Supplementary Materials

Ab initio study of magnetic Cu_2Sb compounds related to antiferromagnetic CuMnAs

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Introduction

This Supplementary Material provides detailed information for each material obtained from our high-throughput calculations. We consider compounds containing two metallic elements selected from Mn, Fe, Cr, Co, Ga, Cu, and Ni, together with As or Sb. In the following, a *material* refers to a fixed chemical composition, independent of the occupation of the two nonequivalent metallic sites M1 and M2.

For a given material containing two different metallic elements A and B, two atomic *configurations* are possible because A and B can occupy the nonequivalent M1 and M2 sites in two different ways. In one configuration, A occupies the M1 site and B occupies the M2 site, while in the second configuration the site occupations are interchanged. Throughout this Supplementary Material, the configuration name specifies the occupation of these sites. For example, CuMnAs denotes the configuration in which Cu occupies the M1 site and Mn occupies the M2 site.

For each configuration, we show an image of the crystal structure and provide the relaxed lattice parameters a and c, together with the two independent fractional z coordinates z_1 and z_2. The structures belong to the $P4/nmm$ space group, and all atomic coordinates can be reconstructed from these two independent coordinates.

The general crystallographic convention used throughout this Supplementary Material is shown in Tab. 1. The M1 atoms occupy the fixed positions at $z = 0$, while z_1 specifies the independent z coordinate of the M2 atoms. The coordinate z_2 specifies the independent z coordinate of the pnictogen atom X, where X is As or Sb.

i	Site	x	y	z
1	M1	0	0	0
2	M1	0.5	0.5	0
3	M2	0	0.5	z_1
4	M2	0.5	0	$1 - z_1$
5	X	0.5	0	z_2
6	X	0	0.5	$1 - z_2$

Table 1: General fractional atomic coordinates used for the $P4/nmm$ structures considered in this work. M1 and M2 denote the two nonequivalent metallic sites and X denotes As or Sb.

The next tables show the results of calculations performed for different magnetic structures. For each calculation, we report the total energy, the energy difference relative to the lowest-energy magnetic structure calculated using the same method, and the magnetic moments of the metallic atoms.

The magnetic structures are calculated using a unit cell doubled along the z direction. The magnetic-moment list therefore contains eight entries corresponding to the eight atoms occupying the M1 and M2 sites in the doubled cell. These atoms are ordered first by increasing fractional z coordinate and, for atoms with the same z coordinate, by increasing fractional x coordinate. The magnetic moments of the four As or Sb atoms are not included because they are zero or very small and are not relevant for distinguishing the magnetic structures considered here.

An example of the atomic coordinates in the doubled cell is shown in Tab. 2. In this example, the indices of the metallic atoms relevant to the magnetic-moment list are $i = 1, \ldots, 8$.

i	SP	x	y	z
1	Cu	0	0	0
2	Cu	0.5	0.5	0
3	Mn	0	0.5	0.175
4	Mn	0.5	0	0.325
5	Cu	0	0	0.5
6	Cu	0.5	0.5	0.5
7	Mn	0	0.5	0.675
8	Mn	0.5	0	0.825
9	As	0.5	0	0.136
10	As	0	0.5	0.364
11	As	0.5	0	0.636
12	As	0	0.5	0.864

Table 2: Example fractional atomic coordinates for a structure doubled along the z direction. The magnetic-moment lists reported in the magnetic-structure tables contain the moments of atoms $i = 1, \ldots, 8$; the As/Sb moments are omitted.

In the Band structure and DOS subsection, we show a combined figure containing results obtained using DFT and DFT+U. Some of the DOS curves are degenerate. Such curves are plotted using the same colour, and the indices of all atoms corresponding to a given curve are indicated. The indices refer to the atomic indices i of the doubled structure, as illustrated in Tab. 2. The As/Sb contributions are not shown in the DOS figures.

For materials with two atomic configurations, both configurations are presented together. The configuration with the lower DFT energy is shown first and marked with ■ lower-energy, while the other configuration is marked with ■ higher-energy. For each atomic configuration, the energy used for this comparison is the lowest DFT total energy among all magnetic structures calculated for that configuration. No energy-status marker is shown when only one atomic configuration is available.

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CoGaAs **54**

CoGaSb **60**

CoMnAs **66**

CoMnSb **73**

CoNiAs **81**

CoNiSb **87**

Cr_2As **93**

Cr_2Sb **97**

CrCuAs **101**

CrCuSb **107**

FeCrAs **113**

CrFeSb **120**

CrGaAs **128**

GaCrSb **134**

CrMnAs **140**

CrMnSb **148**

NiCrAs **156**

CrNiSb **162**

Cu_2As **168**

FeCuAs **171**

FeCuSb **177**

CuGaAs **183**

GaCuSb **189**

CuMnAs **195**

MnCuSb **201**

NiCuAs **207**

NiCuSb **213**

Fe_2As **219**

Fe_2Sb **223**

FeGaAs **227**

FeGaSb **233**

FeMnAs **239**

FeMnSb **246**

FeNiAs **253**

FeNiSb **259**

Ga_2As **265**

Ga_2Sb **268**

GaMnAs **271**

GaMnSb **277**

NiGaAs **283**

GaNiSb **289**

Mn_2As **295**

Mn_2Sb **299**

NiMnAs **303**

NiMnSb **310**

Ni_2As **316**

Ni_2Sb **319**

Summary of lowest-energy magnetic structures

Material	Label	Material	Label	Material	Label	Material	Label
Co_2As	F1	CrCoSb	AF8″	FeCoSb	AF4	GaMnAs	AF2′
Co_2Sb	AF4	CrCuAs	AF8″	FeCrAs	AF2′	GaMnSb	AF2′
CoCrAs	AF4	CrCuSb	AF5″	FeCuAs	AF5″	GaNiSb	NM
CoCuAs	NM	CrFeSb	AF11	FeCuSb	F1″	Mn_2As	AF3
CoCuSb	NM	CrGaAs	AF8″	FeGaAs	F1″	Mn_2Sb	Fi1
CoFeAs	AF4	CrMnAs	AF5	FeGaSb	AF5″	MnCuSb	F1″
CoGaAs	F1″	CrMnSb	AF3	FeMnAs	AF3	Ni_2As	NM
CoGaSb	F1″	CrNiSb	AF8″	FeMnSb	F1	Ni_2Sb	NM
CoMnAs	AF4	Cu_2As	NM	FeNiAs	AF1″	NiCrAs	F1′
CoMnSb	AF4	Cu_2Sb	NM	FeNiSb	F1	NiCuAs	NM
CoNiAs	NM	CuGaAs	NM	Ga_2As	NM	NiCuSb	NM
CoNiSb	NM	CuMnAs	AF2′	Ga_2Sb	NM	NiGaAs	NM
Cr_2As	AF5	Fe_2As	AF4	GaCrSb	AF2′	NiMnAs	AF3′
Cr_2Sb	AF3	Fe_2Sb	AF4	GaCuSb	NM	NiMnSb	F1′

Table 3: Lowest-energy DFT calculation for each material, selected across all available atomic configurations and magnetic structures. The material name identifies the winning configuration. The Label denotes the final magnetic structure of the calculation.

Material	Label	Material	Label	Material	Label	Material	Label
Co_2As	AF10	CrGaSb	AF8″	FeCuAs	F1″	MnGaAs	AF5″
Co_2Sb	AF4	CrMnAs	AF5	FeCuSb	Fi1	MnGaSb	AF5″
CoCrAs	Fi2	Cu_2As	NM	FeGaSb	Fi1	Ni_2As	NM
CoCrSb	AF6	CuCrAs	AF2′	FeMnAs	AF3	Ni_2Sb	NM
CoCuAs	F1″	CuCrSb	Fi1	FeMnSb	Fi1	NiCoAs	AF2′
CoCuSb	F1″	CuGaAs	NM	FeNiSb	F1	NiCrAs	AF3
CoGaAs	F1″	CuMnAs	AF2′	Ga_2As	NM	NiCrSb	AF3′
CoGaSb	Fi1	CuMnSb	AF1′	Ga_2Sb	NM	NiCuAs	NM
CoMnAs	AF3	Fe_2As	Fi1	GaCuSb	NM	NiCuSb	NM
CoMnSb	AF4	Fe_2Sb	AF4	GaFeAs	AF1′	NiFeAs	AF1′
CoNiSb	AF11	FeCoAs	F1	GaNiSb	NM	NiGaAs	NM
Cr_2As	AF11	FeCoSb	F1	Mn_2As	AF3	NiMnAs	AF3
Cr_2Sb	AF5	FeCrAs	Fi2	Mn_2Sb	Fi1	NiMnSb	F1′
CrGaAs	AF8″	FeCrSb	Fi1	MnCrSb	AF3		

Table 4: Lowest-energy DFT+U calculation for each material, selected across all available atomic configurations and magnetic structures. The material name identifies the winning configuration. The Label denotes the final magnetic structure of the calculation.

Material: Co_2As

Configuration: Co_2As

Structure

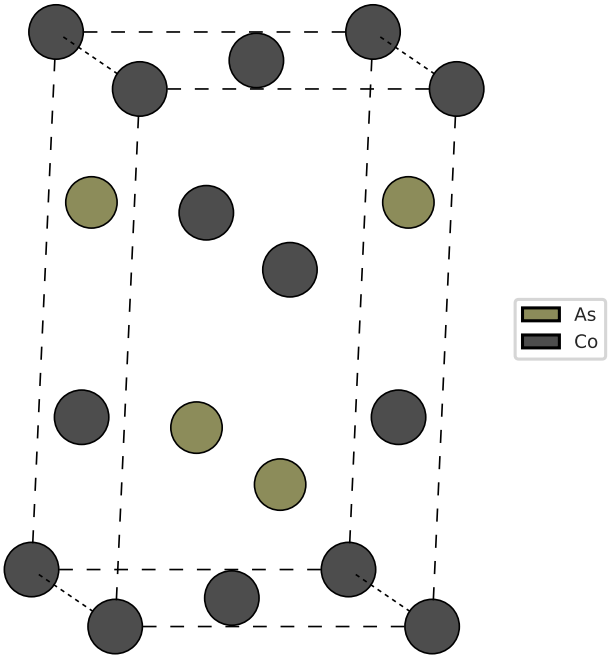


Figure 1: Structure of Co_2As

a (Å)	c (Å)	z_1	z_2
3.5688	5.8686	0.3487	0.2627

Table 5: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-43446.537932	0.000000	0.25, 0.25, 0.72, 0.72, 0.25, 0.25, 0.72, 0.72
AF4	-43446.489451	0.048480	-0.35, -0.35, -0.62, 0.62, 0.35, 0.35, 0.62, -0.62
NM	-43446.433479	0.104452	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 6: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

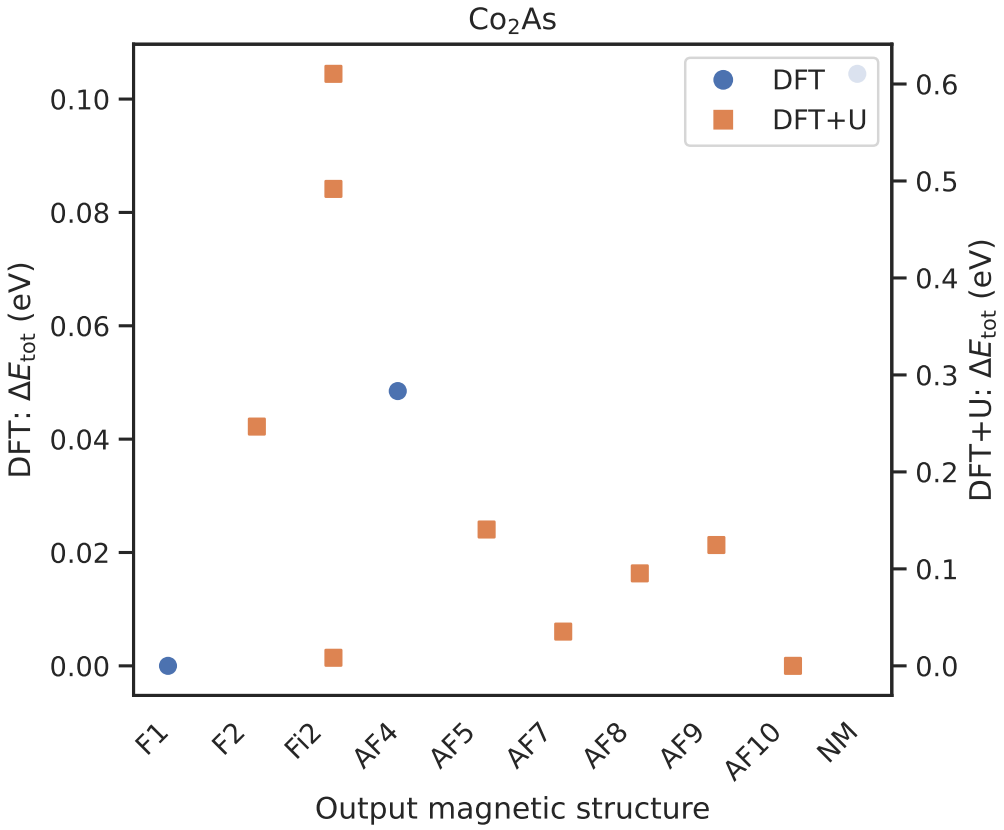


Figure 2: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF10	-43426.899236	0.000000	1.20, -1.20, 1.89, 1.89, -1.20, 1.20, -1.89, -1.89
Fi2	-43426.890900	0.008335	0.39, 0.39, -1.82, 1.75, -1.73, -1.73, 1.75, -1.82
AF7	-43426.863906	0.035330	1.17, -1.17, 1.88, 1.88, 1.17, -1.17, -1.88, -1.88
AF8	-43426.803870	0.095365	1.52, -1.52, -1.81, 1.81, -1.52, 1.52, -1.81, 1.81
AF9	-43426.774635	0.124601	1.47, -1.56, -1.78, 1.78, -1.47, 1.56, 1.78, -1.78
AF5	-43426.758638	0.140598	1.50, -1.50, -1.83, 1.83, 1.50, -1.50, -1.83, 1.83
F2	-43426.652497	0.246738	1.69, 1.69, 1.85, 1.90, 0.00, 0.00, 1.90, 1.85
Fi2	-43426.407416	0.491819	1.47, 1.43, 1.80, -1.82, -1.52, -1.64, -1.79, 1.73
Fi2	-43426.288752	0.610483	1.61, -0.39, -1.85, -1.83, 0.67, -1.51, 0.14, -1.79

Table 7: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

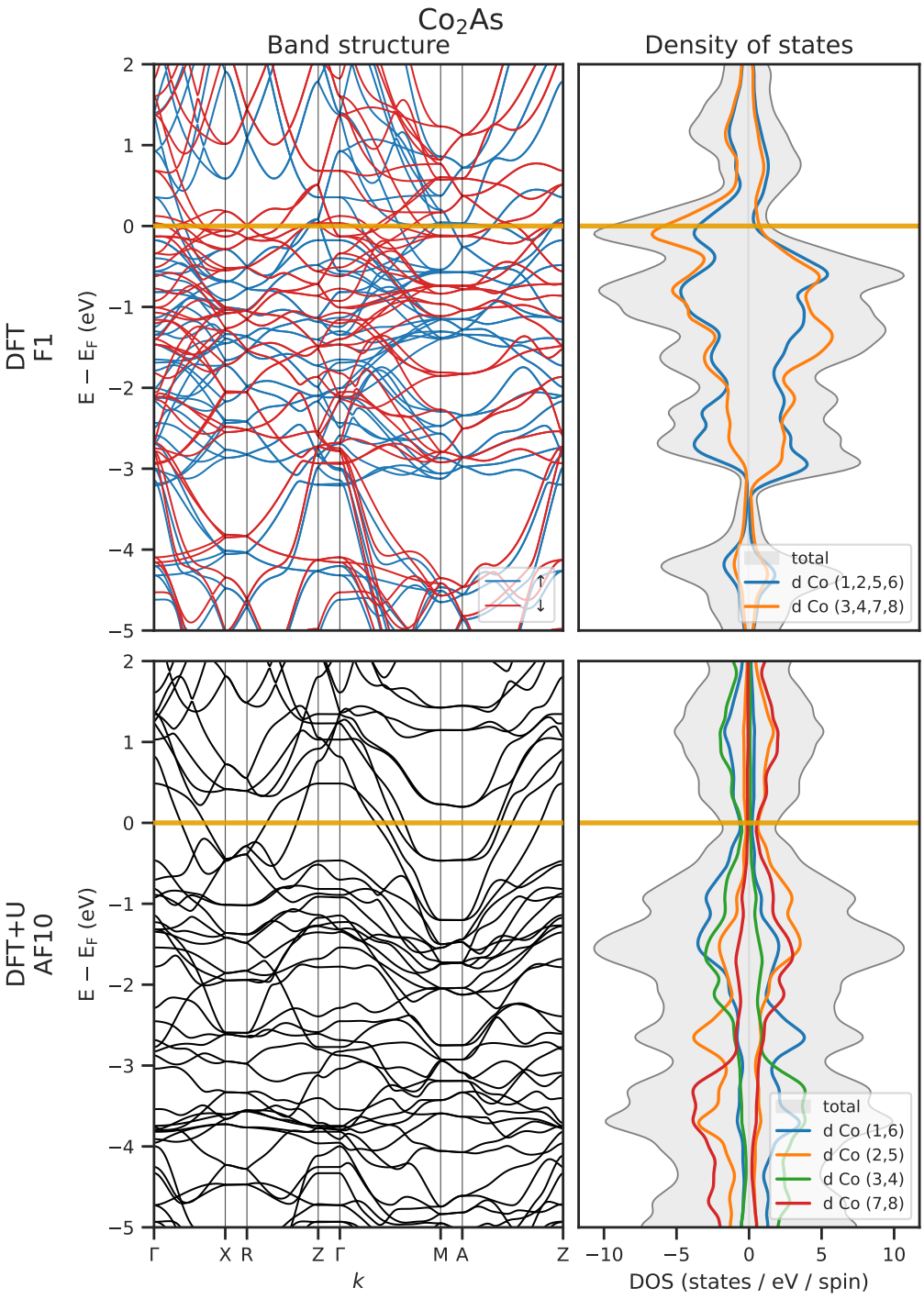


Figure 3: Band structure and Density of states of the lowest in energy calculations.

Material: Co_2Sb

Configuration: Co_2Sb

Structure

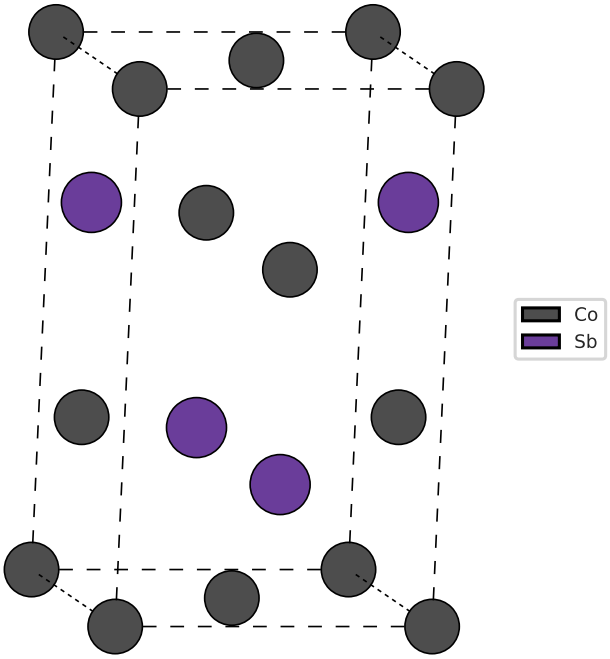


Figure 4: Structure of Co_2Sb

a (Å)	c (Å)	z_1	z_2
3.8543	6.1884	0.2460	0.3132

Table 8: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of an Sb atom in the unit cell.

Magnetic structure and energy

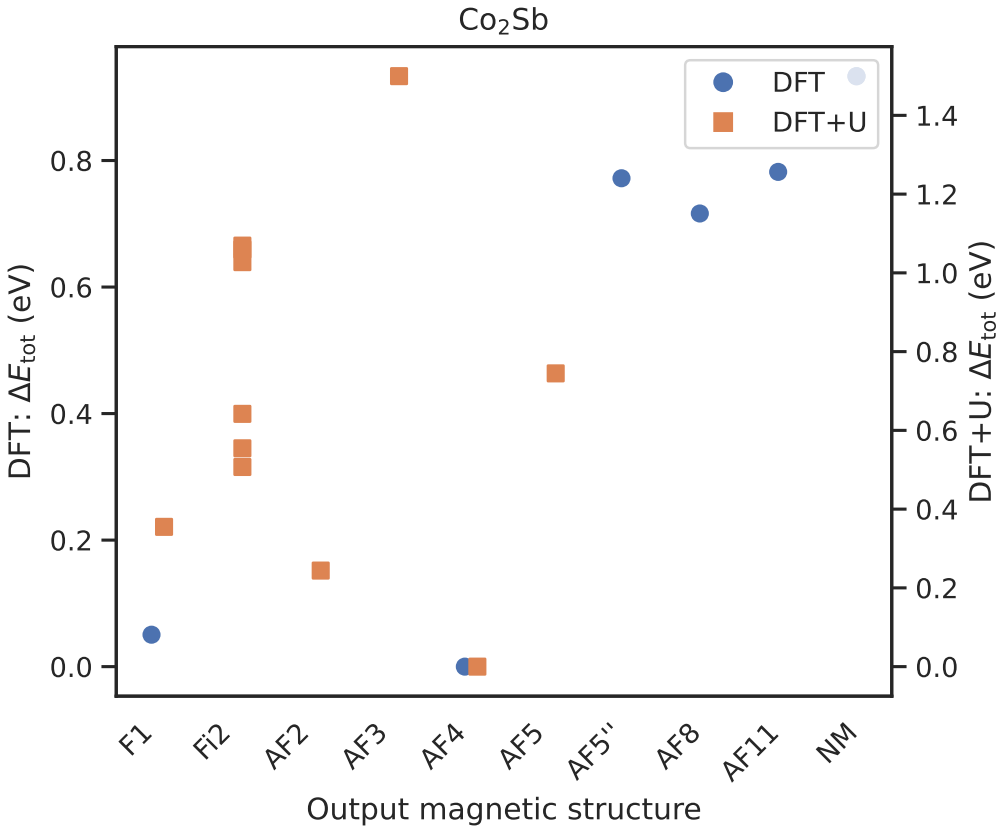


Figure 5: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-41331.835754	0.000000	-1.42, -1.42, -1.38, 1.38, 1.42, 1.42, 1.38, -1.38
F1	-41331.785284	0.050470	1.47, 1.47, 1.36, 1.36, 1.47, 1.47, 1.36, 1.36
AF8	-41331.119480	0.716274	1.18, -1.18, -0.28, 0.28, -1.18, 1.18, -0.28, 0.28
AF5″	-41331.063765	0.771989	1.13, -1.13, 0.00, 0.00, 1.13, -1.13, 0.00, 0.00
AF11	-41331.053713	0.782041	0.94, -0.94, -1.19, 1.33, 0.05, -0.05, -1.33, 1.19
NM	-41330.902586	0.933167	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-41330.902365	0.933389	0.00, 0.00, -0.00, 0.00, 0.00, 0.00, 0.00, -0.00

Table 9: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-41315.514060	0.000000	1.83, 1.86, 1.85, -1.88, -1.85, -1.85, -1.88, 1.85
AF2	-41315.270110	0.243949	1.87, 1.87, -1.95, 1.95, -1.87, -1.87, -1.83, 1.83
F1	-41315.159099	0.354960	1.87, 1.87, 1.90, 1.92, 1.86, 1.86, 1.92, 1.90
Fi2	-41315.007028	0.507032	1.92, 1.93, 1.86, 1.89, -1.87, -1.87, -1.82, -1.84
Fi2	-41314.959580	0.554480	1.86, -2.07, 1.90, 1.91, 1.85, -2.03, -1.94, -1.91
Fi2	-41314.872139	0.641921	1.87, -1.86, 2.01, 1.90, -2.07, 2.07, -1.89, -1.91
AF5	-41314.769322	0.744738	1.88, -1.86, -1.96, 1.93, 1.85, -1.96, -1.94, 1.96
Fi2	-41314.486814	1.027246	1.98, -1.61, -1.98, 1.94, -1.84, 2.06, -1.97, 1.98
Fi2	-41314.454685	1.059375	0.45, -1.98, -1.96, 1.94, -1.74, 1.98, 2.00, -1.98
Fi2	-41314.444865	1.069195	1.91, 1.87, -2.06, -1.88, 1.98, 1.99, -1.91, -2.05
AF3	-41314.014474	1.499586	1.98, 1.98, -1.91, 1.89, -1.91, -1.91, 1.89, -1.91

Table 10: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

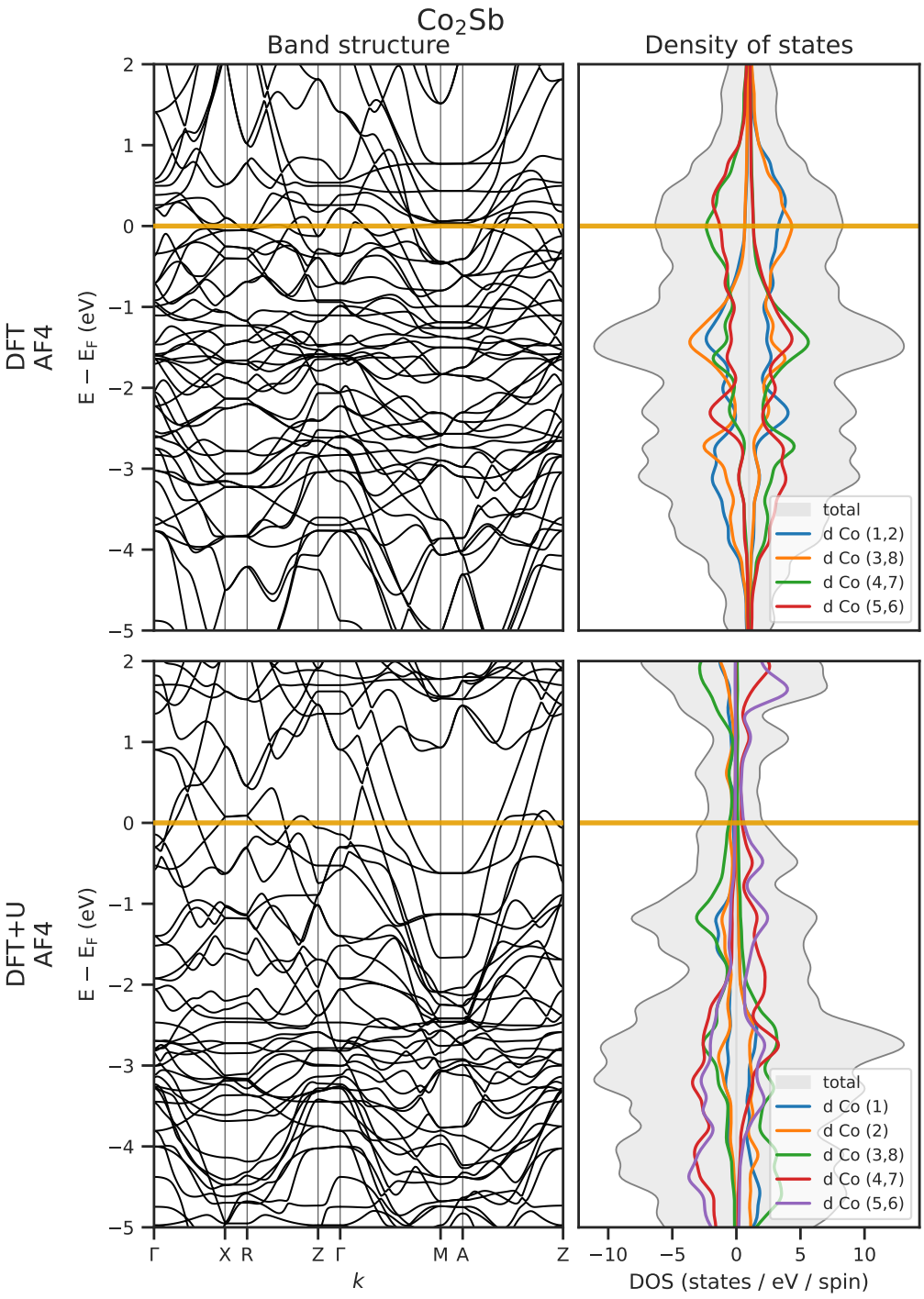


Figure 6: Band structure and Density of states of the lowest in energy calculations.

