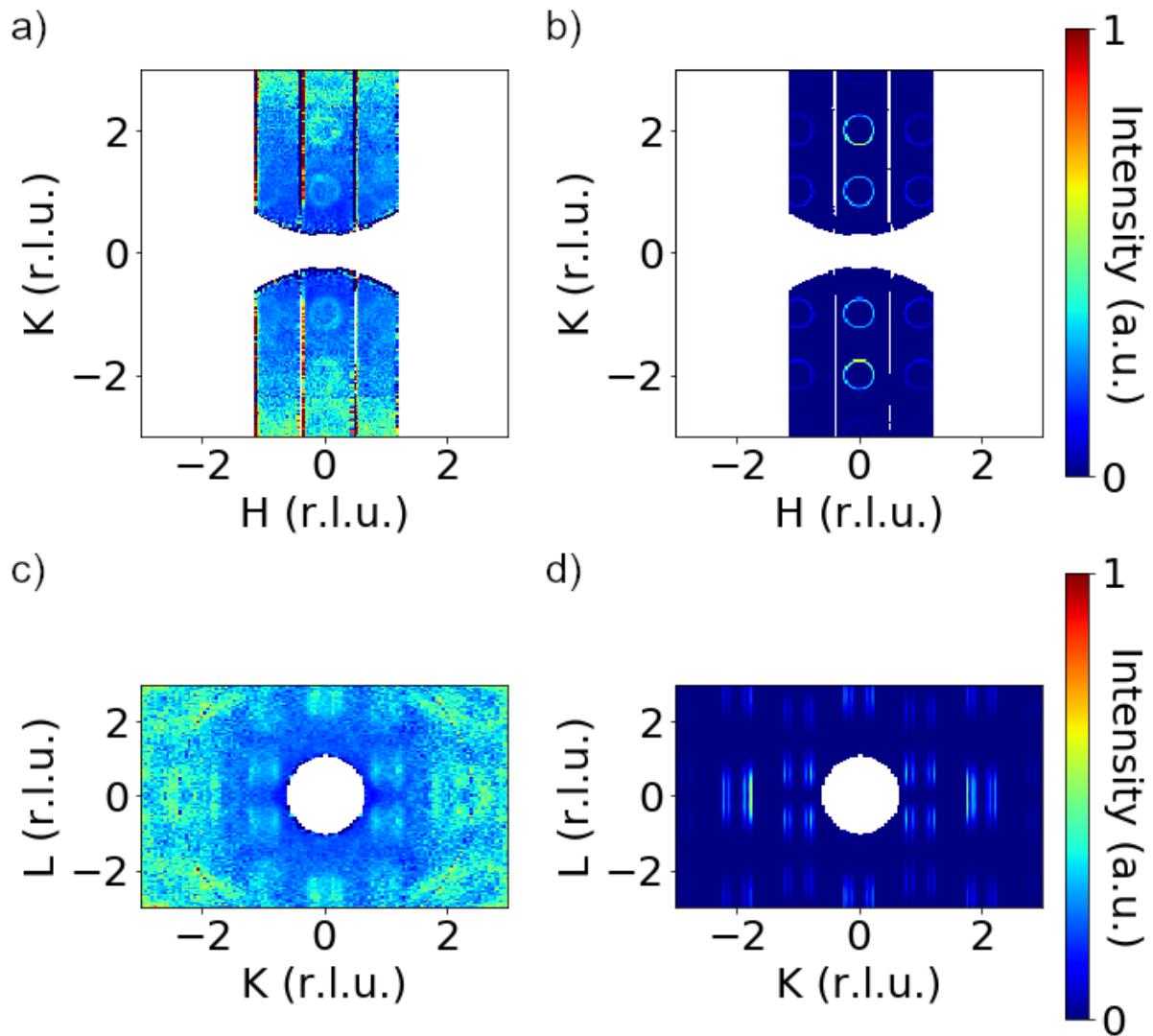


Figure 8.7: Electronic band structure

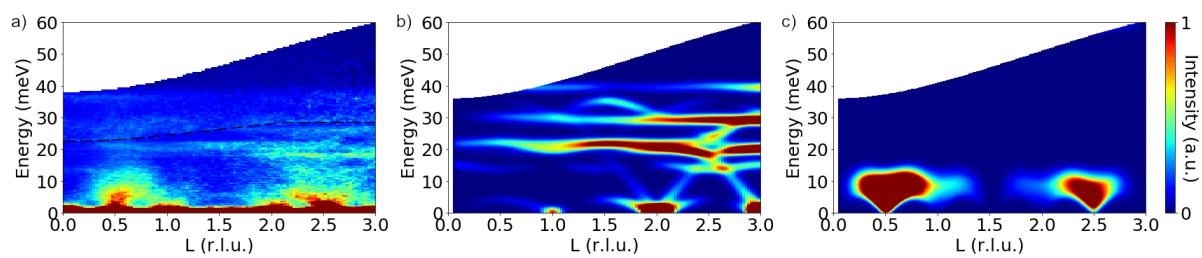


Figure 8.8: Electronic band structure

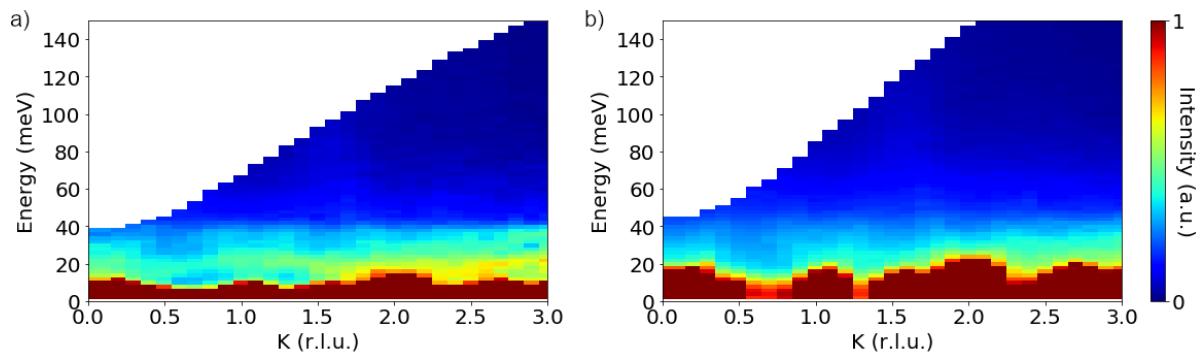