Material: CoCrAs

Configuration: CoCrAs ■ lower-energy

Structure

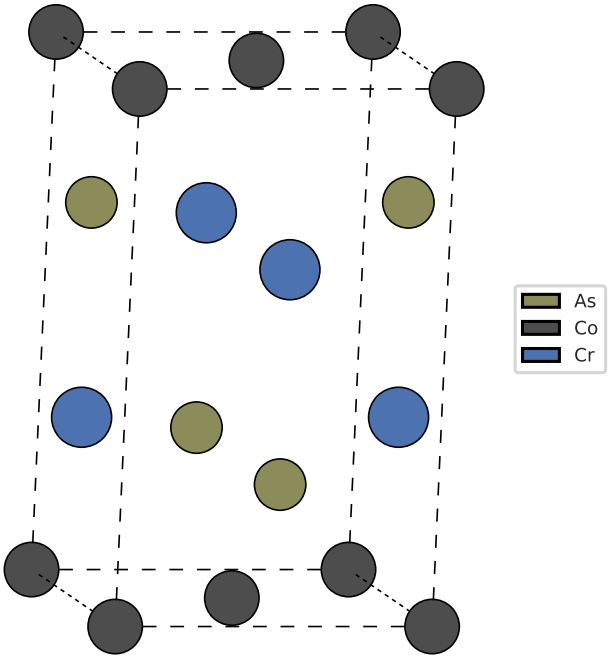


Figure 7: Structure of CoCrAs

a (Å)	c (Å)	z_1	z_2
3.7128	5.9737	0.3341	0.2531

Table 11: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-37020.687814	0.000000	-0.14, -0.14, -3.46, 3.46, 0.14, 0.14, 3.46, -3.46
AF2′	-37020.498288	0.189526	0.00, 0.00, -3.46, 3.46, 0.00, 0.00, -3.46, 3.46
AF1′	-37020.295236	0.392579	0.00, 0.00, 3.14, 3.14, 0.00, 0.00, -3.14, -3.14
Fi1	-37020.243513	0.444301	0.14, 0.14, -3.08, -3.08, 0.14, 0.14, -3.08, -3.08

Table 12: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

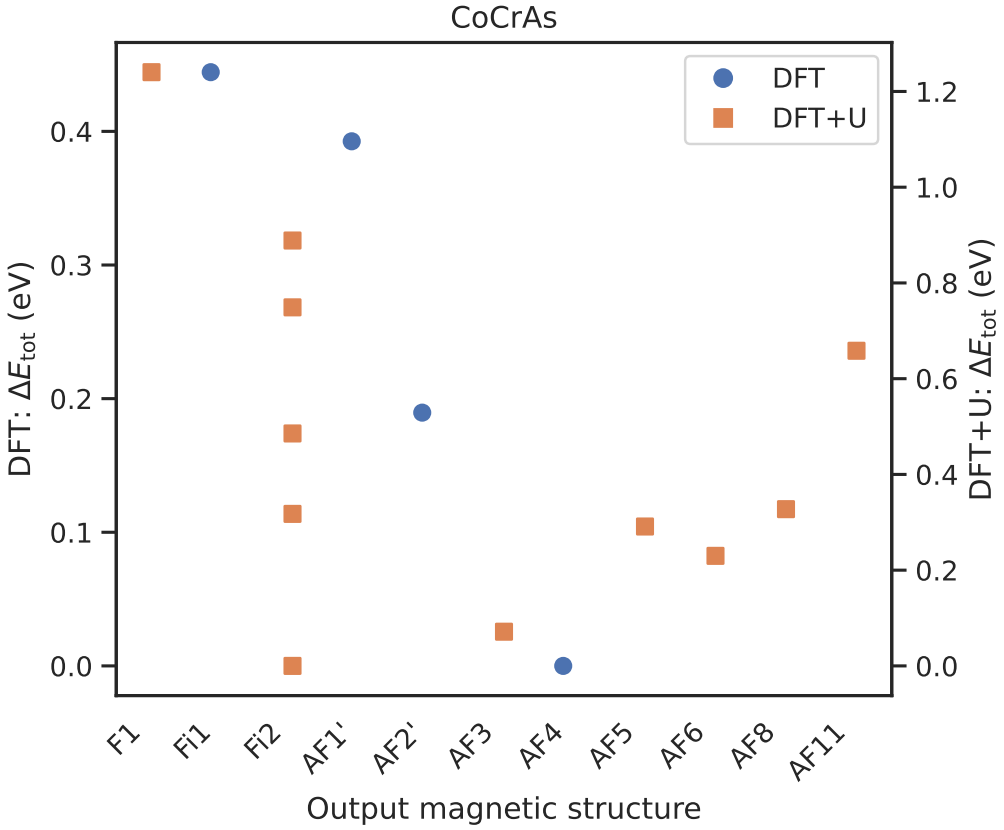


Figure 8: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
Fi2	-37003.846049	0.000000	1.55, 1.55, -4.62, 4.63, -1.49, -1.49, -4.51, 4.52
AF3	-37003.774596	0.071453	1.89, 1.89, -4.60, 4.60, -1.89, -1.89, 4.60, -4.60
AF6	-37003.616169	0.229880	1.61, -1.62, -4.56, 4.56, 1.62, -1.61, 4.56, -4.56
AF5	-37003.554854	0.291196	1.59, -1.59, -4.60, 4.60, 1.59, -1.59, -4.60, 4.60
Fi2	-37003.528495	0.317554	1.62, -1.62, -4.56, 4.55, -1.46, 1.62, 4.55, -4.56
AF8	-37003.518629	0.327420	1.61, -1.61, -4.60, 4.60, -1.60, 1.60, -4.60, 4.60
Fi2	-37003.360474	0.485575	-1.64, 1.63, -4.55, 4.53, 0.20, 0.16, 4.53, -4.57
AF11	-37003.187716	0.658334	1.63, -1.63, 4.54, 4.51, 1.75, -1.75, -4.51, -4.54
Fi2	-37003.097033	0.749016	0.29, 0.29, 4.53, -4.54, -1.59, -1.59, -4.54, 4.53
Fi2	-37002.957419	0.888630	1.66, -1.39, 4.53, 4.53, -1.59, 1.80, -4.50, -4.50
F1	-37002.605771	1.240279	0.18, 0.18, 4.46, 4.46, 0.18, 0.18, 4.46, 4.46

Table 13: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

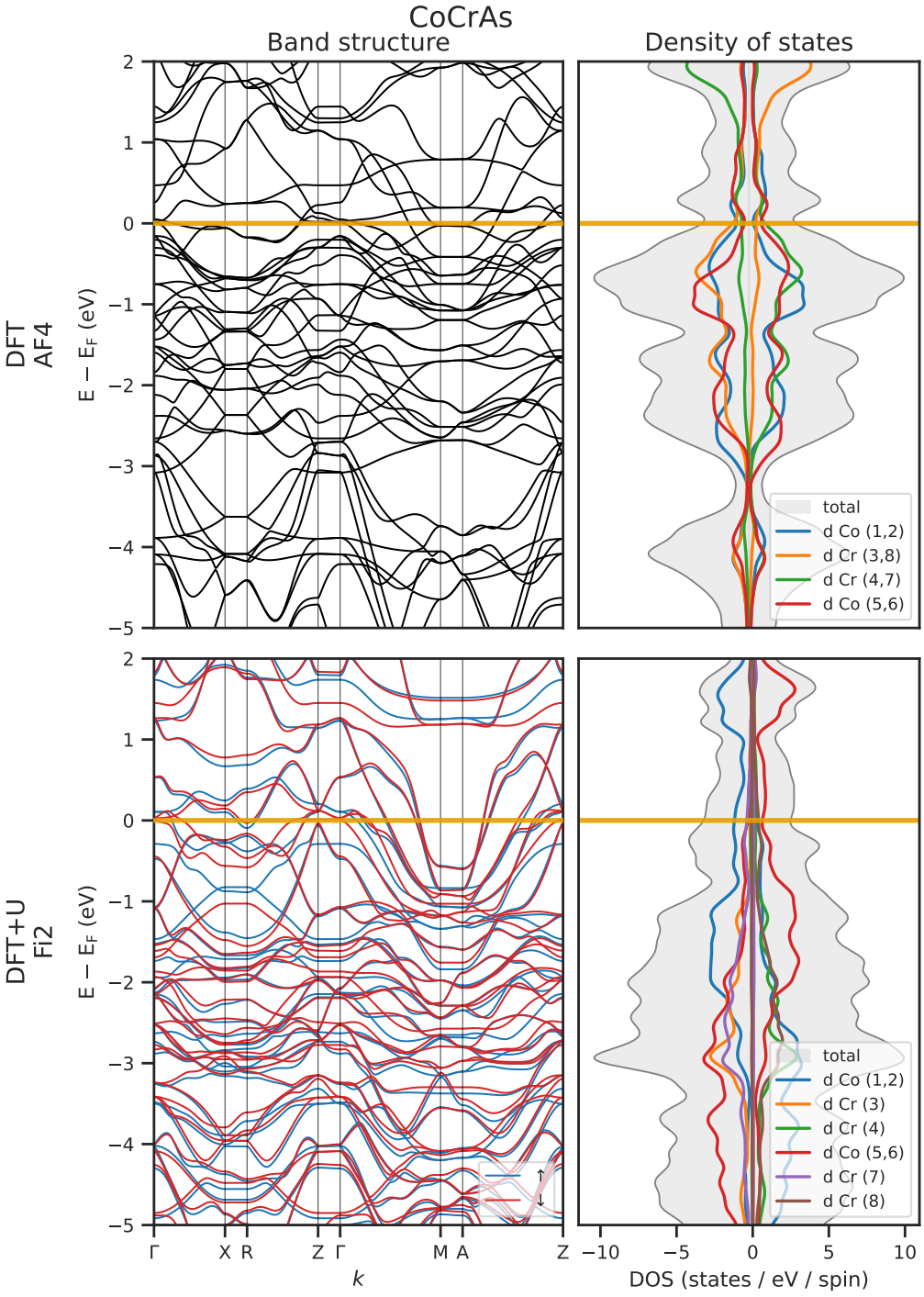


Figure 9: Band structure and Density of states of the lowest in energy calculations.

Configuration: CrCoAs ■ higher-energy

Structure

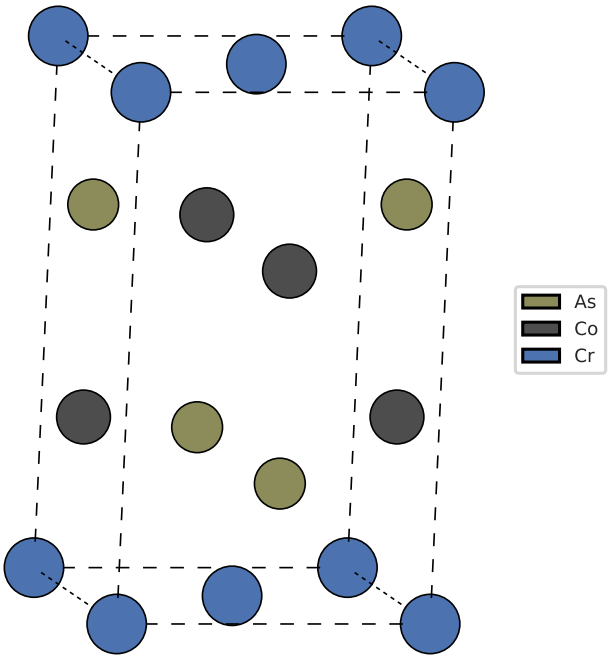


Figure 10: Structure of CrCoAs

a (Å)	c (Å)	z_1	z_2
3.6259	6.1000	0.2990	0.3001

Table 14: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-37019.926893	0.000000	2.35, -2.35, 0.00, 0.00, 2.35, -2.35, 0.00, 0.00
AF8″	-37019.866016	0.060876	2.29, -2.29, 0.00, 0.00, -2.29, 2.29, 0.00, 0.00
F1′	-37019.428625	0.498268	0.03, 0.03, -0.79, -0.79, 0.03, 0.03, -0.79, -0.79
Fi2′	-37019.399228	0.527665	-0.04, -0.04, 0.18, 0.18, -0.04, -0.04, -0.74, -0.74
NM	-37019.379105	0.547787	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 15: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

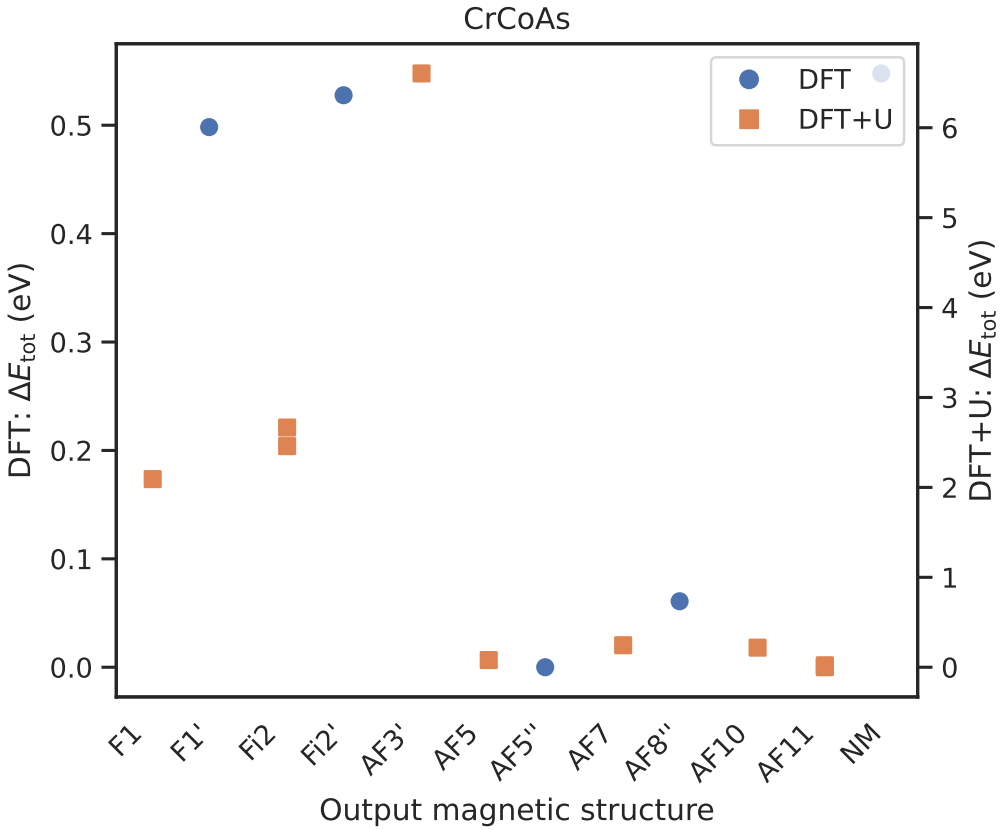


Figure 11: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF11	-37002.066573	0.000000	4.39, -4.20, -1.78, 1.78, -4.39, 4.20, 1.78, -1.78
AF11	-37002.044459	0.022114	4.40, -4.22, -1.83, 1.83, 4.22, -4.40, 1.83, -1.83
AF5	-37001.986763	0.079810	4.29, -4.29, -1.81, 1.81, 4.29, -4.29, -1.81, 1.81
AF10	-37001.848692	0.217881	4.29, -4.29, 1.77, 1.77, -4.29, 4.29, -1.77, -1.77
AF7	-37001.821920	0.244653	4.29, -4.29, 1.82, 1.82, 4.29, -4.29, -1.82, -1.82
F1	-36999.974403	2.092170	3.84, 3.84, 1.51, 1.51, 3.84, 3.84, 1.51, 1.51
Fi2	-36999.607541	2.459032	3.85, 3.86, 1.58, 0.35, -3.97, -4.00, -1.59, 1.57
Fi2	-36999.400810	2.665763	3.87, 3.86, 1.58, -1.63, -3.81, -1.42, -1.63, 1.58
AF3′	-36995.462856	6.603717	0.05, 0.09, -1.91, 1.91, -0.04, -0.09, 1.91, -1.91

Table 16: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

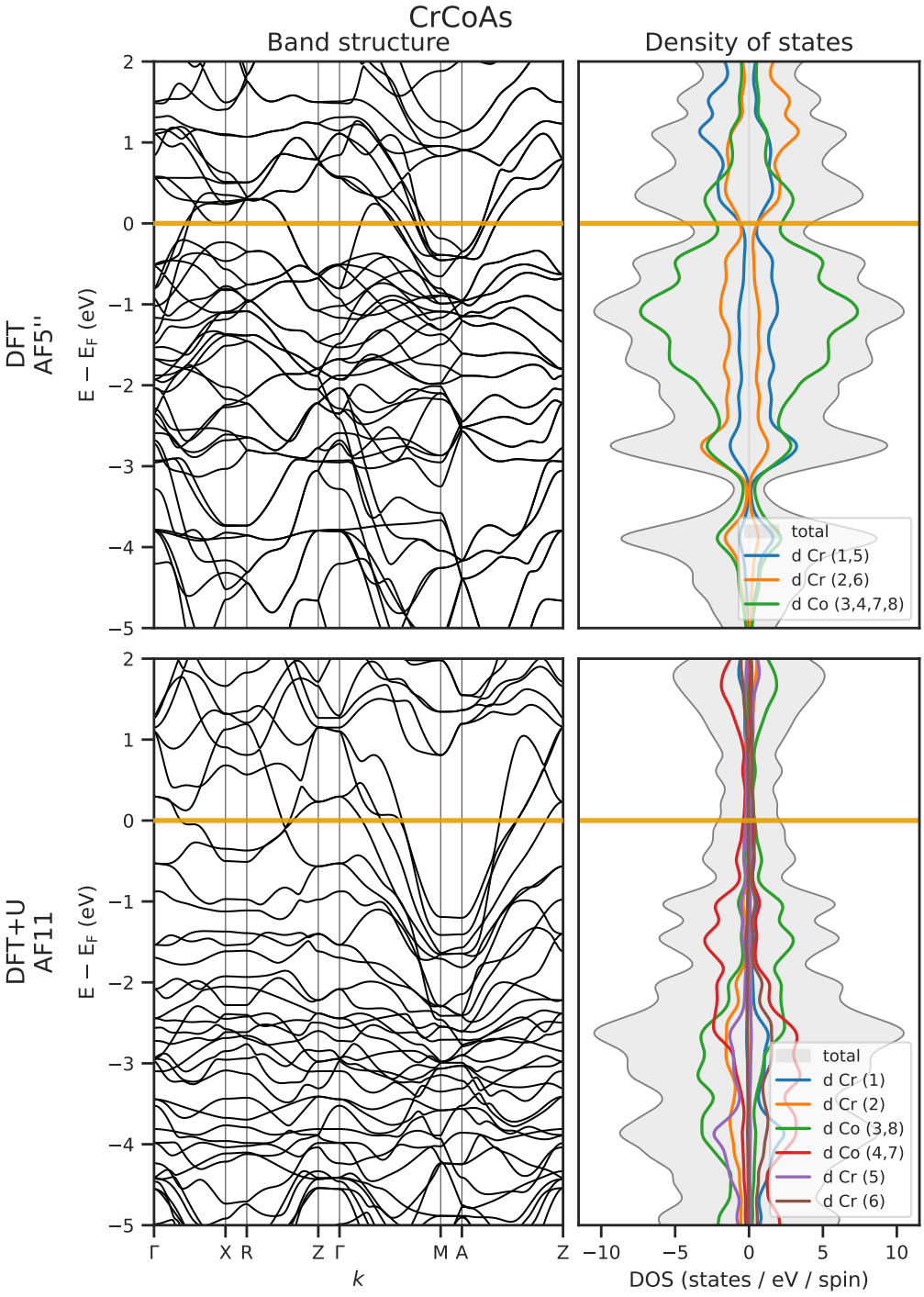


Figure 12: Band structure and Density of states of the lowest in energy calculations.

Material: CrCoSb

Configuration: CrCoSb ■ lower-energy

Structure

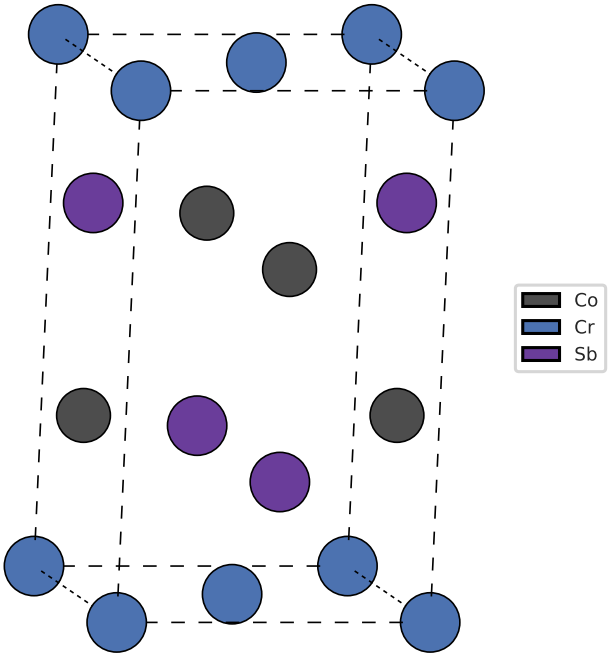


Figure 13: Structure of CrCoSb

a (Å)	c (Å)	z_1	z_2
3.7955	6.5179	0.2655	0.3248

Table 17: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

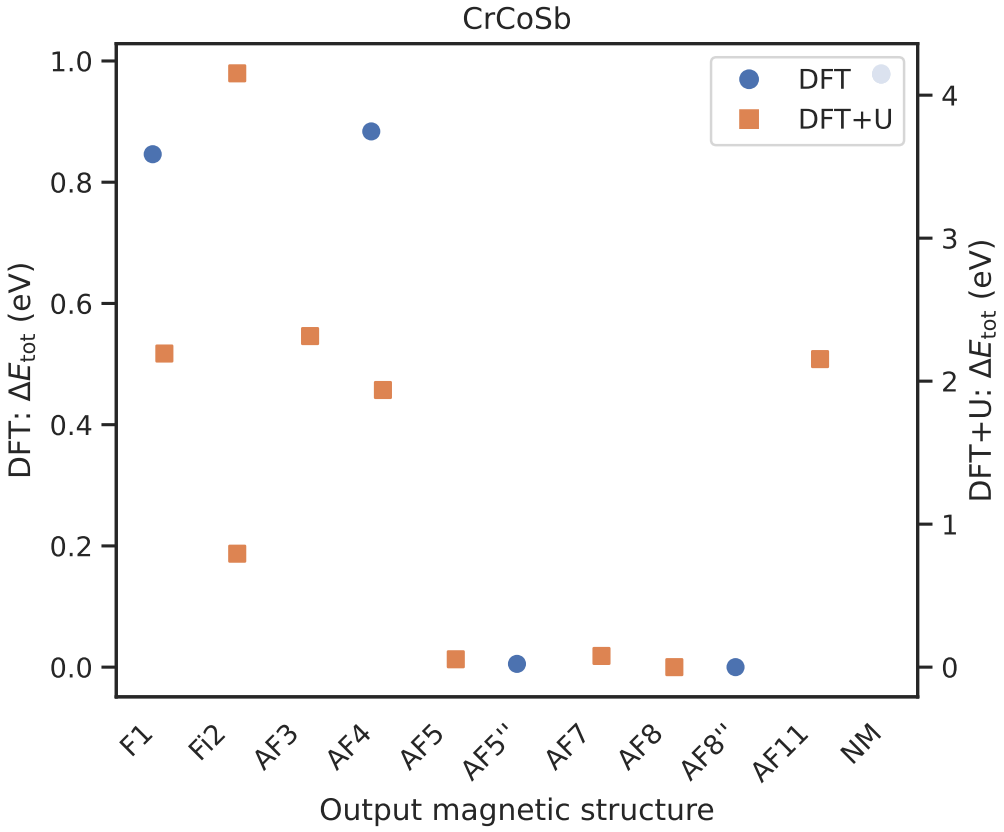


Figure 14: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-34905.193600	0.000000	-2.91, 2.91, 0.00, 0.00, 2.91, -2.91, 0.00, 0.00
AF5″	-34905.188218	0.005382	2.92, -2.92, 0.00, 0.00, 2.92, -2.92, 0.00, 0.00
F1	-34904.347426	0.846174	1.55, 1.55, 0.61, 0.61, 1.55, 1.55, 0.61, 0.61
AF4	-34904.309798	0.883802	1.44, 1.44, 0.64, -0.63, -1.43, -1.43, -0.63, 0.64
NM	-34904.215816	0.977783	0.00, 0.00, 0.00, -0.00, 0.00, 0.00, -0.00, -0.00
NM	-34904.213985	0.979614	-0.00, -0.00, 0.00, 0.00, -0.00, -0.00, 0.00, 0.00

Table 18: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8	-34889.188642	0.000000	4.55, -4.55, -1.79, 1.79, -4.55, 4.55, -1.79, 1.79
AF5	-34889.133619	0.055023	4.55, -4.55, -1.80, 1.80, 4.55, -4.55, -1.80, 1.80
AF7	-34889.110375	0.078267	4.54, -4.54, 1.77, 1.78, 4.54, -4.54, -1.78, -1.77
Fi2	-34888.395206	0.793436	4.54, -4.55, 1.75, 0.22, -4.53, 4.59, -1.79, -1.78
AF4	-34887.250533	1.938108	4.12, 4.12, 1.55, -1.55, -4.12, -4.12, -1.55, 1.55
AF11	-34887.034373	2.154268	4.22, 4.22, -2.10, 2.03, -4.19, -4.19, -1.53, 1.55
F1	-34886.995423	2.193219	4.12, 4.12, 1.53, 1.53, 4.12, 4.12, 1.53, 1.53
AF3	-34886.873354	2.315288	4.33, 4.33, -2.00, 2.07, -4.36, -4.36, 2.07, -2.00
Fi2	-34885.035924	4.152718	4.17, 1.91, 1.56, 2.03, -2.66, -4.22, -1.52, -2.07

Table 19: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

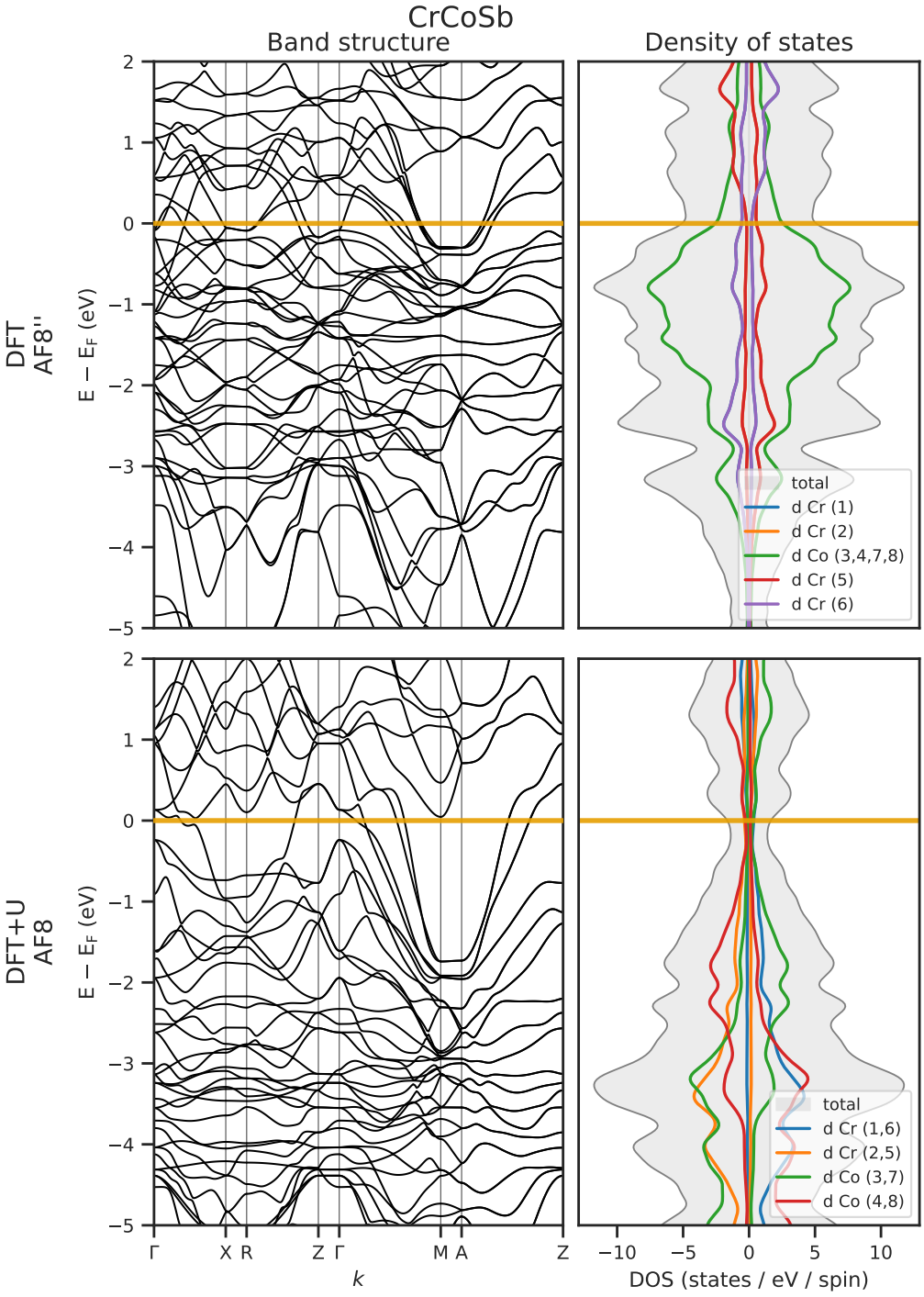


Figure 15: Band structure and Density of states of the lowest in energy calculations.

Configuration: CoCrSb ■ higher-energy

Structure

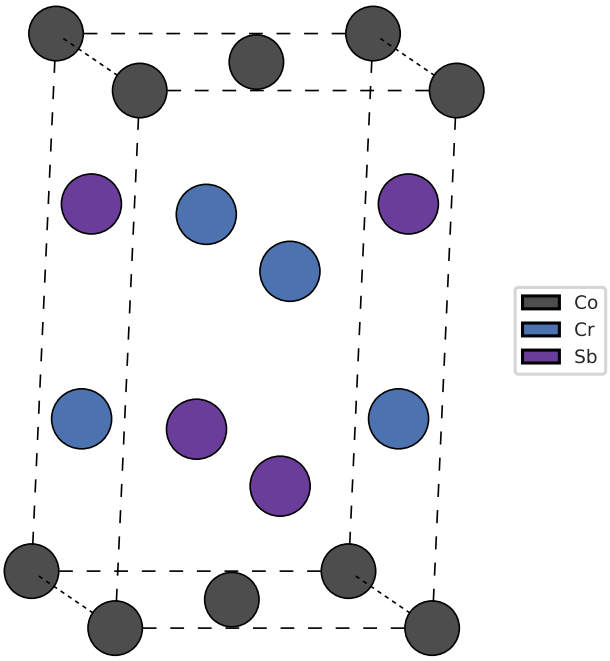


Figure 16: Structure of CoCrSb

a (Å)	c (Å)	z_1	z_2
4.0295	6.1843	0.2853	0.2679

Table 20: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

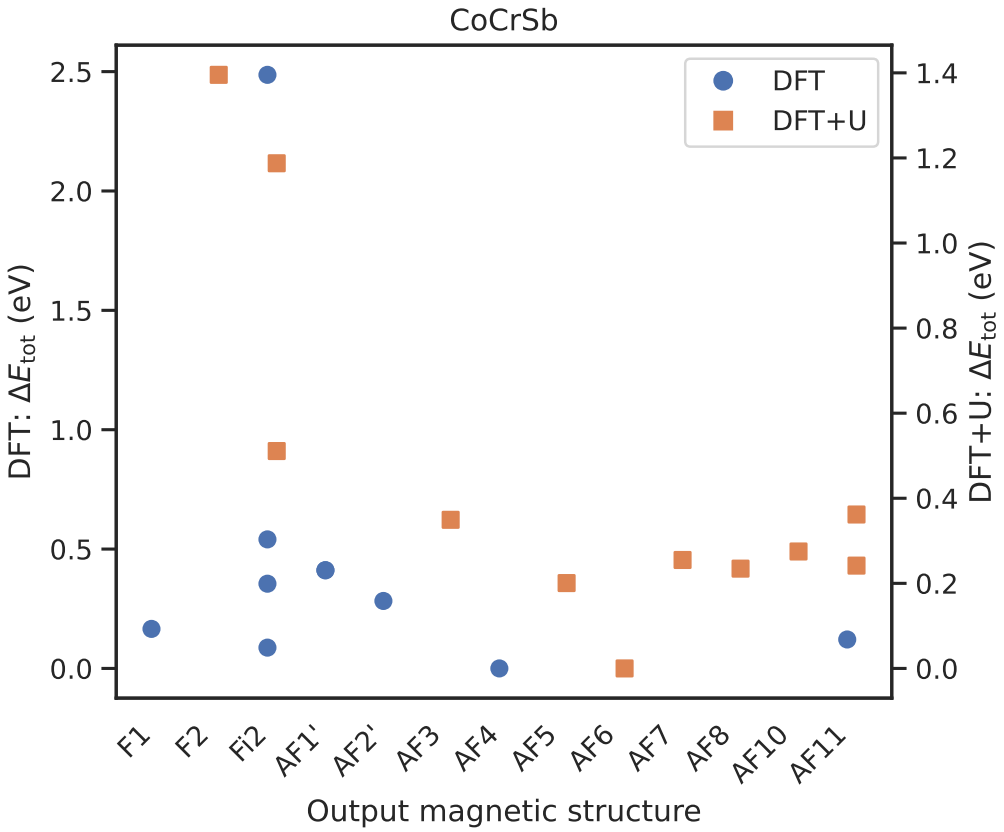


Figure 17: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-34904.595148	0.000000	-0.62, -0.62, -3.64, 3.64, 0.62, 0.62, 3.64, -3.64
Fi2	-34904.508014	0.087134	-0.61, -0.61, -3.68, -3.86, 0.72, 0.72, 3.69, -3.66
AF11	-34904.473885	0.121262	0.74, 0.74, -3.84, 3.84, -0.74, -0.74, -3.72, 3.72
F1	-34904.429533	0.165614	0.60, 0.60, 3.67, 3.67, 0.60, 0.60, 3.67, 3.67
AF2′	-34904.312535	0.282612	0.00, 0.00, -3.80, 3.80, 0.00, 0.00, -3.80, 3.80
Fi2	-34904.240240	0.354908	0.07, 0.07, 3.77, 3.79, -0.84, -0.84, -3.77, -3.88
AF1′	-34904.184050	0.411097	0.00, 0.00, 3.79, 3.79, 0.00, 0.00, -3.79, -3.79
AF1′	-34904.183711	0.411437	0.00, -0.00, 3.79, 3.79, -0.00, 0.00, -3.79, -3.79
Fi2	-34904.054591	0.540557	1.14, 1.14, -3.70, -3.73, 0.54, 0.54, -3.73, -3.70
Fi2	-34902.108629	2.486519	-0.91, -0.91, -0.08, -0.02, 0.82, 0.82, 3.71, 0.07

Table 21: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF6	-34889.764850	0.000000	1.75, -1.79, -4.65, 4.65, 1.79, -1.75, 4.65, -4.65
AF5	-34889.564215	0.200635	1.76, -1.76, -4.69, 4.69, 1.76, -1.76, -4.69, 4.69
AF8	-34889.530250	0.234600	1.75, -1.75, -4.69, 4.69, -1.75, 1.75, -4.69, 4.69
AF11	-34889.523160	0.241690	1.58, 1.58, -4.75, 4.75, -1.58, -1.58, -4.56, 4.56
AF7	-34889.509920	0.254930	1.75, -1.75, 4.71, 4.71, 1.75, -1.75, -4.71, -4.71
AF10	-34889.489955	0.274895	1.73, -1.73, 4.71, 4.71, -1.73, 1.73, -4.71, -4.71
AF3	-34889.415481	0.349369	1.97, 1.97, -4.74, 4.74, -1.97, -1.97, 4.74, -4.74
AF11	-34889.403012	0.361838	1.50, 1.50, 4.60, 4.77, -1.50, -1.50, -4.60, -4.77
Fi2	-34889.253842	0.511007	1.79, -1.73, -4.66, 4.67, -1.67, 1.79, 4.67, -4.66
Fi2	-34888.577365	1.187485	1.12, 0.35, 4.57, -4.57, -0.93, -1.09, -4.56, 4.57
F2	-34888.369509	1.395341	0.89, 0.89, 4.56, 4.57, 0.66, 0.66, 4.57, 4.58

Table 22: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

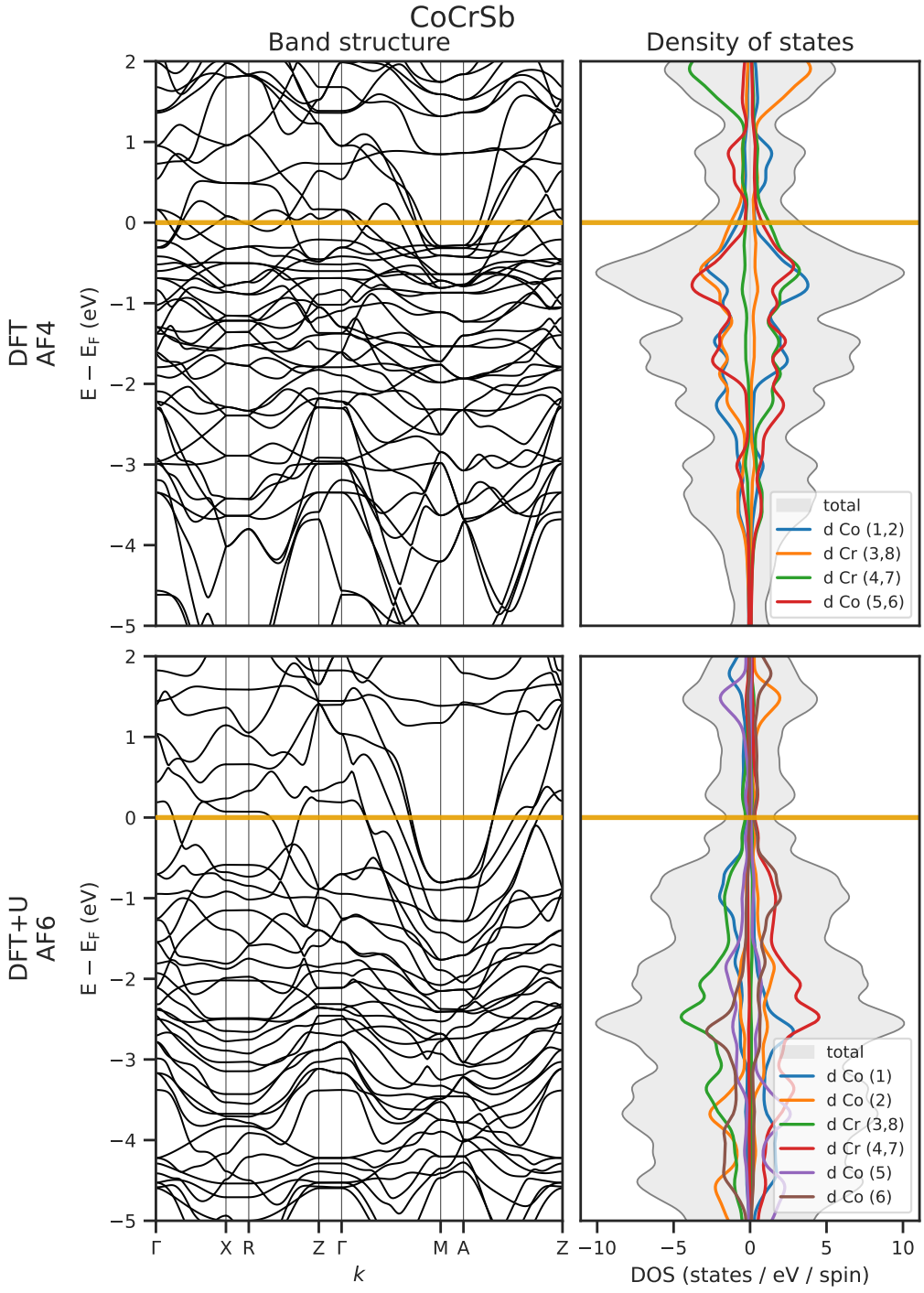


Figure 18: Band structure and Density of states of the lowest in energy calculations.

Material: CoCuAs

Configuration: CoCuAs ■ lower-energy

Structure

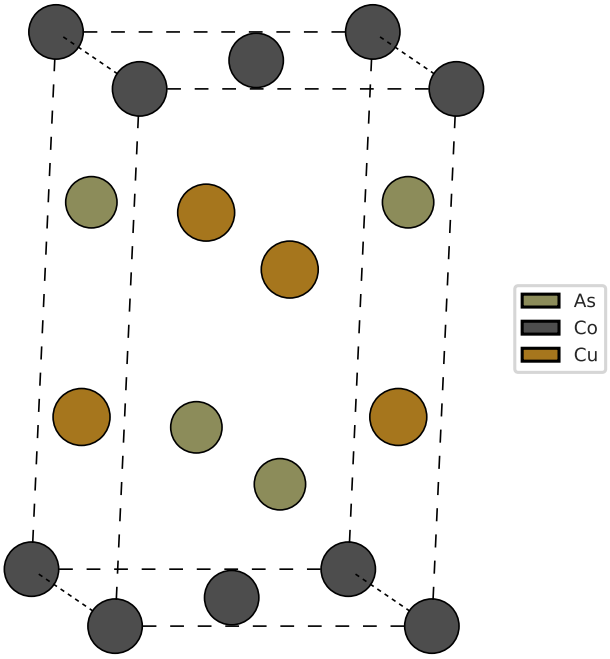


Figure 19: Structure of CoCuAs

a (Å)	c (Å)	z_1	z_2
3.7685	5.7810	0.3174	0.2575

Table 23: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-49016.312851	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 24: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

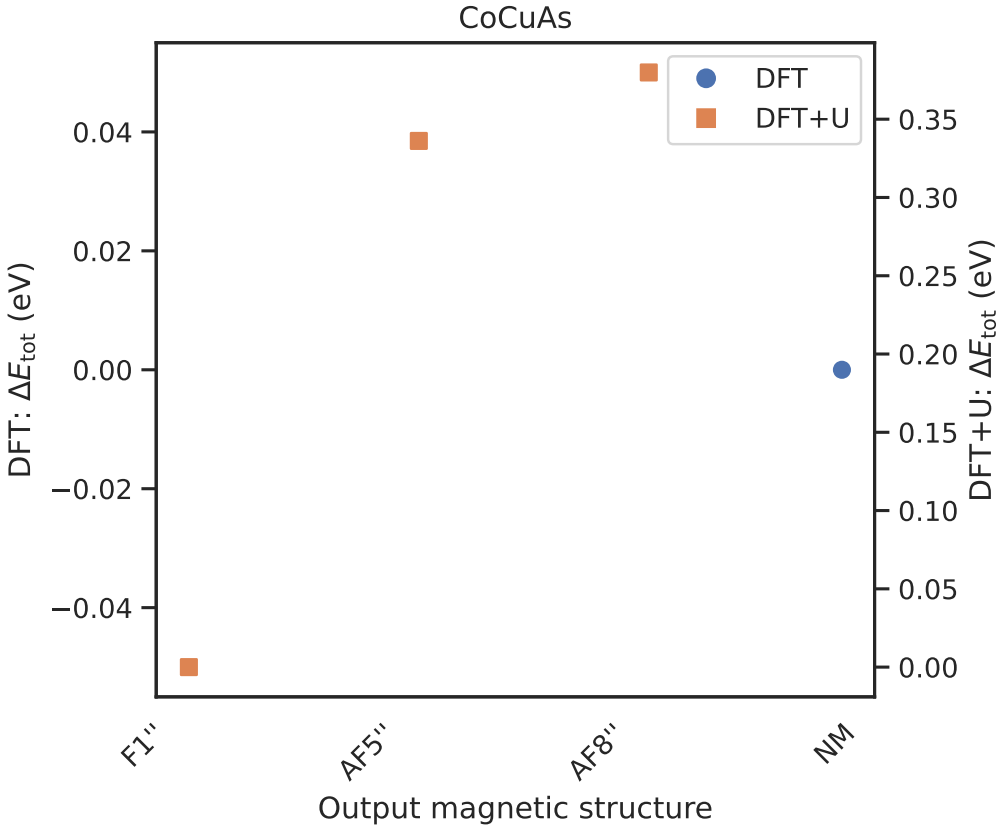


Figure 20: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-49006.455751	0.000000	1.76, 1.76, -0.05, -0.05, 1.76, 1.76, -0.05, -0.05
AF5″	-49006.119627	0.336124	1.69, -1.69, 0.00, 0.00, 1.69, -1.69, 0.00, 0.00
AF8″	-49006.075894	0.379858	1.66, -1.66, 0.00, 0.00, -1.66, 1.66, 0.00, 0.00

Table 25: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

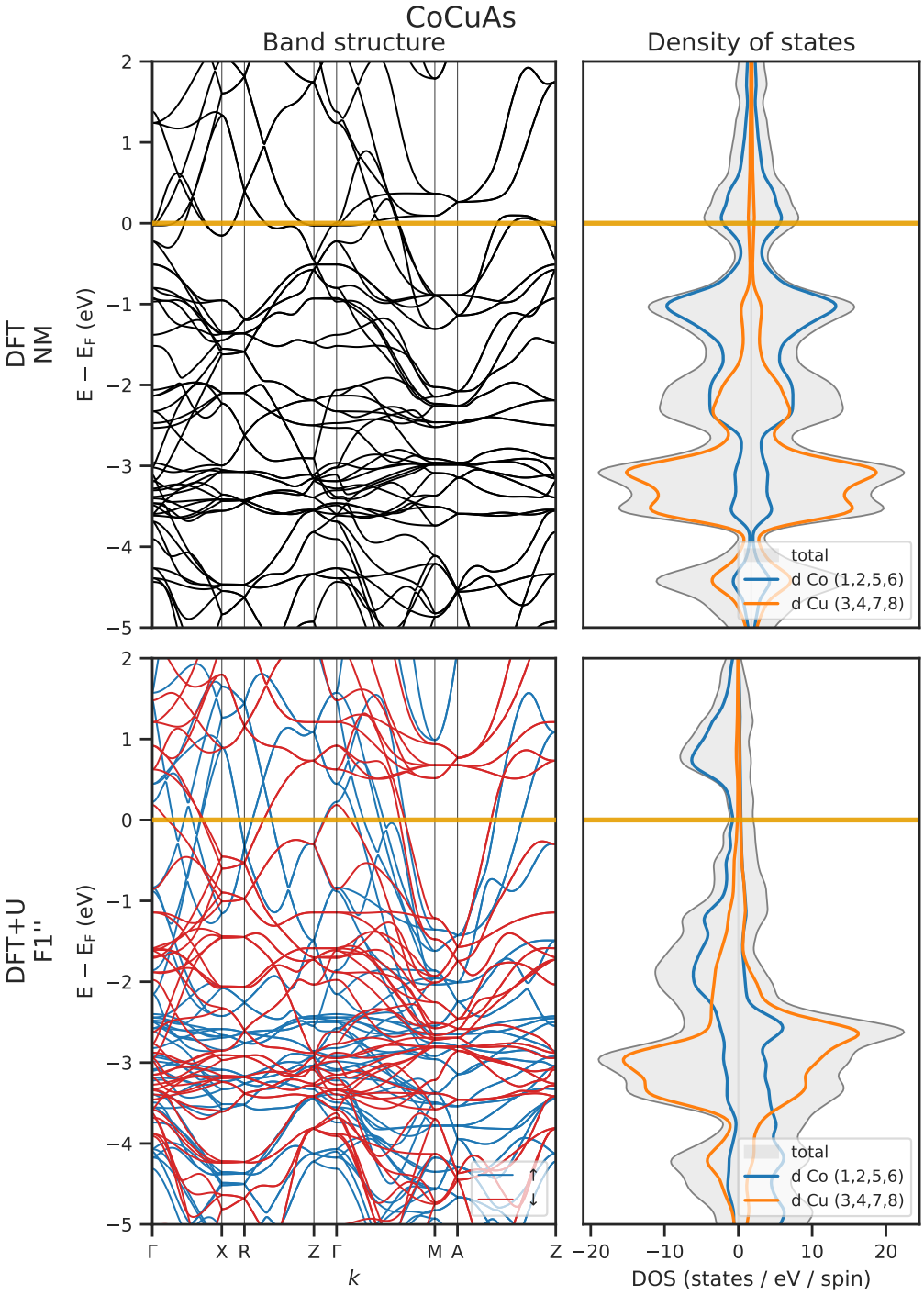


Figure 21: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuCoAs ■ higher-energy