Figure 8.9: Electronic band structure

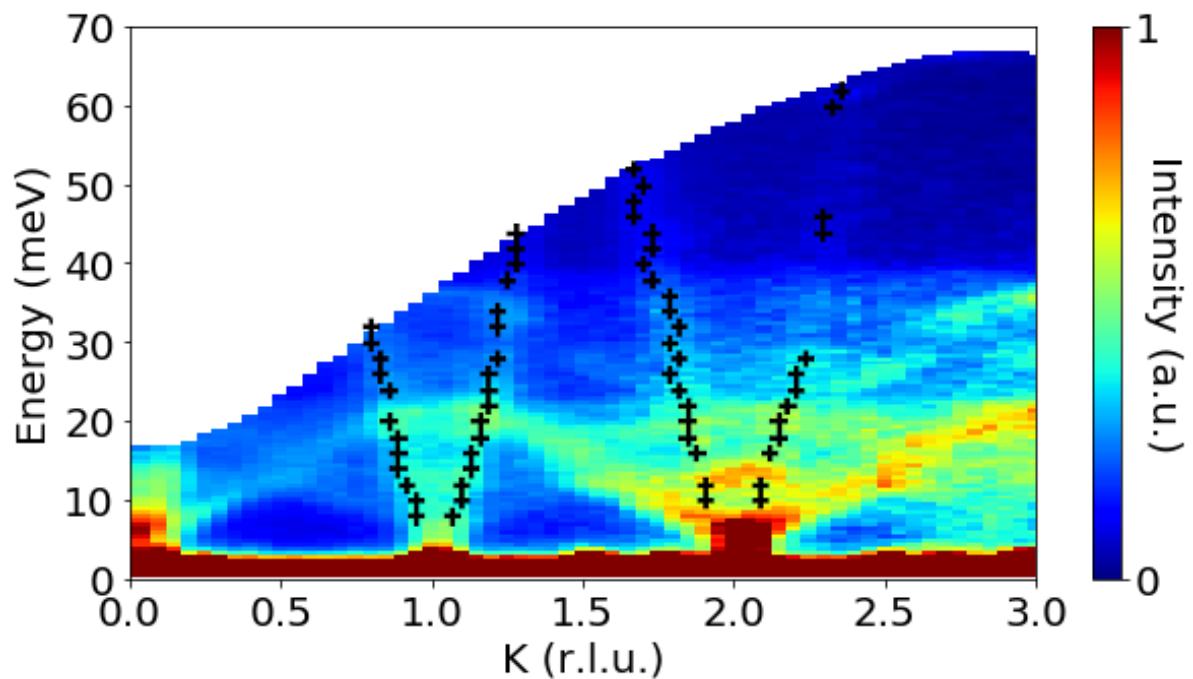


Figure 8.10: Electronic band structure

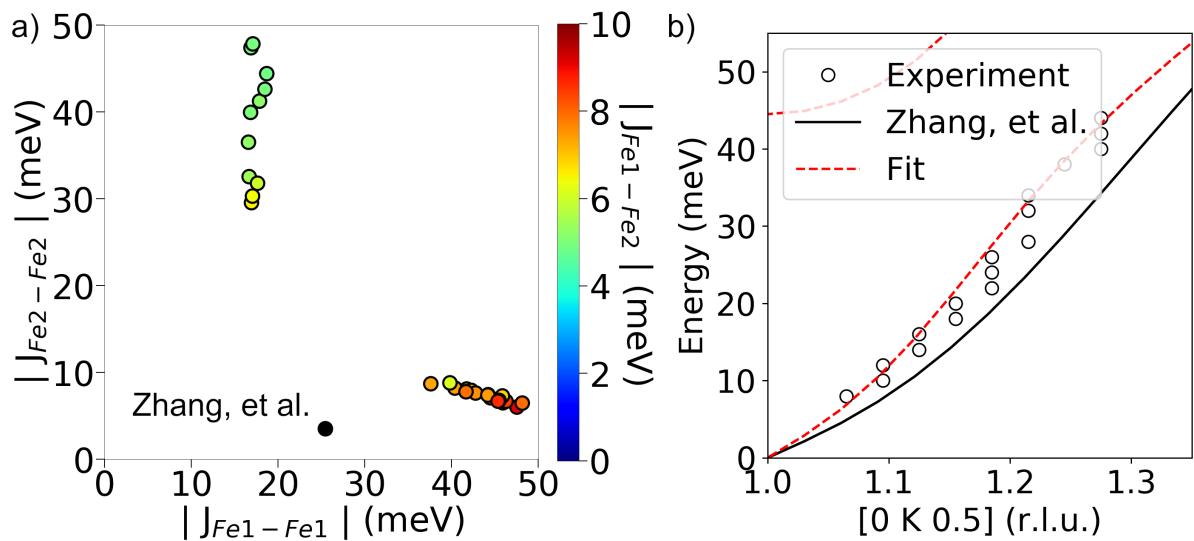


Figure 8.11: Electronic band structure