Structure

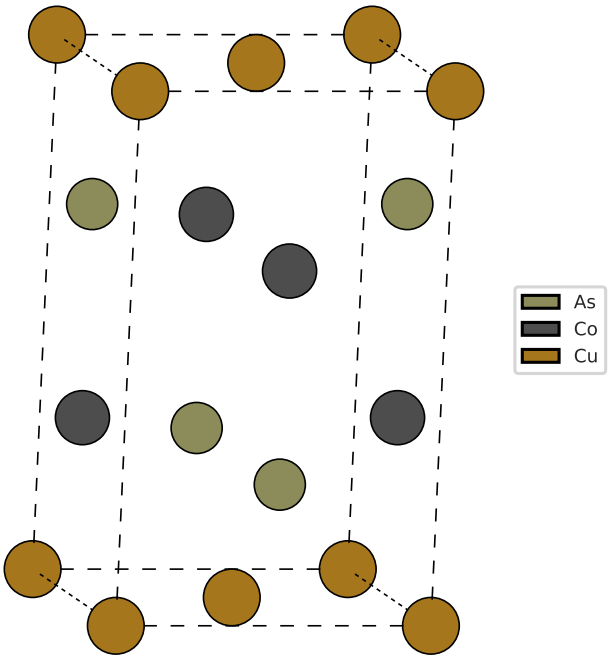


Figure 22: Structure of CuCoAs

a (Å)	c (Å)	z_1	z_2
3.5212	6.4285	0.3563	0.2858

Table 26: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-49014.380723	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 27: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

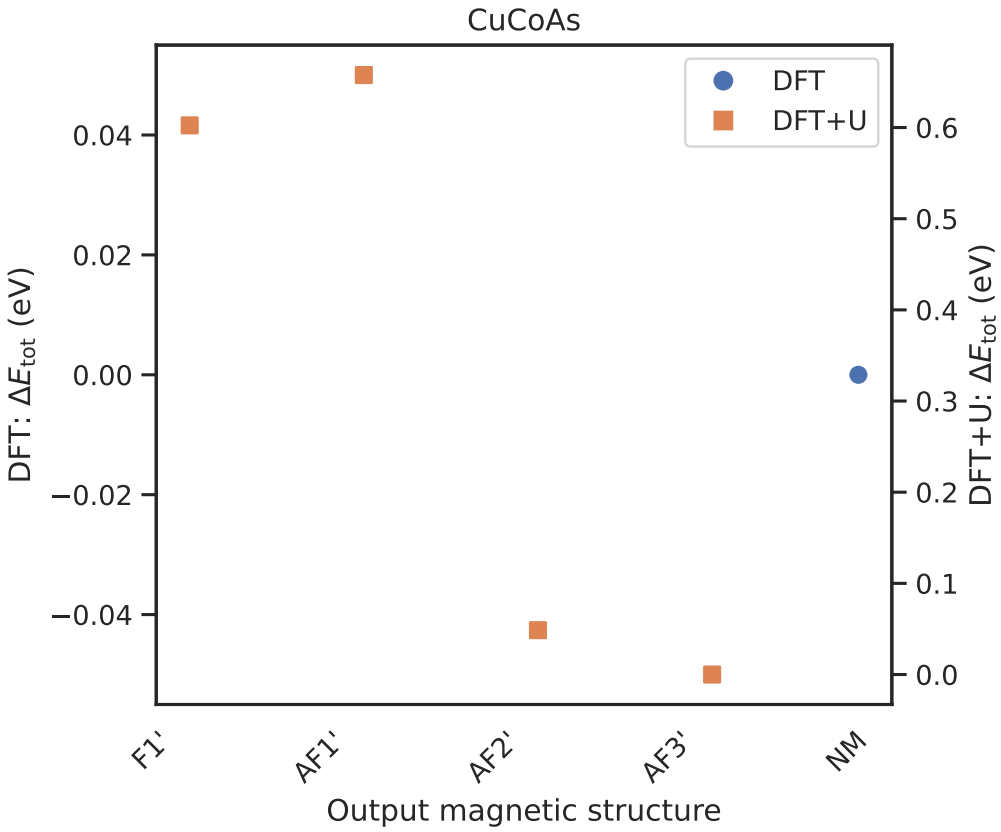


Figure 23: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-49005.713794	0.000000	0.04, 0.04, -1.71, 1.71, -0.04, -0.04, 1.71, -1.71
AF2′	-49005.665141	0.048653	0.00, 0.00, -1.70, 1.70, 0.00, 0.00, -1.70, 1.70
F1′	-49005.111393	0.602401	-0.02, -0.02, 1.82, 1.85, -0.02, -0.02, 1.85, 1.82
AF1′	-49005.056217	0.657577	0.00, 0.00, 1.85, 1.83, 0.00, 0.00, -1.83, -1.85

Table 28: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

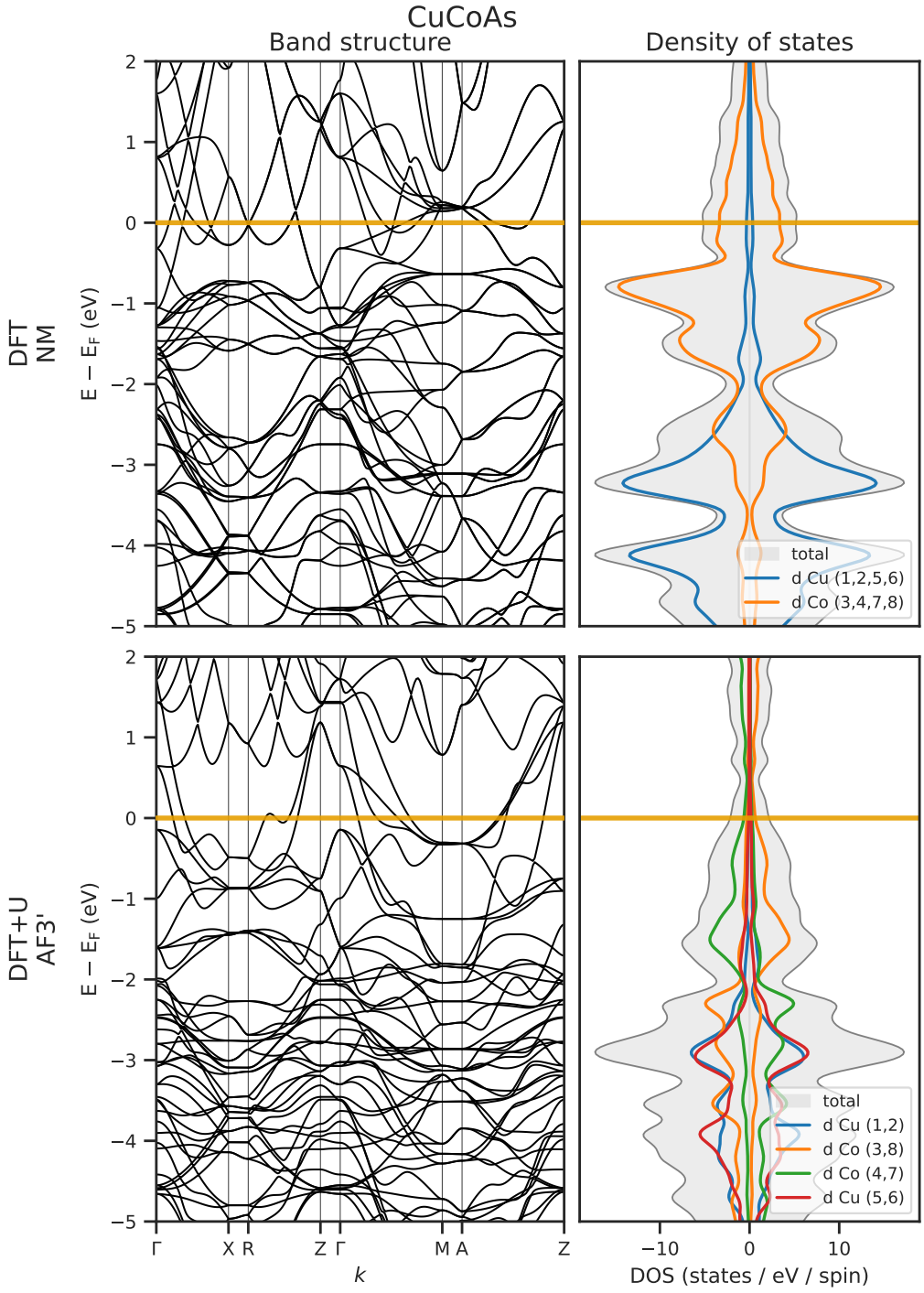


Figure 24: Band structure and Density of states of the lowest in energy calculations.

Material: CoCuSb

Configuration: CoCuSb ■ lower-energy

Structure

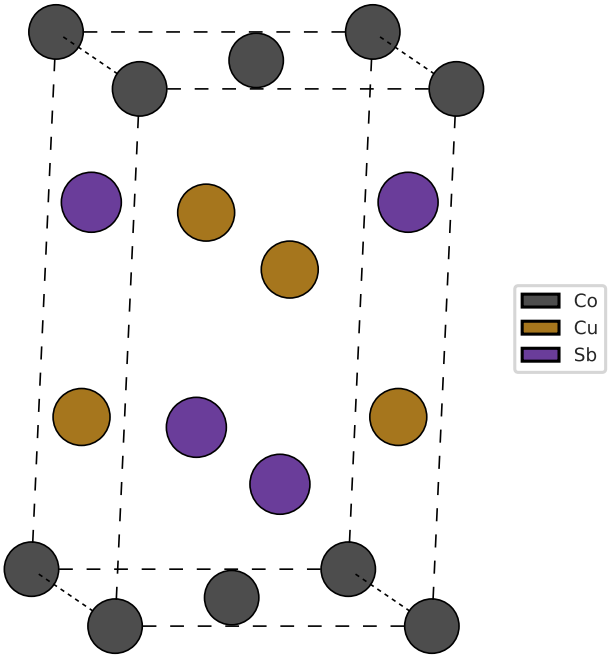


Figure 25: Structure of CoCuSb

a (Å)	c (Å)	z_1	z_2
3.9681	6.0972	0.2719	0.2801

Table 29: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-46901.977037	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-46901.976936	0.000101	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 30: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

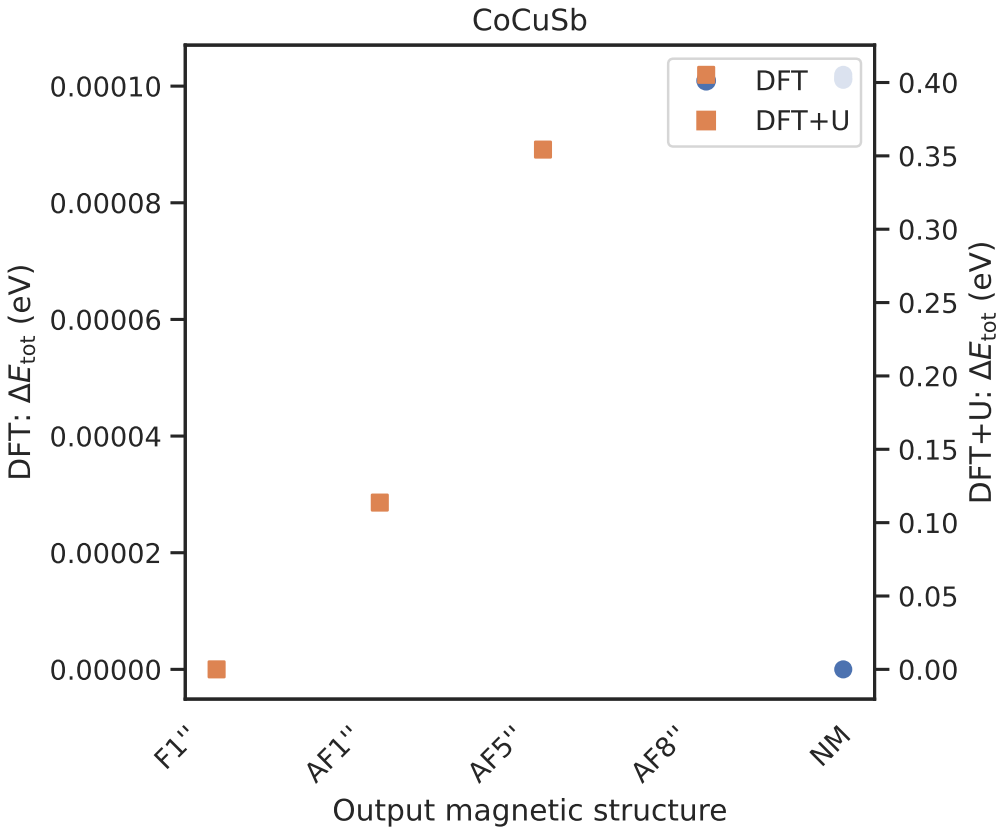


Figure 26: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-46892.982182	0.000000	1.86, 1.86, -0.08, -0.08, 1.86, 1.86, -0.08, -0.08
AF1″	-46892.868500	0.113682	1.91, 1.91, -0.05, 0.05, -1.91, -1.91, 0.05, -0.05
AF5″	-46892.627907	0.354275	1.80, -1.80, 0.00, 0.00, 1.80, -1.80, 0.00, 0.00
AF8″	-46892.576963	0.405219	1.76, -1.76, 0.00, 0.00, -1.76, 1.76, 0.00, 0.00

Table 31: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

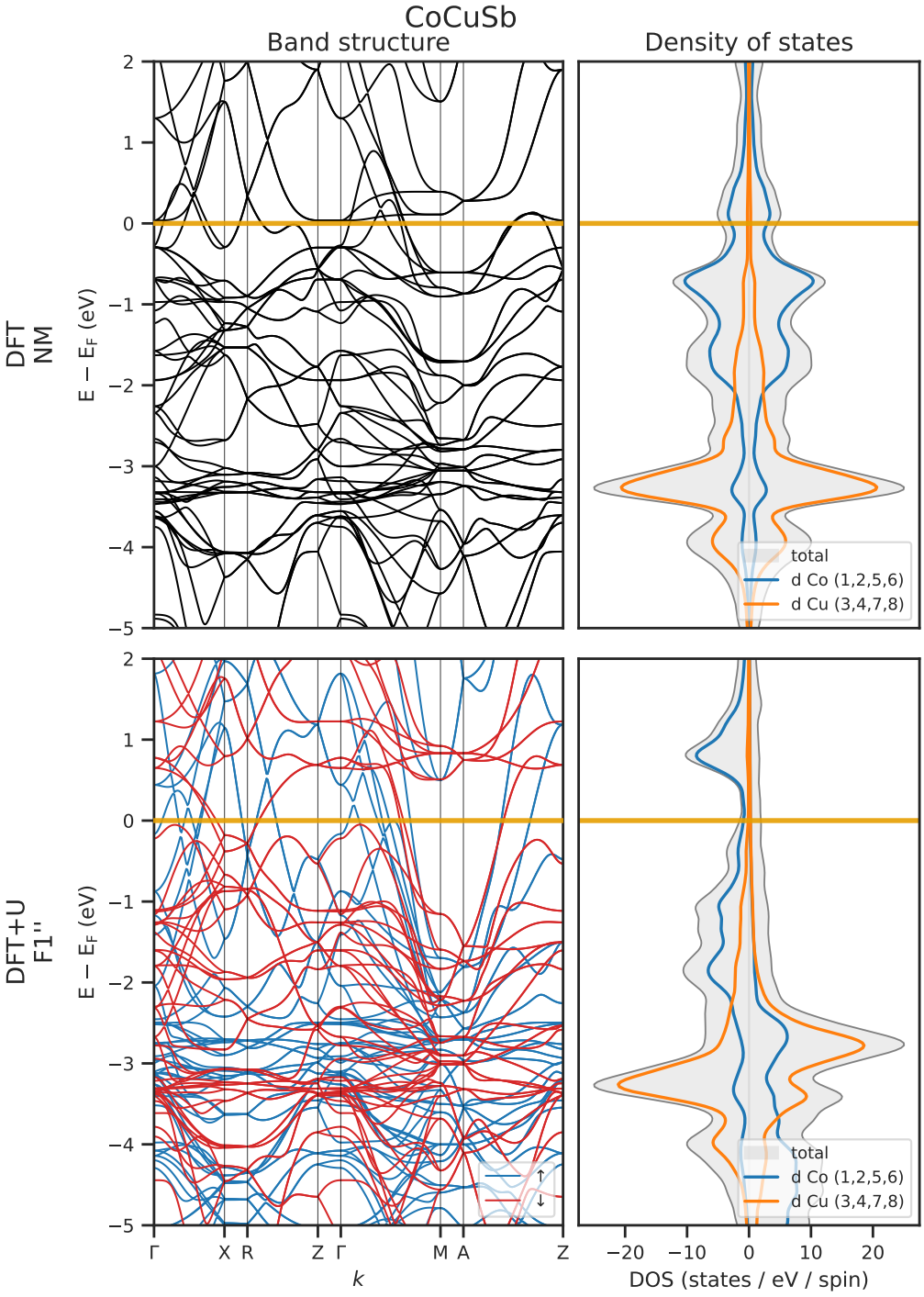


Figure 27: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuCoSb ■ higher-energy

Structure

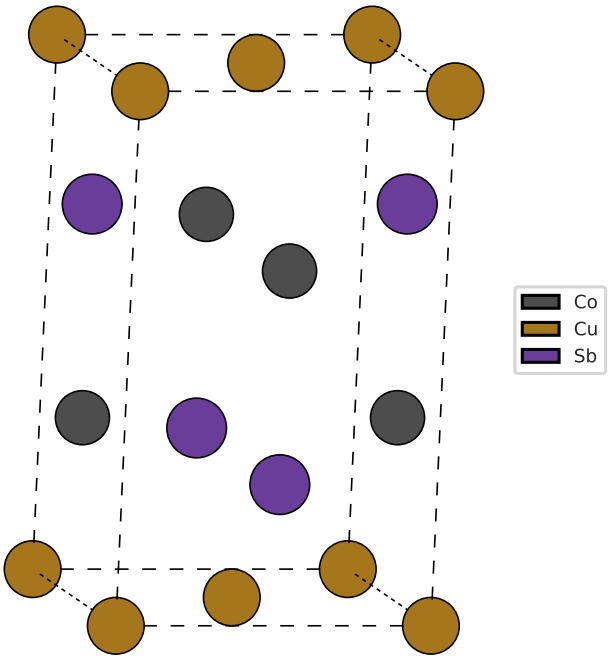


Figure 28: Structure of CuCoSb

a (Å)	c (Å)	z_1	z_2
3.7489	6.5975	0.2639	0.3323

Table 32: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-46900.466236	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 33: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

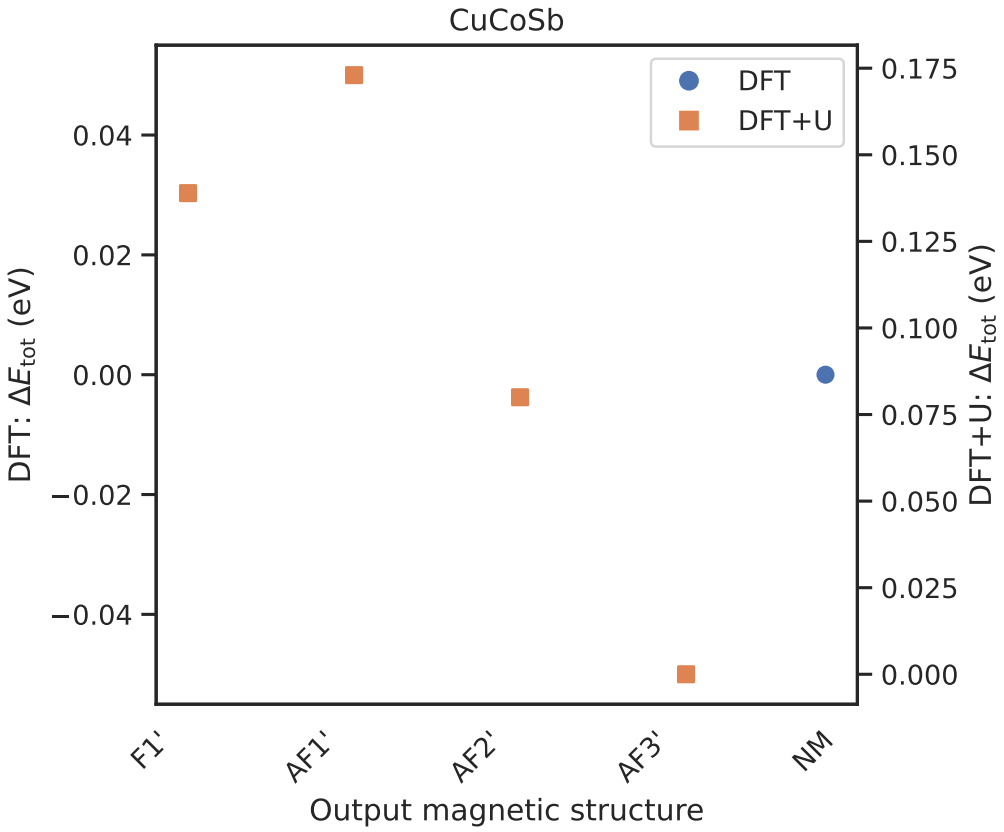


Figure 29: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-46892.883525	0.000000	0.05, 0.05, -1.77, 1.77, -0.05, -0.05, 1.77, -1.77
AF2′	-46892.803535	0.079990	0.00, 0.00, -1.80, 1.80, 0.00, 0.00, -1.80, 1.80
F1′	-46892.744597	0.138928	-0.03, -0.03, 1.75, 1.75, -0.03, -0.03, 1.75, 1.75
AF1′	-46892.710525	0.172999	0.00, 0.00, 1.74, 1.74, 0.00, 0.00, -1.74, -1.74

Table 34: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

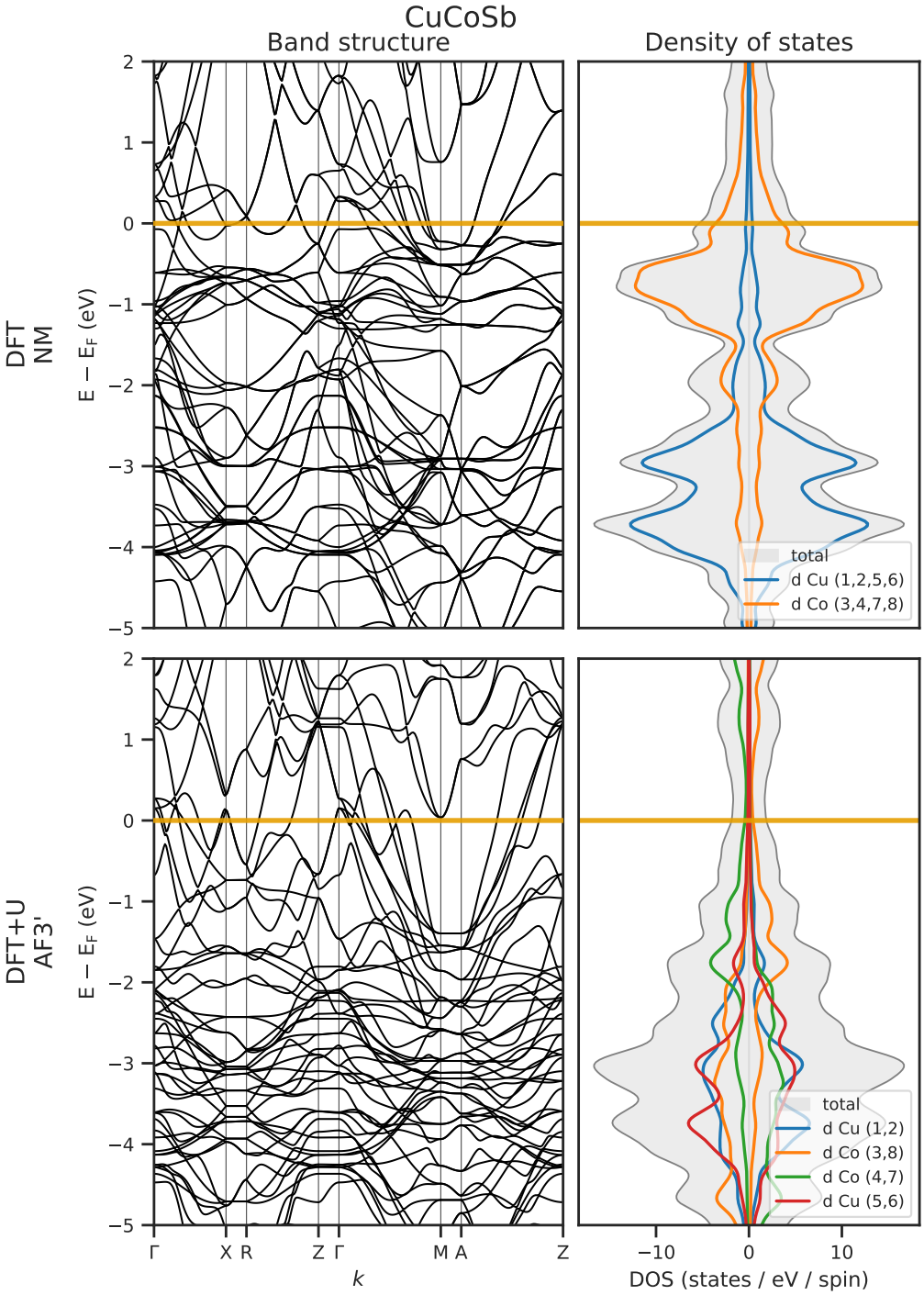


Figure 30: Band structure and Density of states of the lowest in energy calculations.

Material: CoFeAs

Configuration: CoFeAs ■ lower-energy

Structure

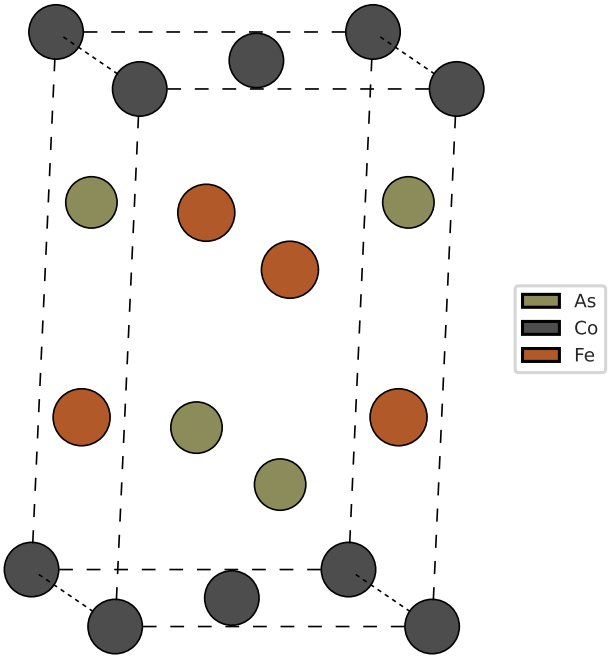


Figure 31: Structure of CoFeAs

a (Å)	c (Å)	z_1	z_2
3.6144	5.9530	0.3411	0.2563

Table 35: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-41050.913581	0.000000	0.50, 0.50, 2.53, -2.53, -0.50, -0.50, -2.53, 2.53
F1′	-41050.845460	0.068120	0.03, 0.03, 2.38, 2.38, 0.03, 0.03, 2.38, 2.38
AF1′	-41050.498696	0.414884	0.00, 0.00, 2.62, 2.62, 0.00, 0.00, -2.62, -2.62
AF2′	-41050.467323	0.446258	0.00, 0.00, -2.57, 2.57, 0.00, 0.00, -2.57, 2.57

Table 36: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

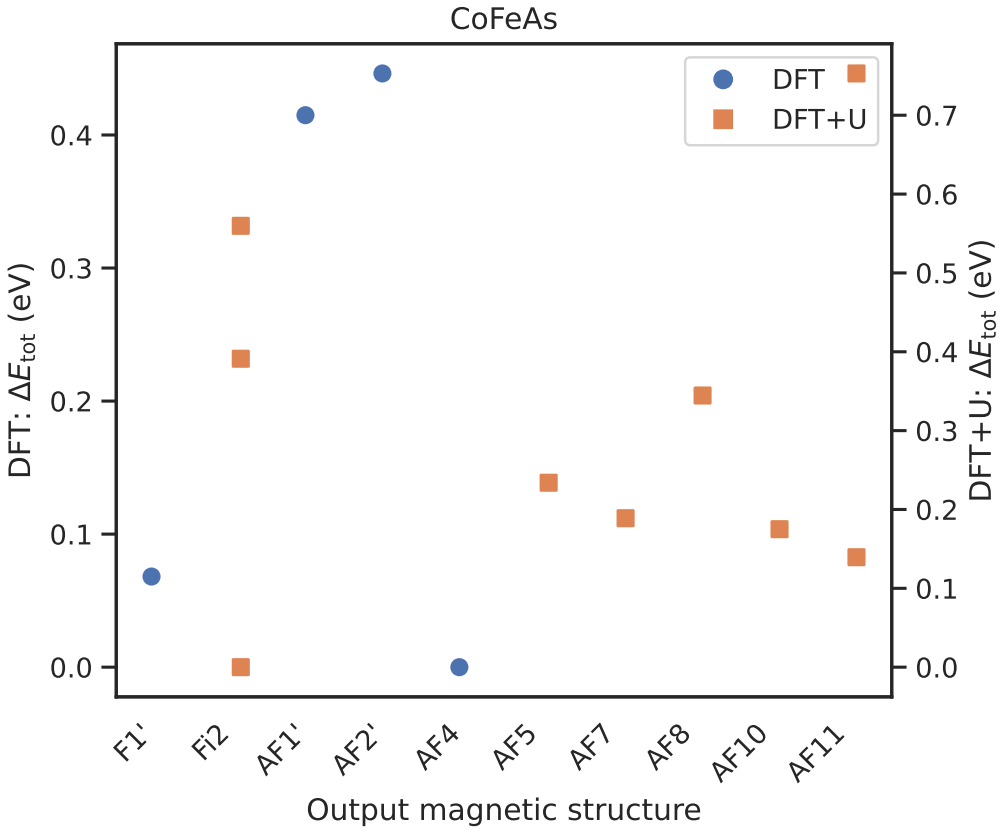


Figure 32: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi2	-41032.386951	0.000000	1.65, 1.66, -3.23, -3.21, 0.32, 0.93, -3.21, -3.23
AF11	-41032.247505	0.139446	1.07, -1.42, -3.23, 3.23, 1.42, -1.07, 3.23, -3.23
AF10	-41032.211963	0.174988	1.17, -1.17, 3.15, 3.15, -1.17, 1.17, -3.15, -3.15
AF7	-41032.198018	0.188933	1.13, -1.13, 3.16, 3.16, 1.13, -1.13, -3.16, -3.16
AF5	-41032.153038	0.233913	1.35, -1.35, -3.18, 3.18, 1.35, -1.35, -3.18, 3.18
AF8	-41032.042409	0.344542	1.42, -1.42, -3.20, 3.20, -1.41, 1.41, -3.20, 3.20
Fi2	-41031.995767	0.391184	-0.01, 1.45, 3.17, -3.20, -1.26, -0.16, -3.19, 3.08
Fi2	-41031.827191	0.559760	-0.42, -0.42, 3.21, 3.14, 0.48, 0.48, 3.14, 3.21
AF11	-41031.633964	0.752987	1.31, 1.31, -3.32, 3.32, -1.30, -1.30, -3.13, 3.13

Table 37: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

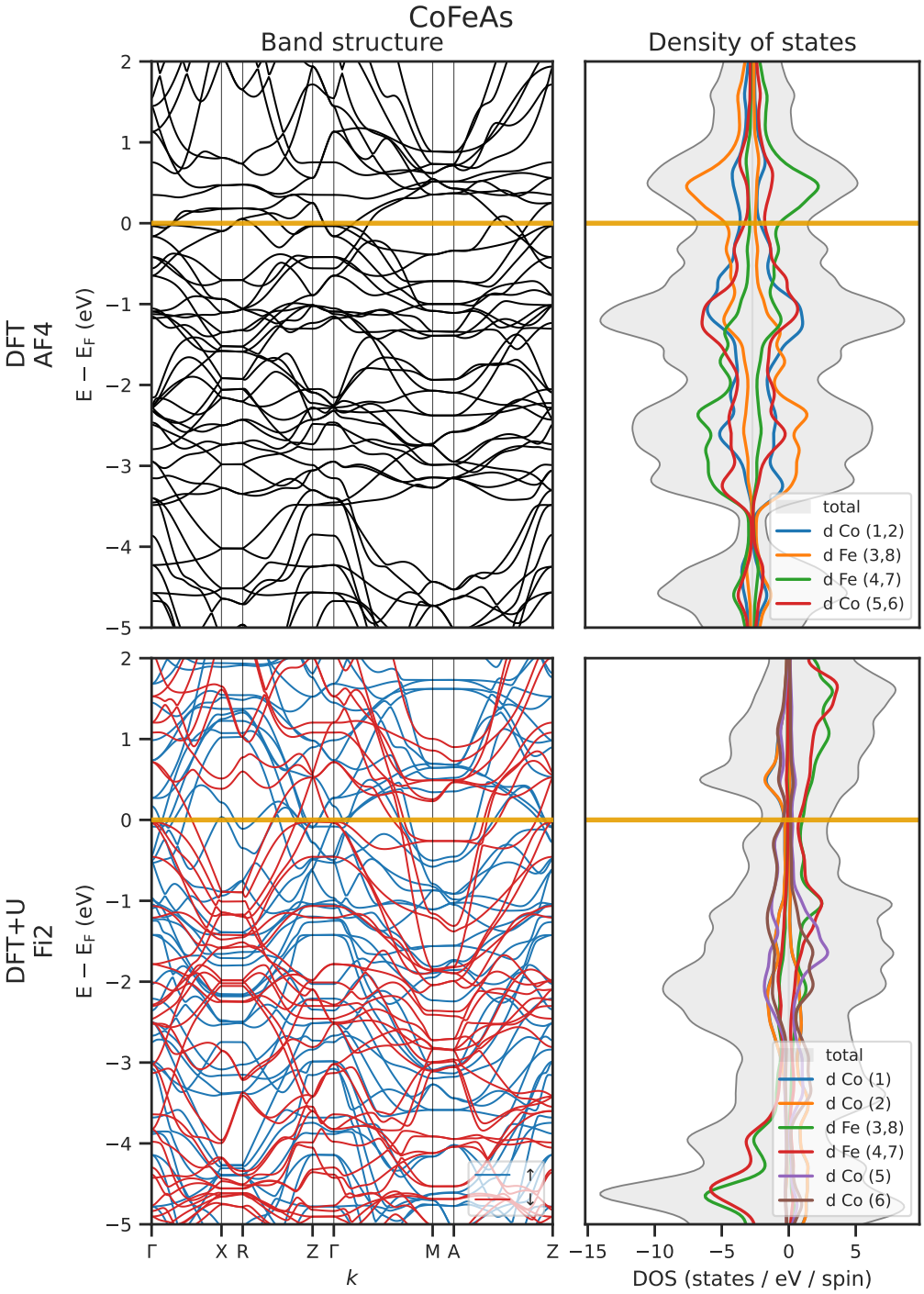


Figure 33: Band structure and Density of states of the lowest in energy calculations.

Configuration: FeCoAs ■ higher-energy

Structure

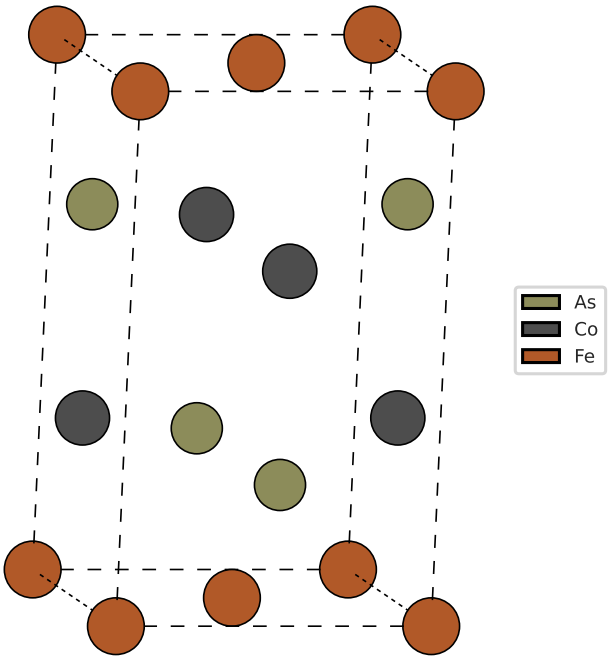


Figure 34: Structure of FeCoAs

a (Å)	c (Å)	z_1	z_2
3.5971	6.0624	0.3035	0.2980

Table 38: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

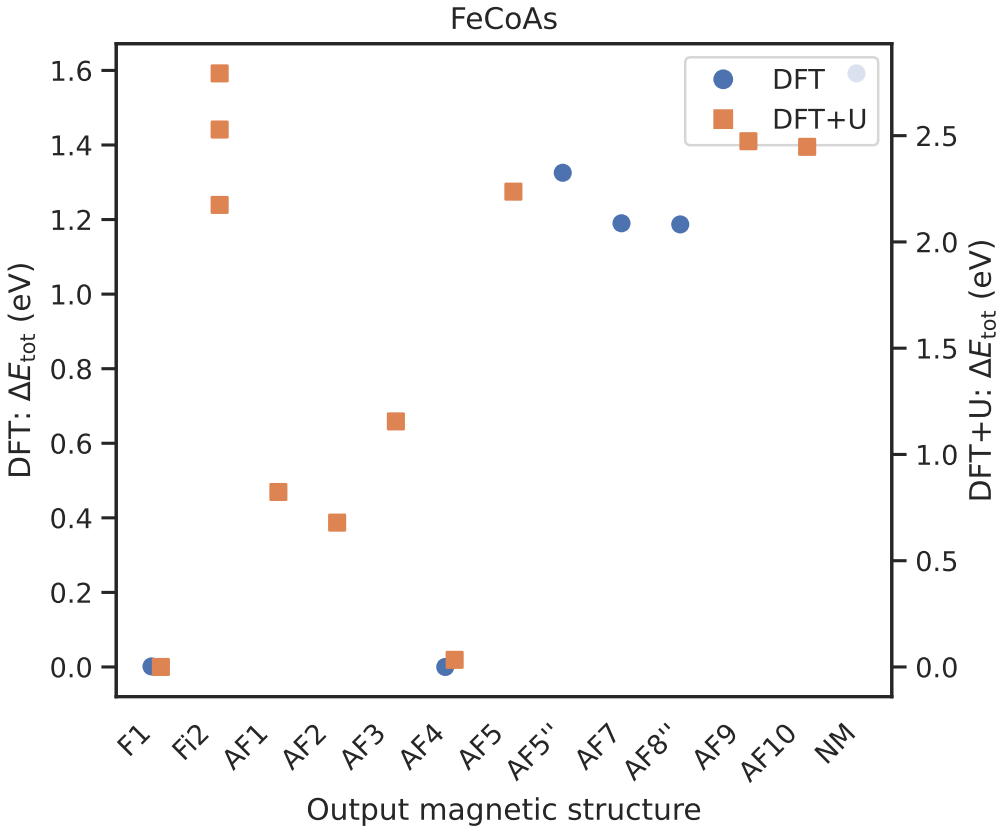


Figure 35: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-41050.462806	0.000000	2.22, 2.22, 1.08, -1.08, -2.22, -2.22, -1.09, 1.09
F1	-41050.461348	0.001458	2.29, 2.29, 1.11, 1.11, 2.29, 2.29, 1.11, 1.11
AF8″	-41049.275827	1.186978	2.09, -2.09, 0.00, 0.00, -2.10, 2.10, 0.00, 0.00
AF7	-41049.272783	1.190023	1.97, -1.97, 1.02, 1.02, 1.97, -1.97, -1.02, -1.02
AF5″	-41049.137263	1.325543	2.03, -2.03, 0.00, 0.00, 2.03, -2.03, 0.00, 0.00
NM	-41048.870741	1.592064	0.00, 0.00, 0.00, -0.00, 0.00, 0.00, 0.00, 0.00

Table 39: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-41034.647003	0.000000	3.02, 3.02, 1.75, 1.75, 3.02, 3.02, 1.75, 1.75
AF4	-41034.613496	0.033508	-3.06, -3.06, -1.79, 1.79, 3.06, 3.06, 1.79, -1.79
AF2	-41033.967757	0.679246	3.06, 3.06, -1.79, 1.79, -3.06, -3.06, -1.78, 1.78
AF1	-41033.823631	0.823372	3.06, 3.06, 1.77, 1.76, -3.06, -3.06, -1.77, -1.76
AF3	-41033.491518	1.155485	3.03, 3.03, -1.77, 1.77, -3.03, -3.03, 1.77, -1.77
Fi2	-41032.472876	2.174127	3.24, -3.08, -1.80, 1.80, 3.11, -3.12, 1.80, -1.80
AF5	-41032.410352	2.236651	3.19, -3.19, -1.80, 1.79, 3.17, -3.17, -1.79, 1.80
AF10	-41032.199614	2.447389	3.20, -3.20, 1.80, 1.80, -3.20, 3.20, -1.80, -1.80
AF9	-41032.173176	2.473827	3.06, -3.04, -1.85, 1.84, -3.10, 3.04, 1.84, -1.85
Fi2	-41032.118180	2.528823	3.00, 3.00, -1.77, -1.79, 2.97, 2.97, -2.18, -2.07
Fi2	-41031.853961	2.793042	3.03, -3.24, 1.72, 1.90, 3.17, -3.10, -1.89, -1.95

Table 40: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

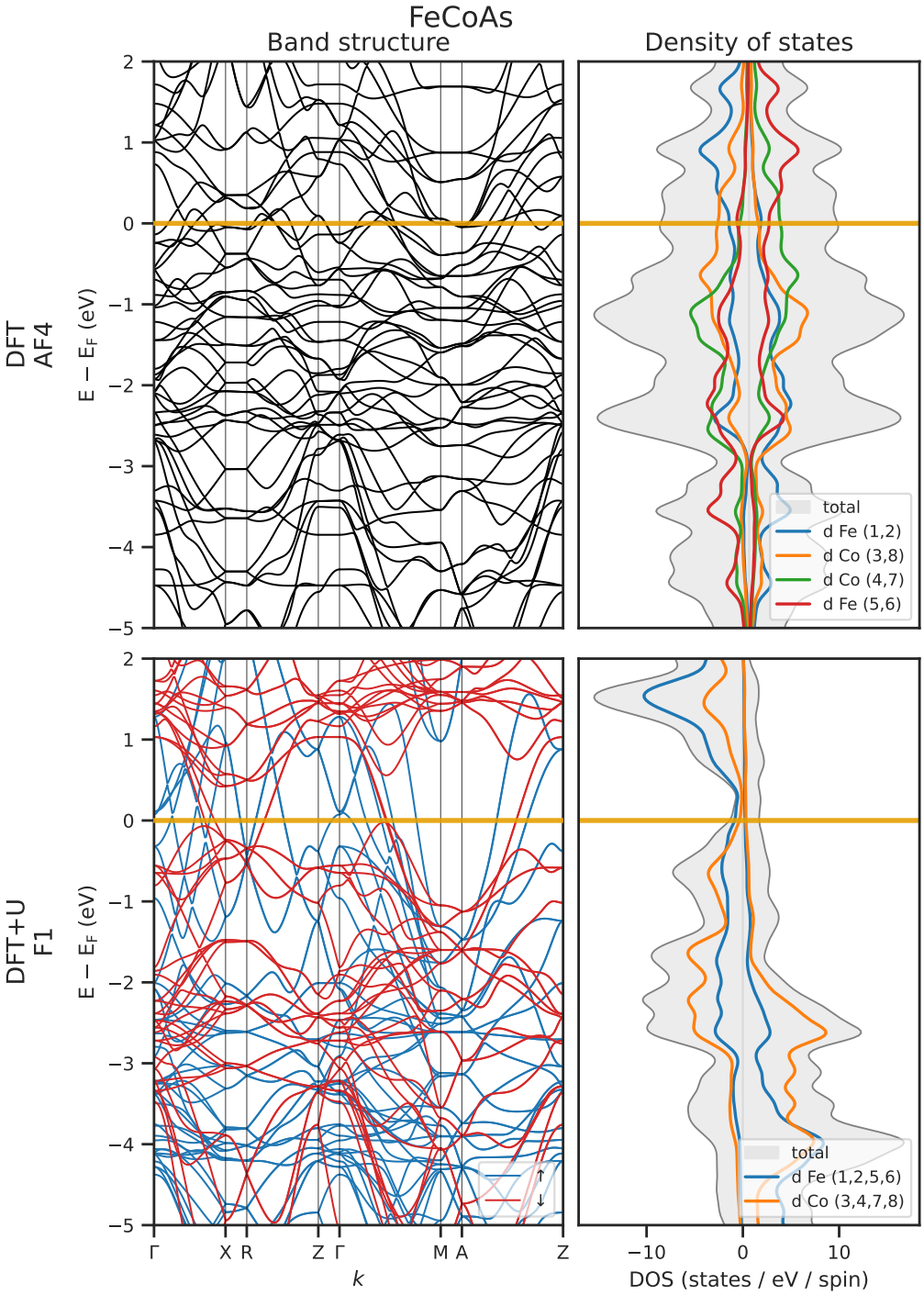


Figure 36: Band structure and Density of states of the lowest in energy calculations.

Material: FeCoSb

Configuration: FeCoSb ■ lower-energy

Structure

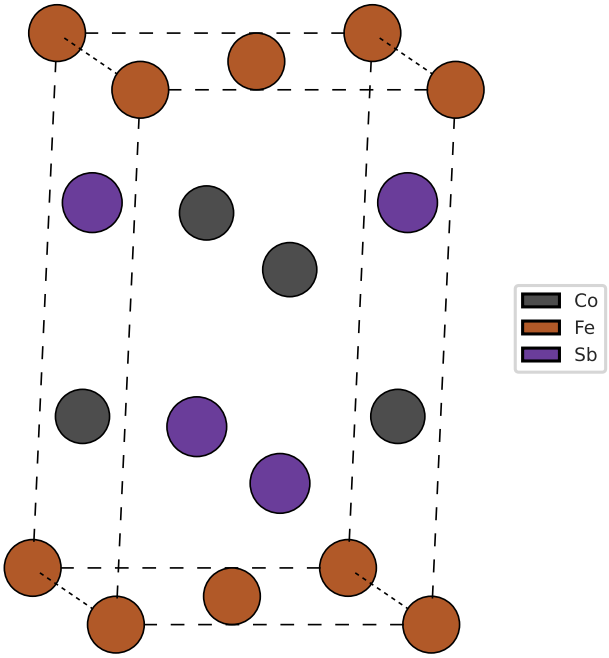


Figure 37: Structure of FeCoSb

a (Å)	c (Å)	z_1	z_2
3.7813	6.2750	0.2534	0.3216

Table 41: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

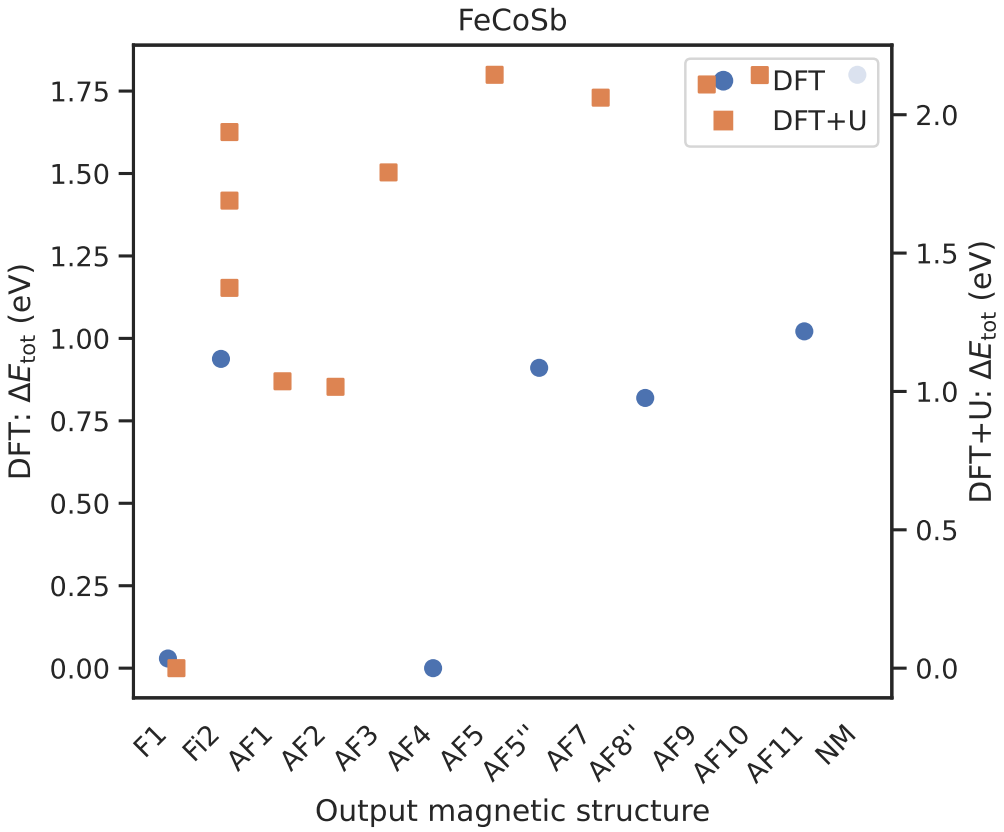


Figure 38: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-38936.402010	0.000000	2.55, 2.55, 1.23, -1.23, -2.55, -2.55, -1.23, 1.23
F1	-38936.372723	0.029287	2.57, 2.57, 1.18, 1.18, 2.57, 2.57, 1.18, 1.18
AF8″	-38935.582598	0.819412	2.37, -2.37, 0.00, 0.00, -2.37, 2.37, 0.00, 0.00
AF5″	-38935.491287	0.910724	2.37, -2.37, 0.00, 0.00, 2.37, -2.37, 0.00, 0.00
Fi2	-38935.464178	0.937832	1.06, -2.62, -0.74, -0.10, 2.34, -2.51, -0.10, -0.74
AF11	-38935.380653	1.021357	0.90, -2.61, -0.74, 0.74, -0.90, 2.61, 0.74, -0.74
NM	-38934.602681	1.799329	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 42: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-38920.985339	0.000000	3.08, 3.08, 1.77, 1.77, 3.08, 3.08, 1.77, 1.77
AF2	-38919.968588	1.016751	3.09, 3.09, -1.89, 1.89, -3.09, -3.09, -1.80, 1.80
AF1	-38919.948620	1.036719	3.09, 3.09, 1.77, 1.85, -3.09, -3.09, -1.77, -1.85
Fi2	-38919.611062	1.374277	-3.09, -3.08, -1.79, -1.83, 3.08, -3.17, -1.82, -1.78
Fi2	-38919.295704	1.689635	3.03, -3.14, 1.78, -1.91, 3.11, 3.05, 1.79, -1.84
AF3	-38919.193793	1.791546	3.08, 3.08, -1.90, 1.90, -3.08, -3.08, 1.90, -1.90
Fi2	-38919.048008	1.937331	2.99, 3.15, -1.87, -2.13, 2.97, 2.97, -1.88, -1.87
AF7	-38918.923662	2.061677	3.22, -3.22, 1.82, 1.82, 3.22, -3.22, -1.82, -1.82
AF9	-38918.876021	2.109318	3.19, -3.20, -1.88, 1.88, -3.19, 3.20, 1.88, -1.88
AF10	-38918.842037	2.143302	3.21, -3.21, 1.83, 1.83, -3.21, 3.21, -1.83, -1.83
AF5	-38918.841075	2.144264	3.21, -3.21, -1.85, 1.85, 3.21, -3.21, -1.85, 1.85