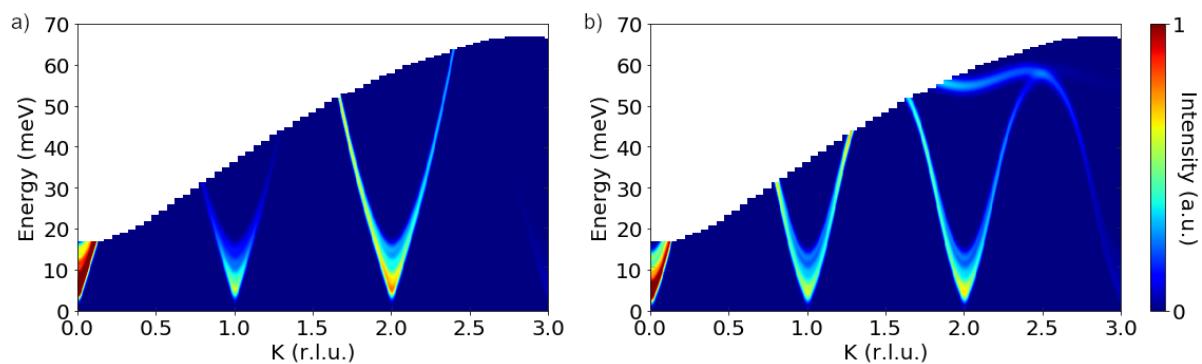


Figure 8.12: Electronic band structure

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Chapter 9

Conclusions

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