Table 43: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

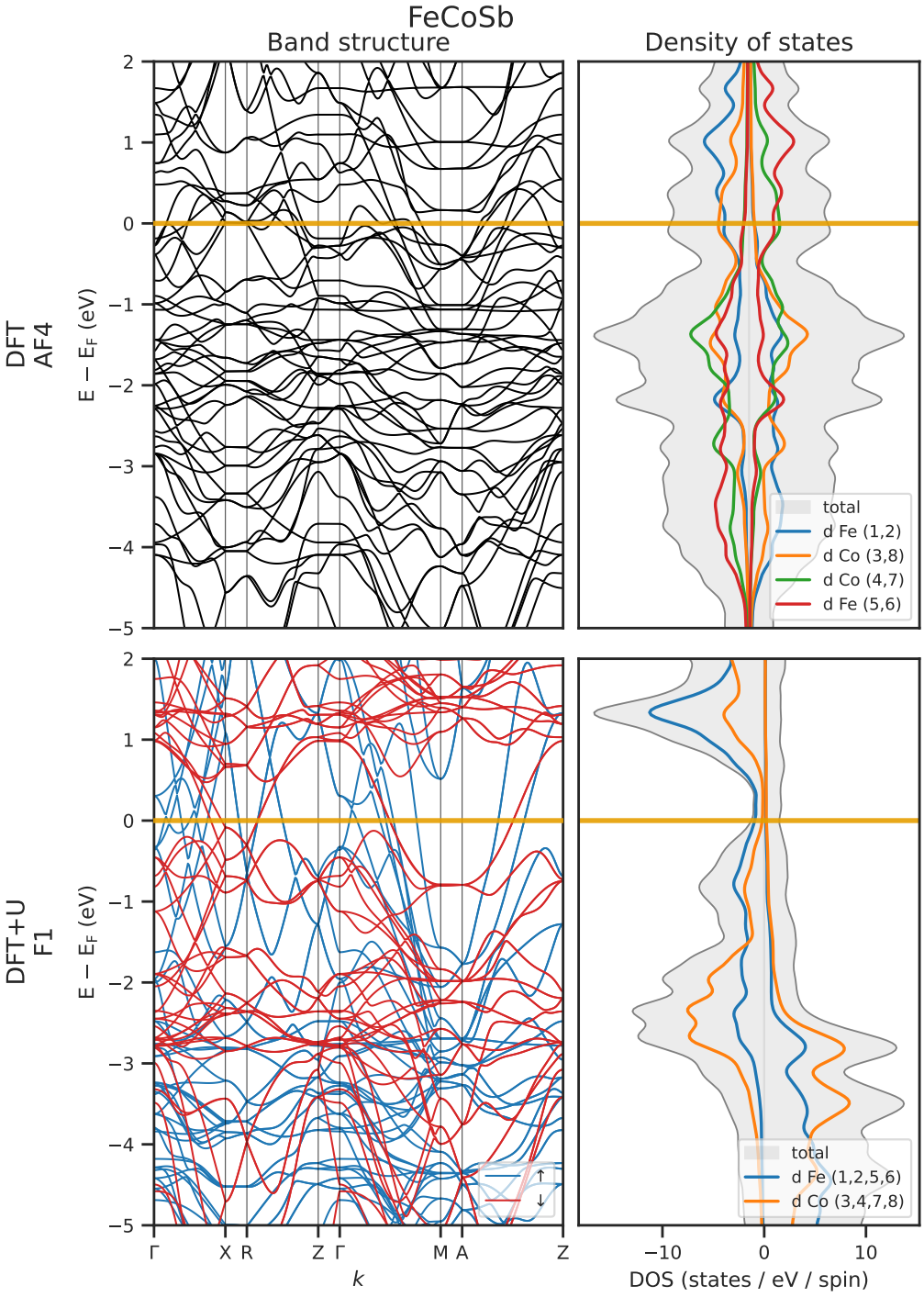


Figure 39: Band structure and Density of states of the lowest in energy calculations.

Configuration: CoFeSb ■ higher-energy

Structure

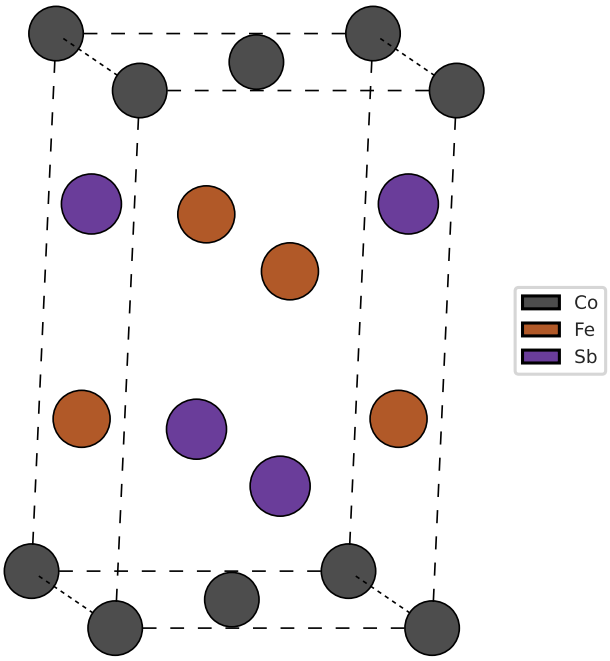


Figure 40: Structure of CoFeSb

a (Å)	c (Å)	z_1	z_2
3.9195	6.1417	0.2609	0.2928

Table 44: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

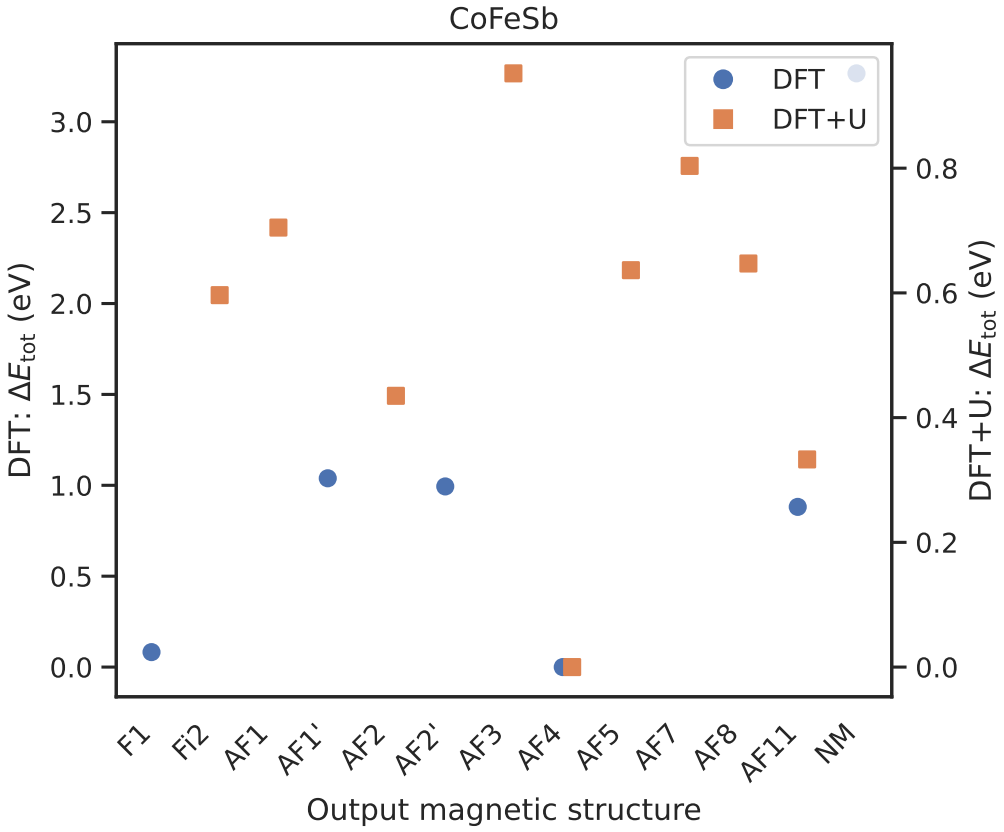


Figure 41: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-38936.190145	0.000000	-1.33, -1.33, -2.85, 2.85, 1.33, 1.33, 2.85, -2.85
F1	-38936.107826	0.082319	1.36, 1.36, 2.91, 2.91, 1.36, 1.36, 2.91, 2.91
AF11	-38935.308865	0.881280	1.01, 1.01, 2.97, 2.83, -1.02, -1.02, -2.97, -2.83
AF2′	-38935.196380	0.993765	0.00, 0.00, -2.90, 2.90, 0.00, 0.00, -2.90, 2.90
AF1′	-38935.151525	1.038620	0.00, 0.00, 2.97, 2.97, 0.00, 0.00, -2.97, -2.97
NM	-38932.923857	3.266288	-0.00, 0.00, -0.00, 0.00, 0.00, -0.00, 0.00, 0.00

Table 45: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-38919.469840	0.000000	1.64, 1.64, 3.22, -3.22, -1.64, -1.64, -3.22, 3.22
AF11	-38919.136863	0.332977	1.08, -1.91, -3.32, 3.32, 1.91, -1.08, 3.32, -3.32
AF2	-38919.034863	0.434976	1.71, 1.71, -3.22, 3.22, -1.71, -1.71, -3.24, 3.24
Fi2	-38918.873435	0.596405	1.73, -1.61, 3.27, 3.34, -1.90, 1.92, -3.34, -3.22
AF5	-38918.833401	0.636439	1.66, -1.66, -3.21, 3.22, 1.66, -1.66, -3.22, 3.21
AF8	-38918.822687	0.647153	1.68, -1.68, -3.23, 3.23, -1.68, 1.68, -3.23, 3.23
AF1	-38918.765077	0.704763	1.72, 1.71, 3.29, 3.23, -1.73, -1.73, -3.29, -3.23
AF7	-38918.666195	0.803645	1.59, -1.59, 3.37, 3.37, 1.59, -1.59, -3.37, -3.37
AF3	-38918.517792	0.952048	1.86, 1.86, -3.16, 3.16, -1.86, -1.86, 3.16, -3.16

Table 46: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

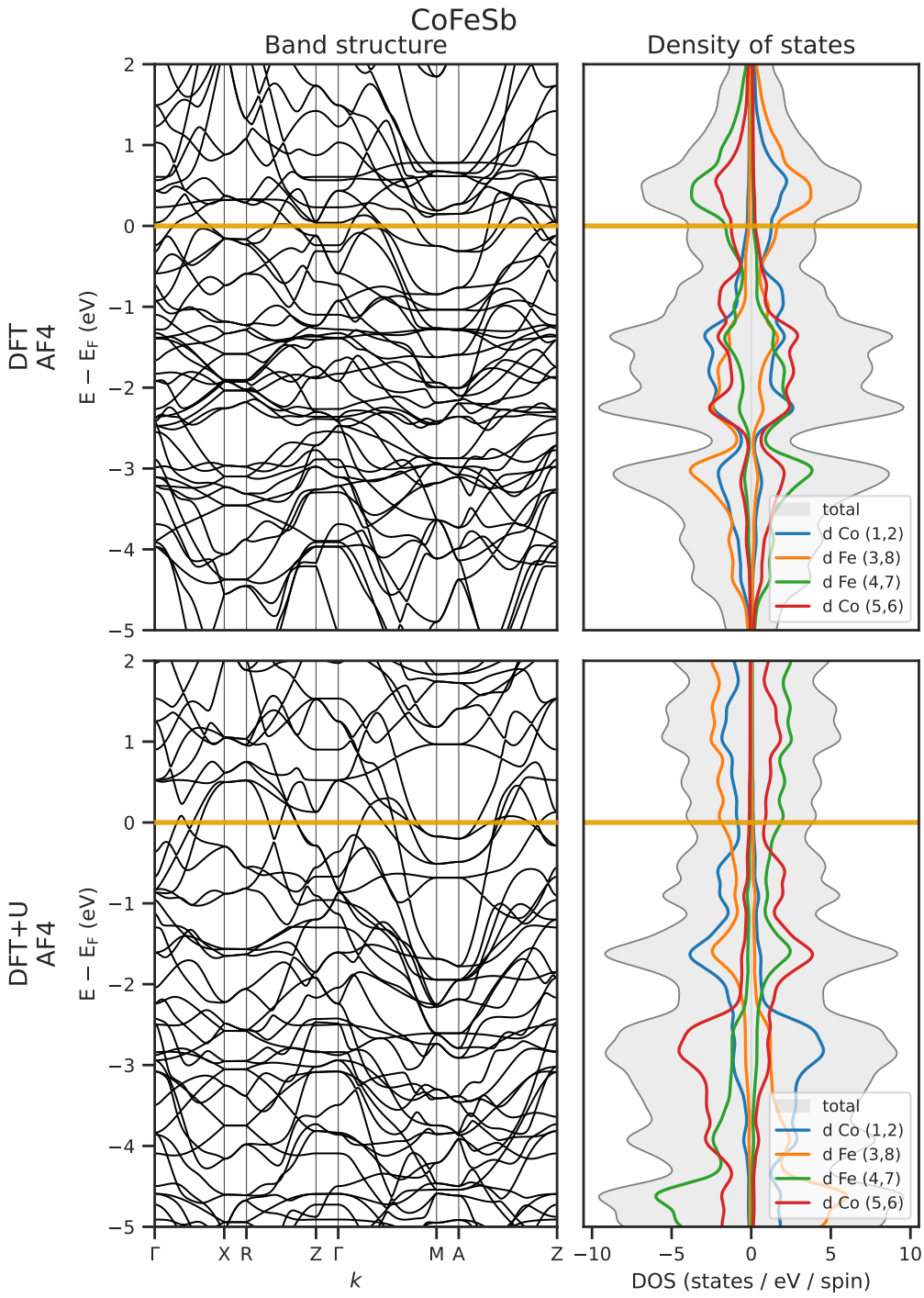


Figure 42: Band structure and Density of states of the lowest in energy calculations.

Material: CoGaAs

Configuration: CoGaAs ■ lower-energy

Structure

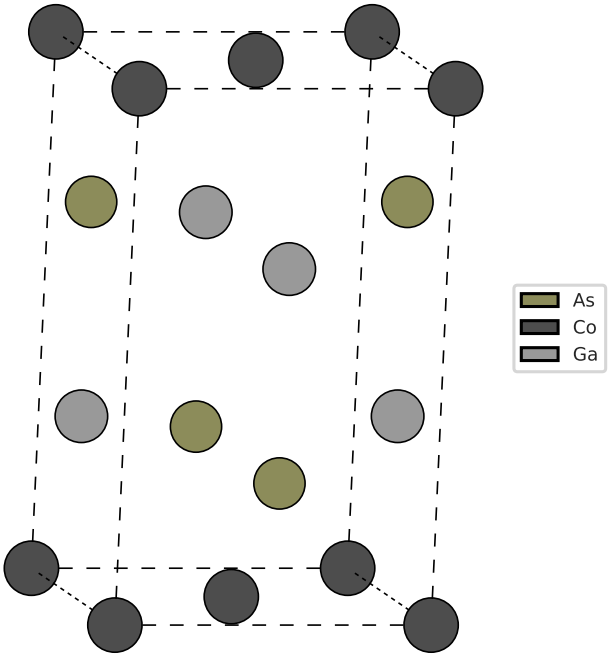


Figure 43: Structure of CoGaAs

a (Å)	c (Å)	z_1	z_2
4.1186	5.4723	0.2775	0.2550

Table 47: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-35858.626254	0.000000	0.76, 0.76, -0.04, -0.04, 0.76, 0.76, -0.04, -0.04
AF1″	-35858.604184	0.022069	0.73, 0.73, -0.03, 0.03, -0.73, -0.73, 0.03, -0.03
NM	-35858.451682	0.174572	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 48: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

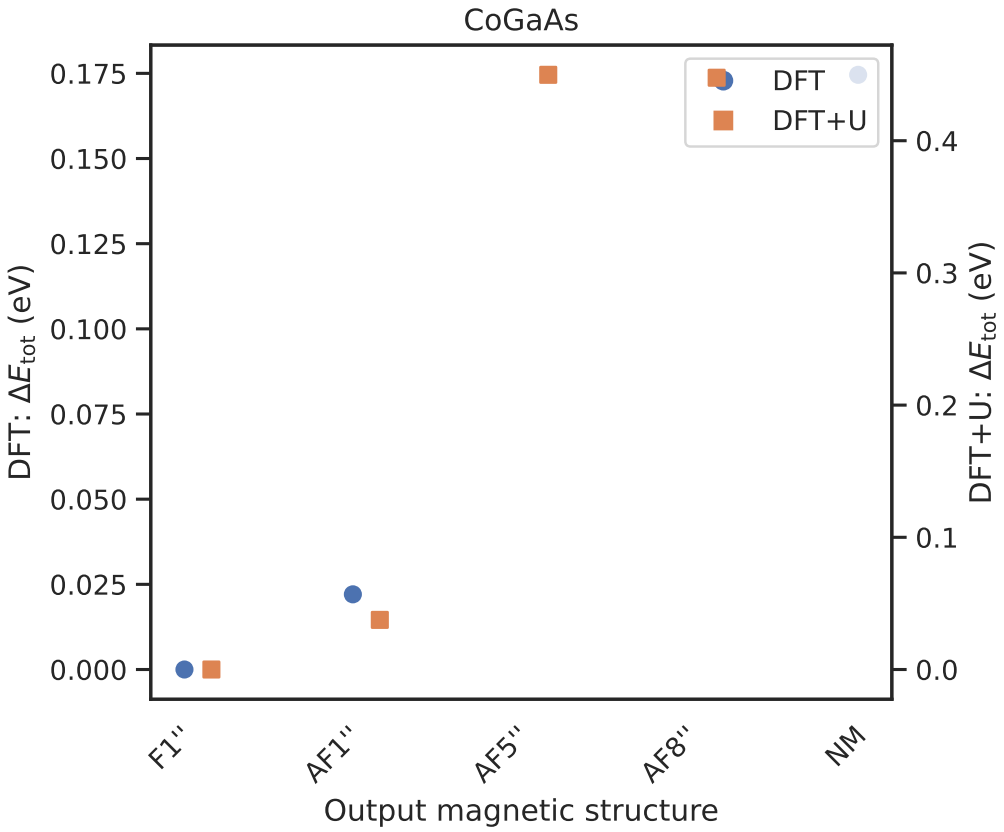


Figure 44: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-35848.997896	0.000000	1.15, 1.15, -0.10, -0.10, 1.15, 1.15, -0.10, -0.10
AF1″	-35848.960361	0.037535	1.11, 1.11, -0.09, 0.09, -1.11, -1.11, 0.09, -0.09
AF8″	-35848.550250	0.447646	1.31, -1.31, 0.00, 0.00, -1.31, 1.31, 0.00, 0.00
AF5″	-35848.548047	0.449849	1.31, -1.31, 0.00, 0.00, 1.31, -1.31, 0.00, 0.00

Table 49: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

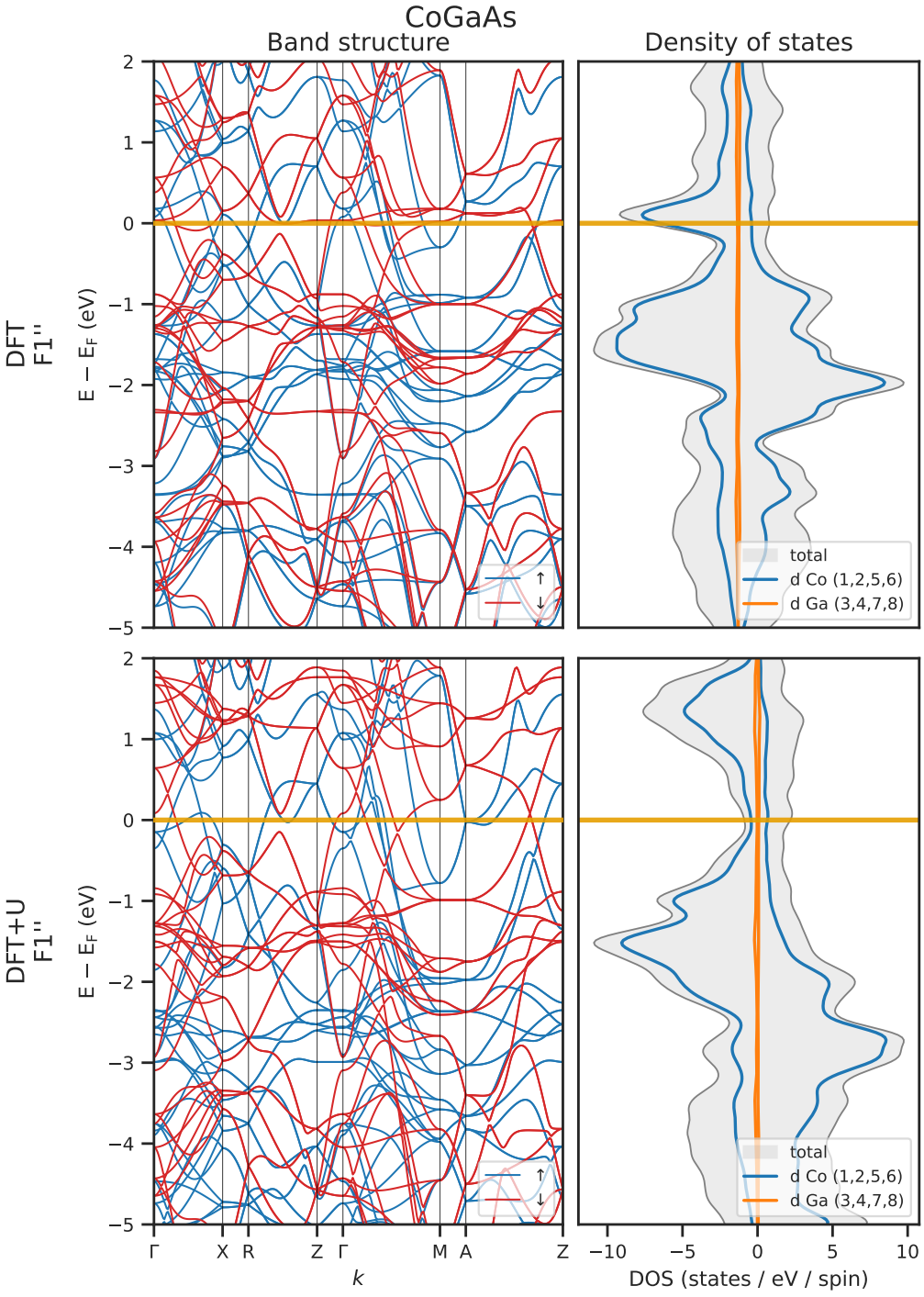


Figure 45: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaCoAs ■ higher-energy

Structure

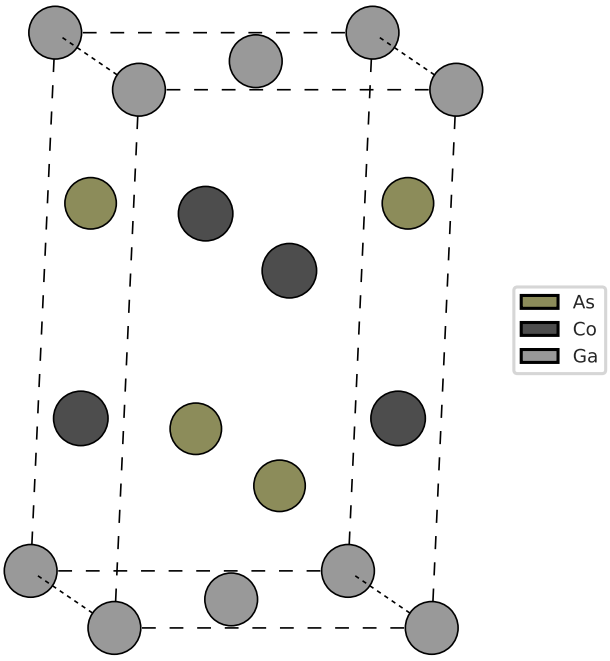


Figure 46: Structure of GaCoAs

a (Å)	c (Å)	z_1	z_2
3.6078	6.7807	0.2621	0.3736

Table 50: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-35857.828641	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 51: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

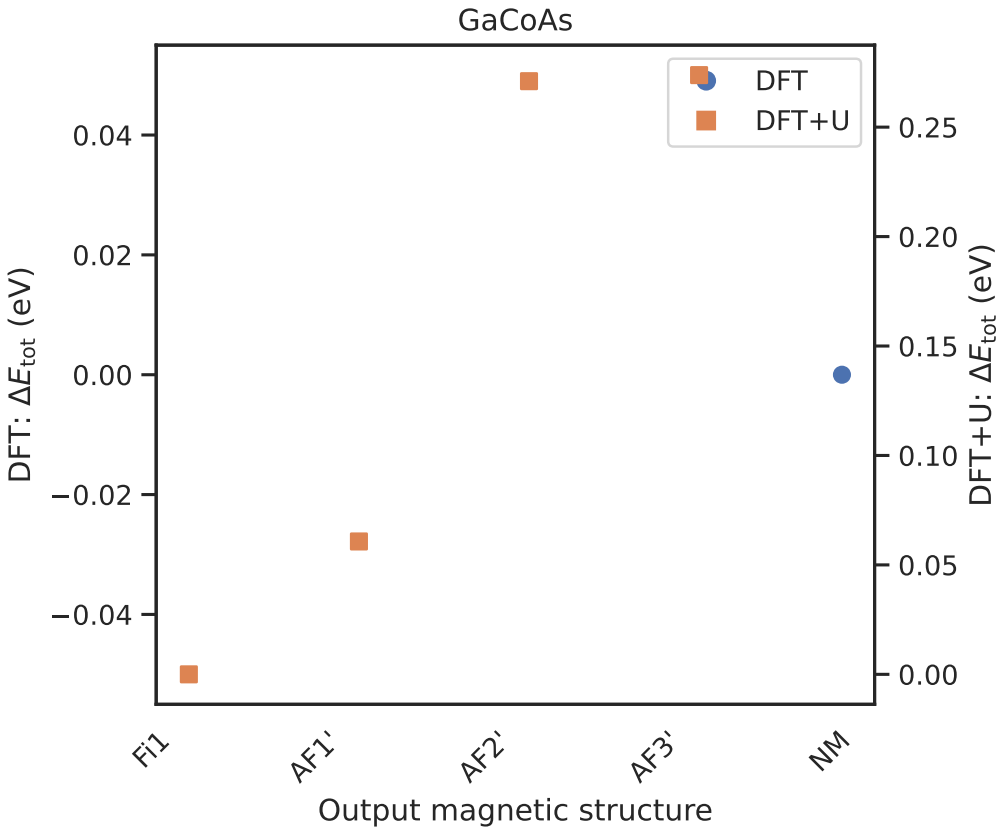


Figure 47: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-35848.667693	0.000000	-0.10, -0.10, 1.61, 1.61, -0.10, -0.10, 1.61, 1.61
AF1′	-35848.606983	0.060710	0.00, 0.00, 1.66, 1.66, 0.00, 0.00, -1.66, -1.66
AF2′	-35848.396696	0.270997	0.00, 0.00, -1.68, 1.68, 0.00, 0.00, -1.68, 1.68
AF3′	-35848.393922	0.273771	0.09, 0.09, -1.66, 1.66, -0.09, -0.09, 1.66, -1.66

Table 52: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

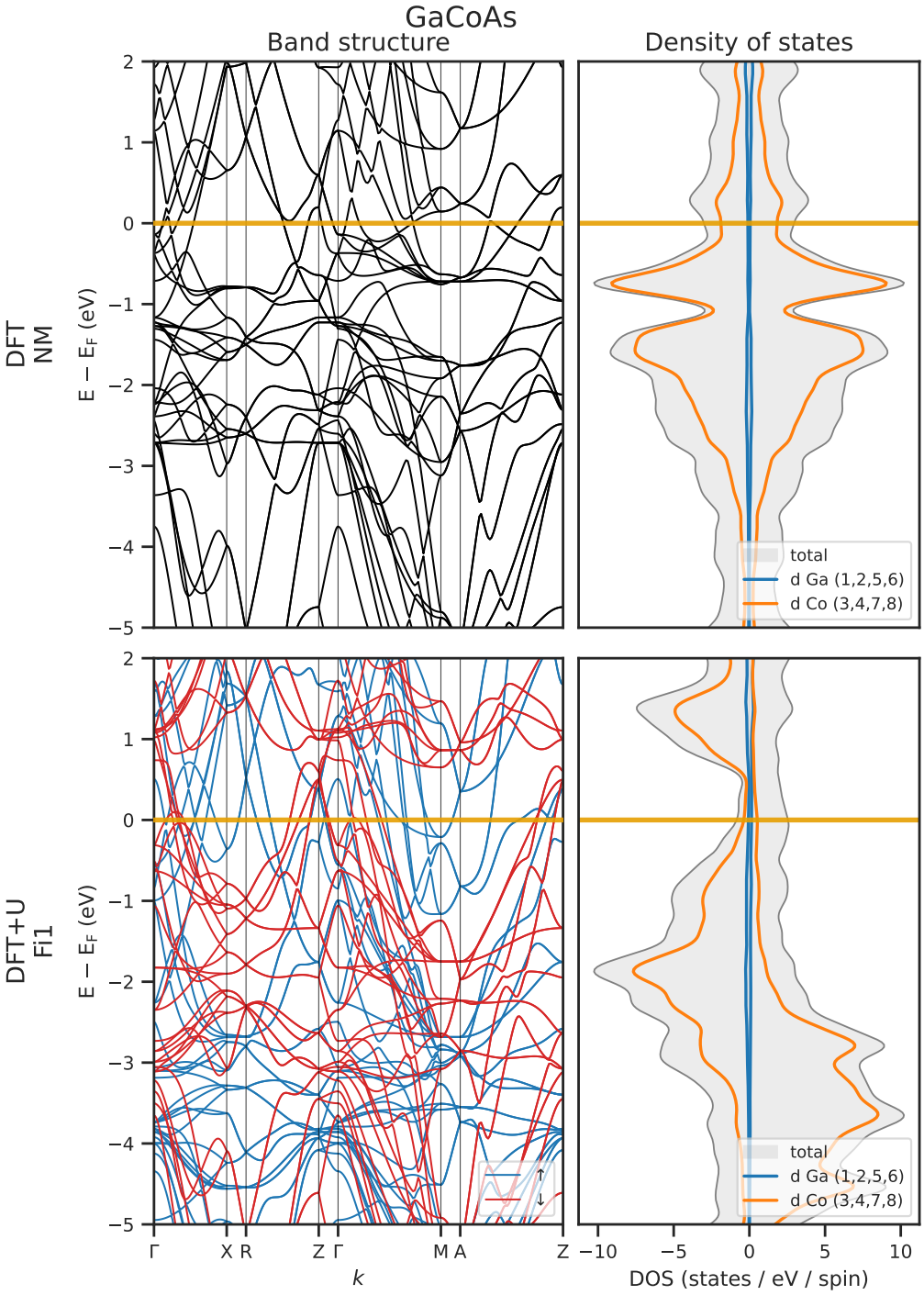


Figure 48: Band structure and Density of states of the lowest in energy calculations.

Material: CoGaSb

Configuration: CoGaSb ■ lower-energy

Structure

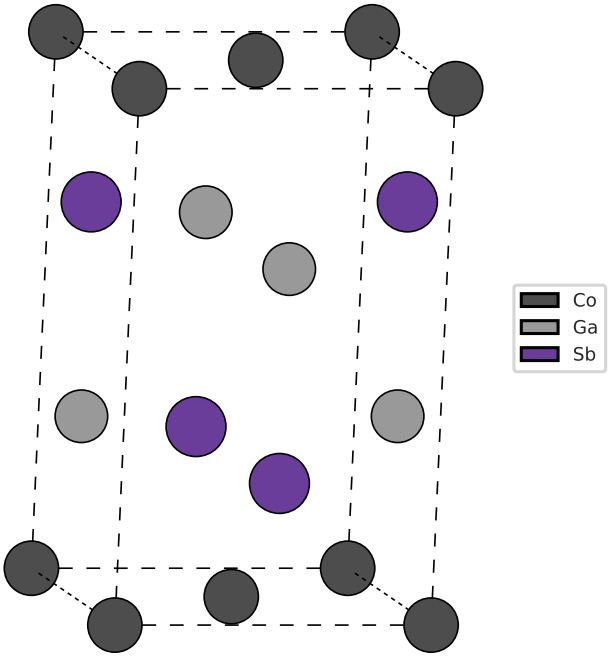


Figure 49: Structure of CoGaSb

a (Å)	c (Å)	z_1	z_2
4.3022	5.8162	0.2384	0.2786

Table 53: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-33744.669798	0.000000	0.77, 0.77, -0.03, -0.03, 0.77, 0.77, -0.03, -0.03
AF1″	-33744.635533	0.034264	0.71, 0.71, -0.02, 0.02, -0.72, -0.71, 0.02, -0.02
NM	-33744.533821	0.135977	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 54: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

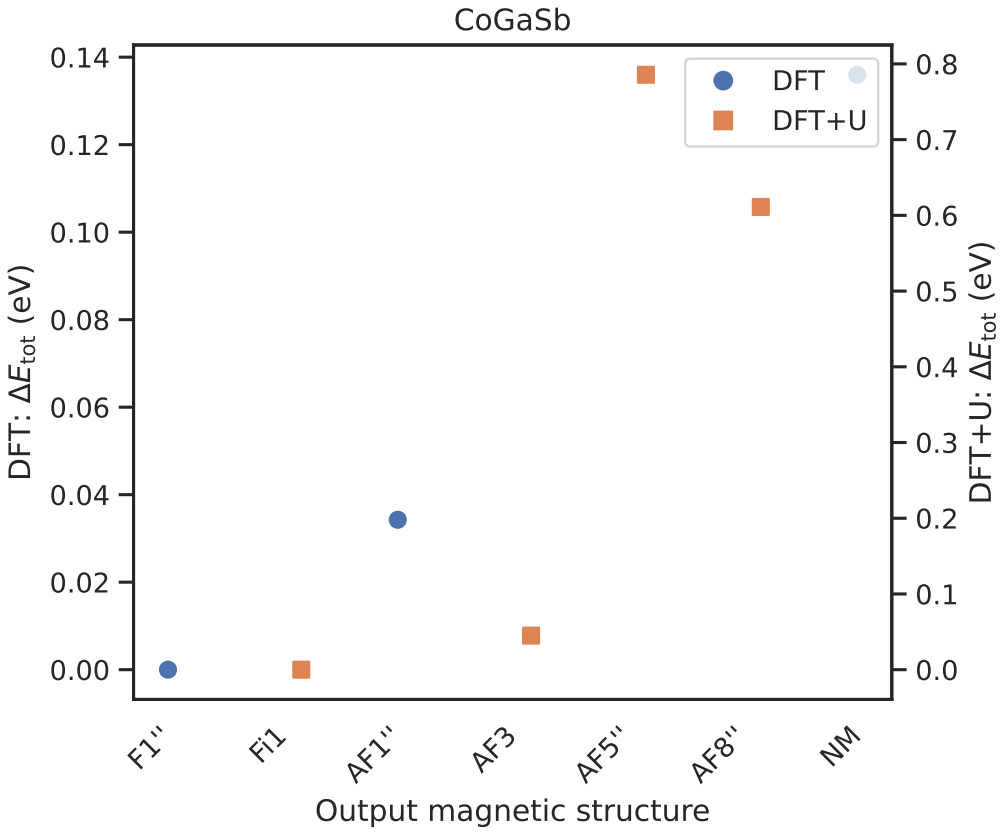


Figure 50: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-33735.314783	0.000000	1.21, 1.21, -0.10, -0.10, 1.21, 1.21, -0.10, -0.10
AF3	-33735.269762	0.045021	1.15, 1.15, -0.10, 0.10, -1.15, -1.15, 0.10, -0.10
AF8″	-33734.703672	0.611111	1.41, -1.41, -0.00, 0.00, -1.46, 1.45, 0.00, 0.00
AF5″	-33734.529116	0.785667	1.49, -1.48, -0.00, -0.00, 1.49, -1.48, -0.00, -0.00

Table 55: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

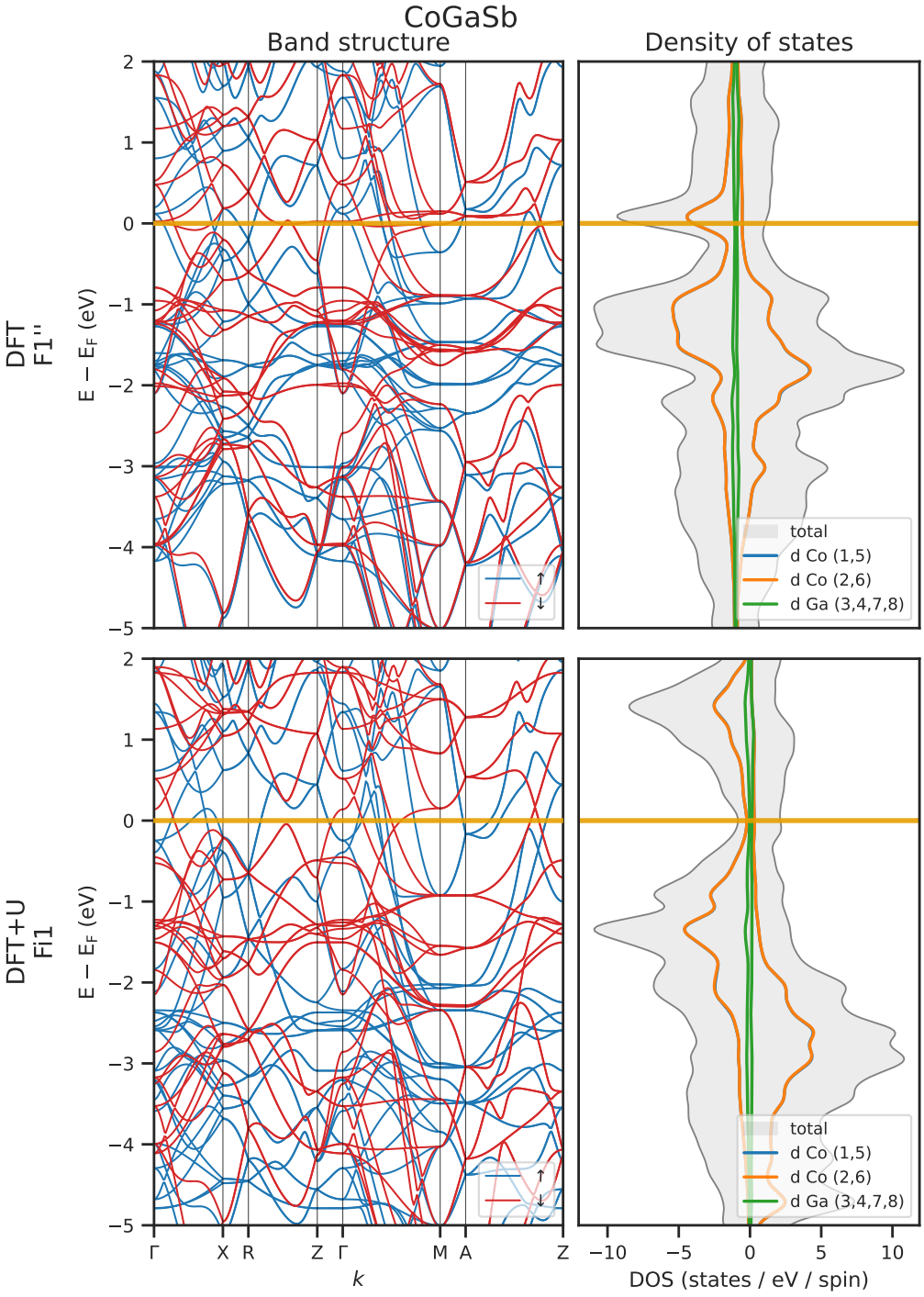


Figure 51: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaCoSb ■ higher-energy

Structure

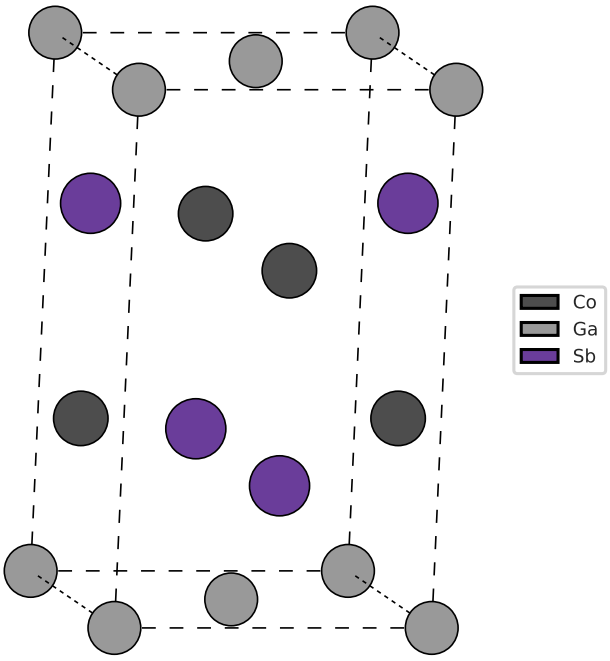


Figure 52: Structure of GaCoSb

a (Å)	c (Å)	z_1	z_2
3.6446	8.7766	0.4019	0.3132

Table 56: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-33740.319773	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 57: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

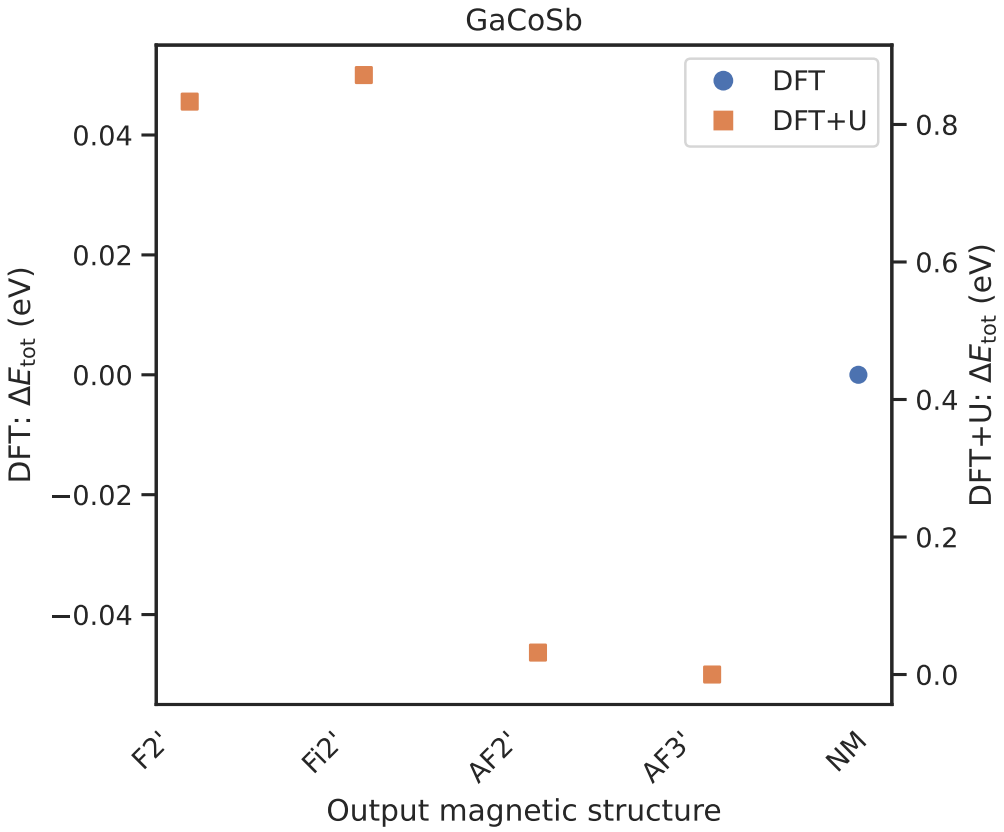


Figure 53: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-33732.046973	0.000000	0.01, 0.01, -1.82, 1.82, -0.01, -0.01, 1.82, -1.82
AF2′	-33732.015050	0.031923	0.00, 0.00, -1.82, 1.82, 0.00, 0.00, -1.82, 1.82
F2′	-33731.213712	0.833261	0.02, 0.02, 1.94, 1.94, 0.02, 0.02, 1.75, 1.75
Fi2′	-33731.175109	0.871864	-0.00, -0.00, 1.99, 1.99, -0.00, -0.00, -1.81, -1.81

Table 58: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

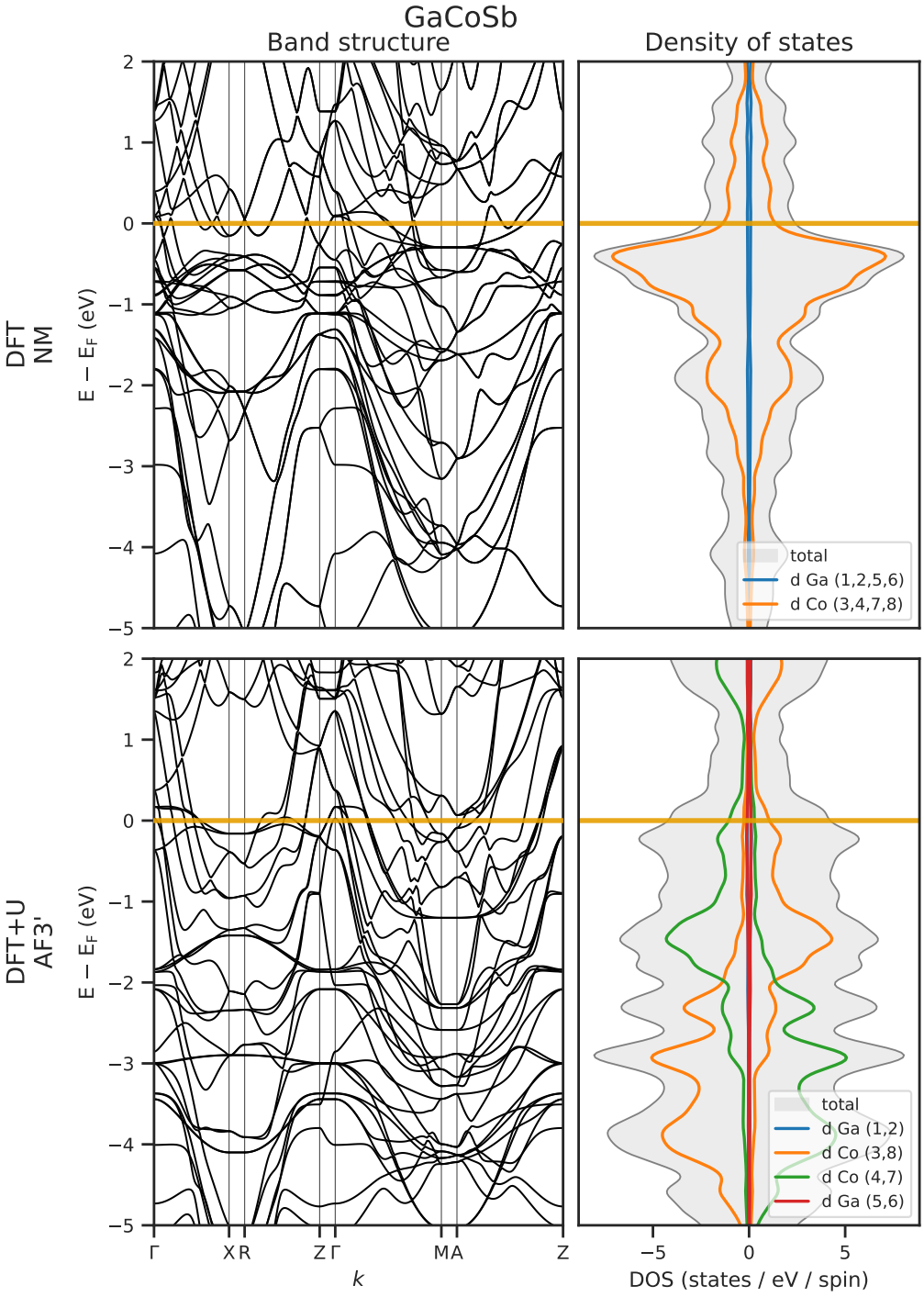


Figure 54: Band structure and Density of states of the lowest in energy calculations.

Material: CoMnAs

Configuration: CoMnAs ■ lower-energy

Structure

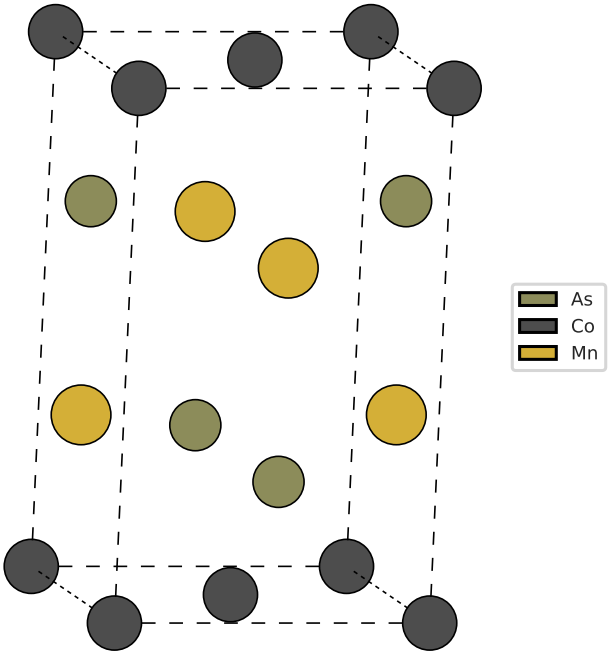


Figure 55: Structure of CoMnAs

a (Å)	c (Å)	z_1	z_2
3.7095	5.9660	0.3399	0.2524

Table 59: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-38923.687902	0.000000	-0.38, -0.38, -3.68, 3.68, 0.38, 0.38, 3.68, -3.68
Fi1	-38923.575101	0.112801	0.19, 0.19, -3.64, -3.64, 0.19, 0.19, -3.64, -3.64
AF2′	-38923.272664	0.415238	0.00, 0.00, -3.75, 3.75, 0.00, 0.00, -3.75, 3.75
AF1′	-38922.913505	0.774398	0.00, 0.00, 3.65, 3.65, 0.00, 0.00, -3.65, -3.65

Table 60: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

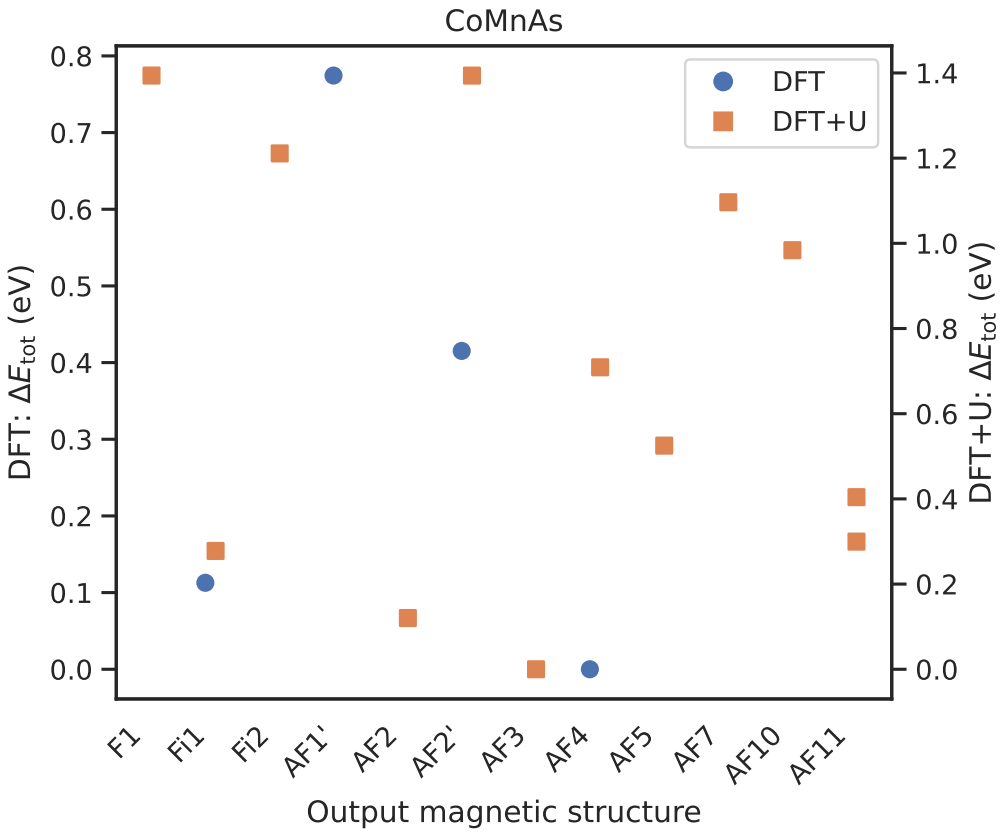


Figure 56: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-38907.813970	0.000000	1.73, 1.73, -4.66, 4.66, -1.73, -1.73, 4.66, -4.66
AF2	-38907.693653	0.120317	1.50, 1.50, -4.67, 4.67, -1.50, -1.50, -4.62, 4.62
Fi1	-38907.536145	0.277825	1.68, 1.68, -4.64, -4.64, 1.68, 1.68, -4.64, -4.64
AF11	-38907.514269	0.299701	1.26, -1.71, -4.61, 4.61, 1.71, -1.26, 4.61, -4.61
AF11	-38907.409885	0.404085	1.25, -1.67, -4.60, 4.60, -1.25, 1.67, 4.60, -4.60
AF5	-38907.288894	0.525076	1.61, -1.61, -4.64, 4.64, 1.61, -1.61, -4.64, 4.64
AF4	-38907.105042	0.708928	0.55, 0.55, 4.56, -4.56, -0.55, -0.55, -4.56, 4.56
AF10	-38906.830023	0.983947	1.64, -1.64, 4.60, 4.60, -1.63, 1.63, -4.60, -4.60
AF7	-38906.717524	1.096446	1.61, -1.61, 4.59, 4.61, 1.63, -1.63, -4.61, -4.59
Fi2	-38906.602871	1.211099	1.56, 0.04, 4.56, 4.63, -1.72, -1.70, -4.63, -4.63
AF2′	-38906.420143	1.393827	0.00, 0.00, -4.62, 4.62, 0.00, 0.00, -4.62, 4.62
F1	-38906.420050	1.393920	0.57, 0.57, 4.55, 4.55, 0.57, 0.57, 4.55, 4.55

Table 61: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

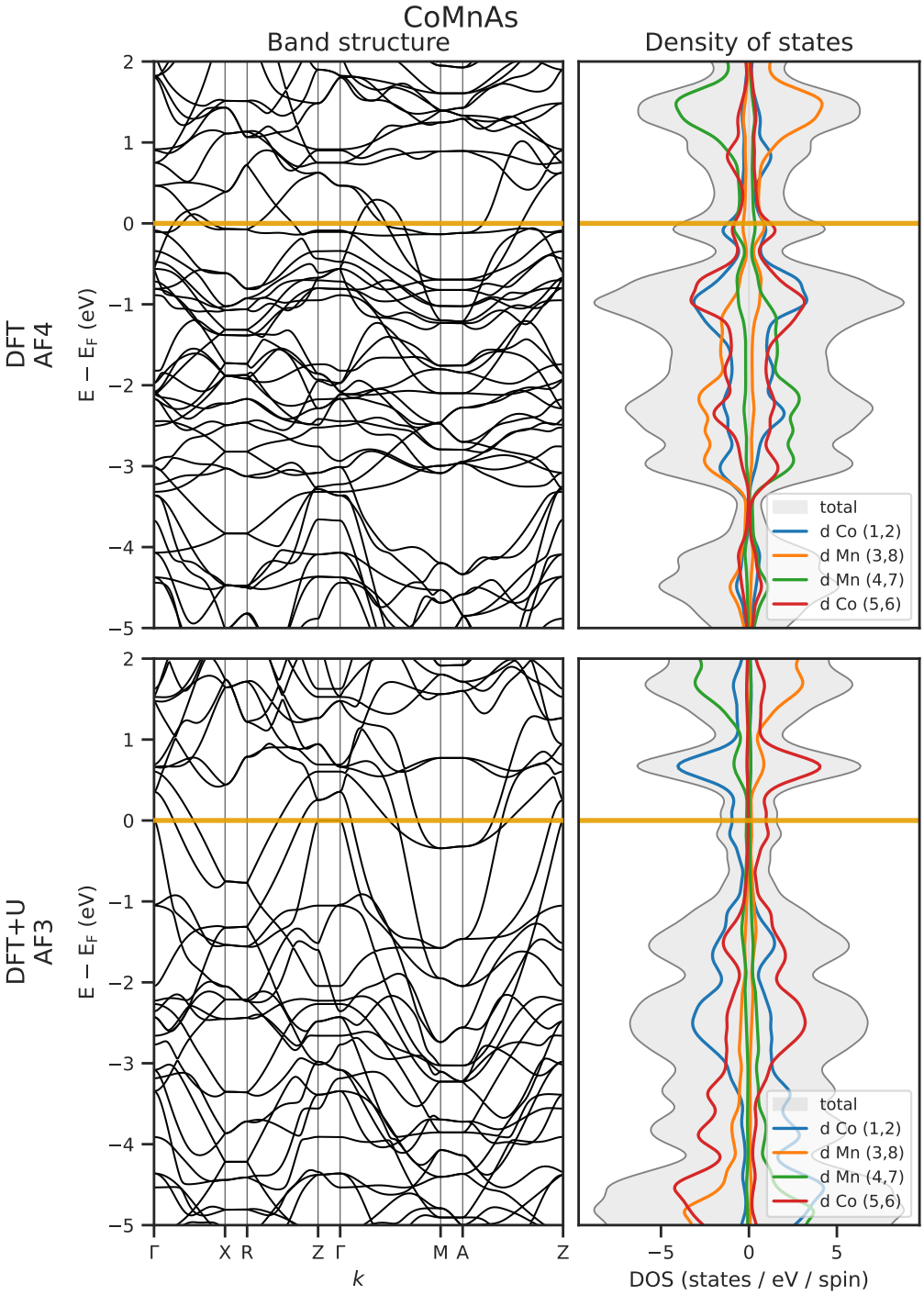


Figure 57: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnCoAs ■ higher-energy

Structure

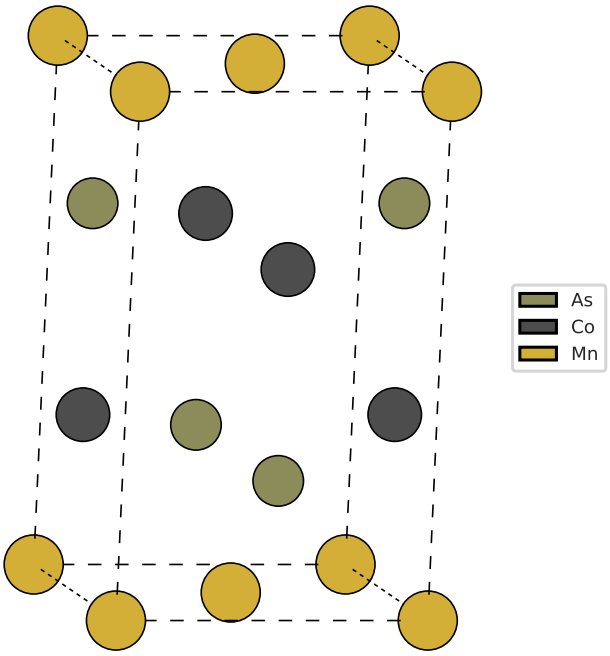


Figure 58: Structure of MnCoAs

a (Å)	c (Å)	z_1	z_2
3.6154	5.8562	0.2990	0.2925

Table 62: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

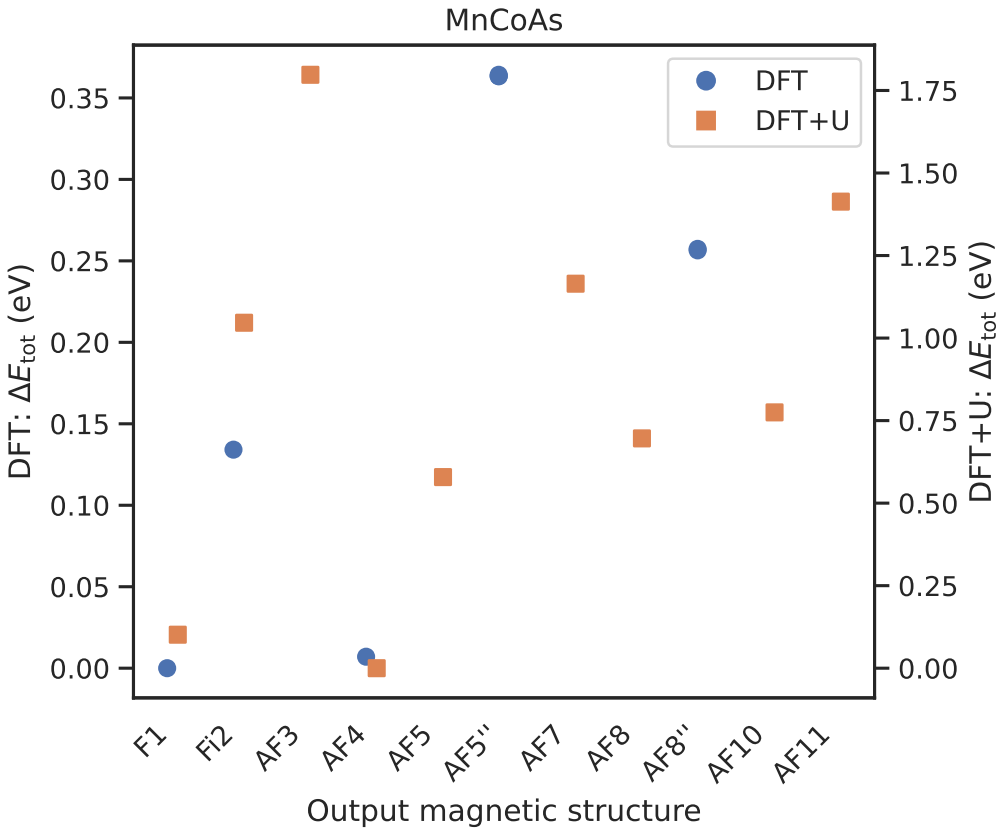


Figure 59: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-38920.823303	0.000000	2.27, 2.27, 1.01, 1.01, 2.27, 2.27, 1.01, 1.01
AF4	-38920.816253	0.007049	2.24, 2.24, 0.99, -0.99, -2.24, -2.24, -0.99, 0.99
Fi2	-38920.689174	0.134129	2.22, -2.16, 0.05, 0.96, 2.27, 2.30, 0.96, 0.05
AF8″	-38920.566856	0.256447	2.33, -2.33, 0.00, 0.00, -2.33, 2.33, 0.00, 0.00
AF8″	-38920.565938	0.257365	2.33, -2.33, 0.00, 0.00, -2.33, 2.33, 0.00, 0.00
AF5″	-38920.459954	0.363348	2.22, -2.22, 0.00, 0.00, 2.22, -2.22, 0.00, 0.00
AF5″	-38920.459095	0.364207	2.22, -2.22, 0.00, 0.00, 2.22, -2.22, 0.00, 0.00

Table 63: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-38903.203560	0.000000	4.01, 4.01, 1.69, -1.69, -4.01, -4.01, -1.69, 1.69
F1	-38903.102090	0.101469	3.99, 3.99, 1.64, 1.64, 3.99, 3.99, 1.64, 1.64
AF5	-38902.624667	0.578893	4.19, -4.19, -1.82, 1.82, 4.19, -4.19, -1.82, 1.82
AF8	-38902.507429	0.696131	4.19, -4.19, -1.83, 1.83, -4.19, 4.19, -1.83, 1.83
AF10	-38902.428637	0.774923	4.21, -4.21, 1.82, 1.82, -4.21, 4.21, -1.82, -1.82
Fi2	-38902.157103	1.046456	4.09, 4.09, -1.96, 1.75, -4.11, -4.11, -1.67, 1.69
AF7	-38902.038855	1.164705	4.19, -4.19, 1.80, 1.87, 4.21, -4.21, -1.87, -1.80
AF11	-38901.790249	1.413311	4.11, 4.11, 1.65, 0.82, -4.11, -4.11, -1.65, -0.82
AF3	-38901.406027	1.797533	4.25, 4.25, -1.66, 1.66, -4.25, -4.25, 1.66, -1.66

Table 64: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

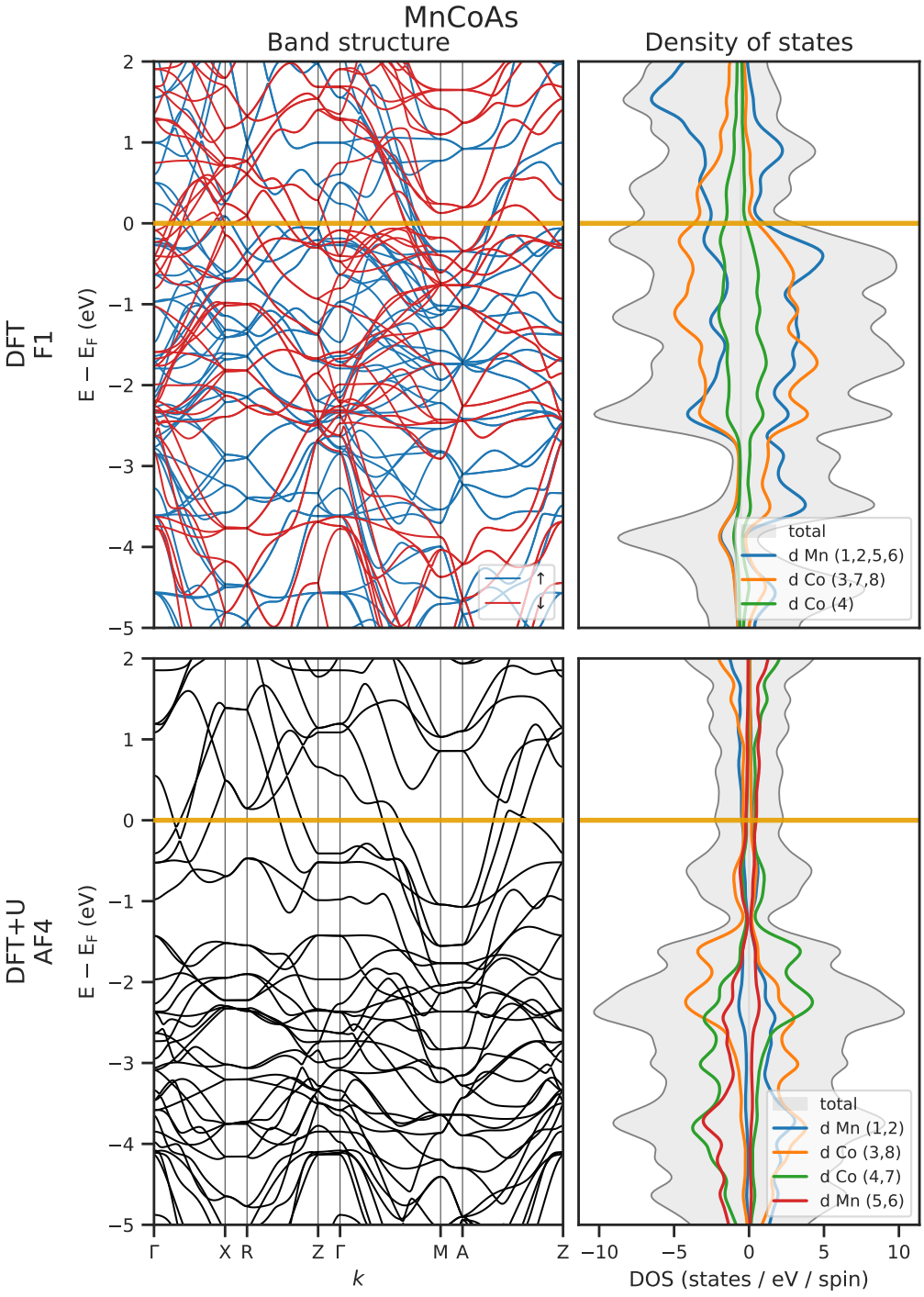


Figure 60: Band structure and Density of states of the lowest in energy calculations.

Material: CoMnSb

Configuration: CoMnSb ■ lower-energy

Structure

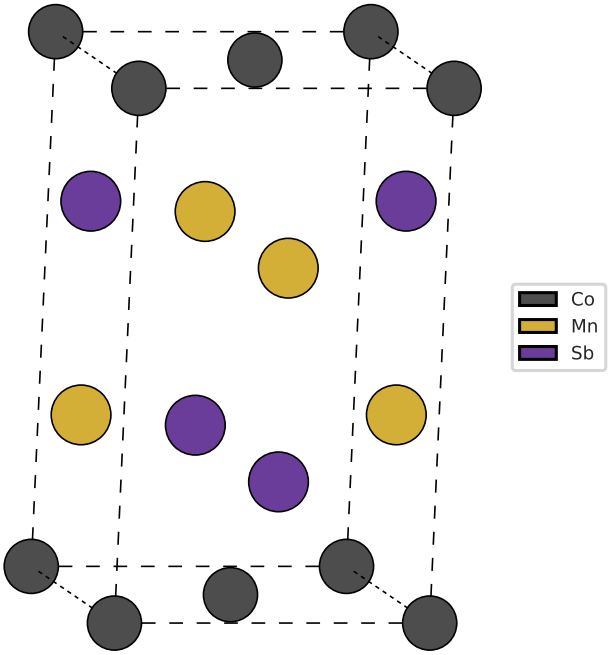


Figure 61: Structure of CoMnSb

a (Å)	c (Å)	z_1	z_2
4.0670	6.1217	0.2726	0.2741

Table 65: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

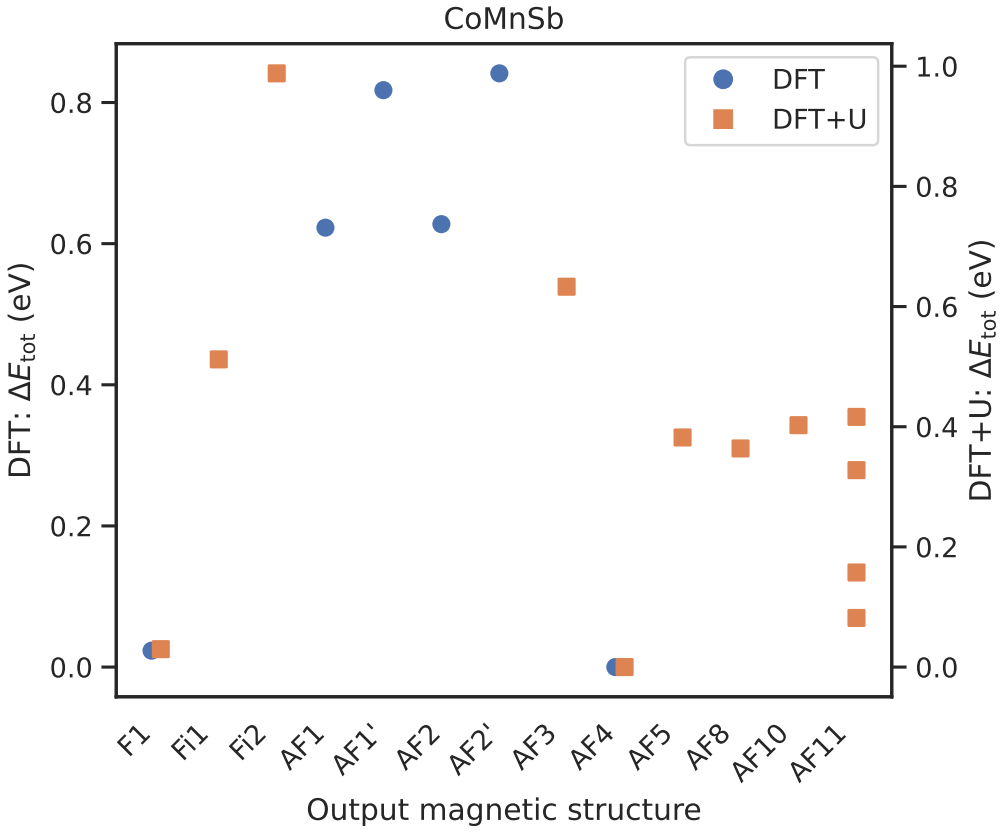


Figure 62: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF4	-36808.453789	0.000000	-0.97, -0.97, -3.96, 3.96, 0.97, 0.97, 3.96, -3.96
F1	-36808.430526	0.023263	-0.99, -0.99, -4.00, -4.00, -0.99, -0.99, -4.00, -4.00
AF1	-36807.831115	0.622674	0.88, 0.88, 4.08, 4.14, -0.88, -0.88, -4.08, -4.14
AF2	-36807.826151	0.627638	0.88, 0.88, -4.09, 4.09, -0.88, -0.88, -4.03, 4.03
AF1′	-36807.636294	0.817494	0.00, 0.00, 4.09, 4.09, 0.00, 0.00, -4.09, -4.09
AF2′	-36807.612474	0.841314	0.00, 0.00, -4.09, 4.09, 0.00, 0.00, -4.09, 4.09

Table 66: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-36794.122408	0.000000	1.58, 1.58, 4.59, -4.59, -1.58, -1.58, -4.59, 4.59
F1	-36794.092571	0.029837	1.54, 1.54, 4.64, 4.64, 1.54, 1.54, 4.64, 4.64
AF11	-36794.040661	0.081747	1.56, 1.56, 4.70, 4.89, -1.56, -1.56, -4.70, -4.89
AF11	-36793.964971	0.157438	1.54, 1.54, -4.84, 4.84, -1.54, -1.54, -4.66, 4.66
AF11	-36793.794639	0.327769	0.31, -1.71, -4.66, 4.66, 1.71, -0.31, 4.66, -4.66
AF8	-36793.758562	0.363847	1.63, -1.63, -4.74, 4.74, -1.63, 1.63, -4.74, 4.74
AF5	-36793.740277	0.382132	1.64, -1.64, -4.74, 4.74, 1.64, -1.64, -4.74, 4.74
AF10	-36793.719806	0.402603	1.65, -1.65, 4.79, 4.79, -1.65, 1.65, -4.79, -4.79
AF11	-36793.706021	0.416387	0.31, -1.70, -4.66, 4.66, -0.31, 1.70, 4.66, -4.66
Fi1	-36793.610331	0.512077	1.76, 1.76, -4.84, -4.84, 1.76, 1.76, -4.84, -4.84
AF3	-36793.489363	0.633046	1.76, 1.76, -4.79, 4.79, -1.76, -1.76, 4.79, -4.79
Fi2	-36793.134289	0.988120	-0.39, 0.38, 4.78, 4.70, 1.55, 1.54, -4.88, -4.78

Table 67: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

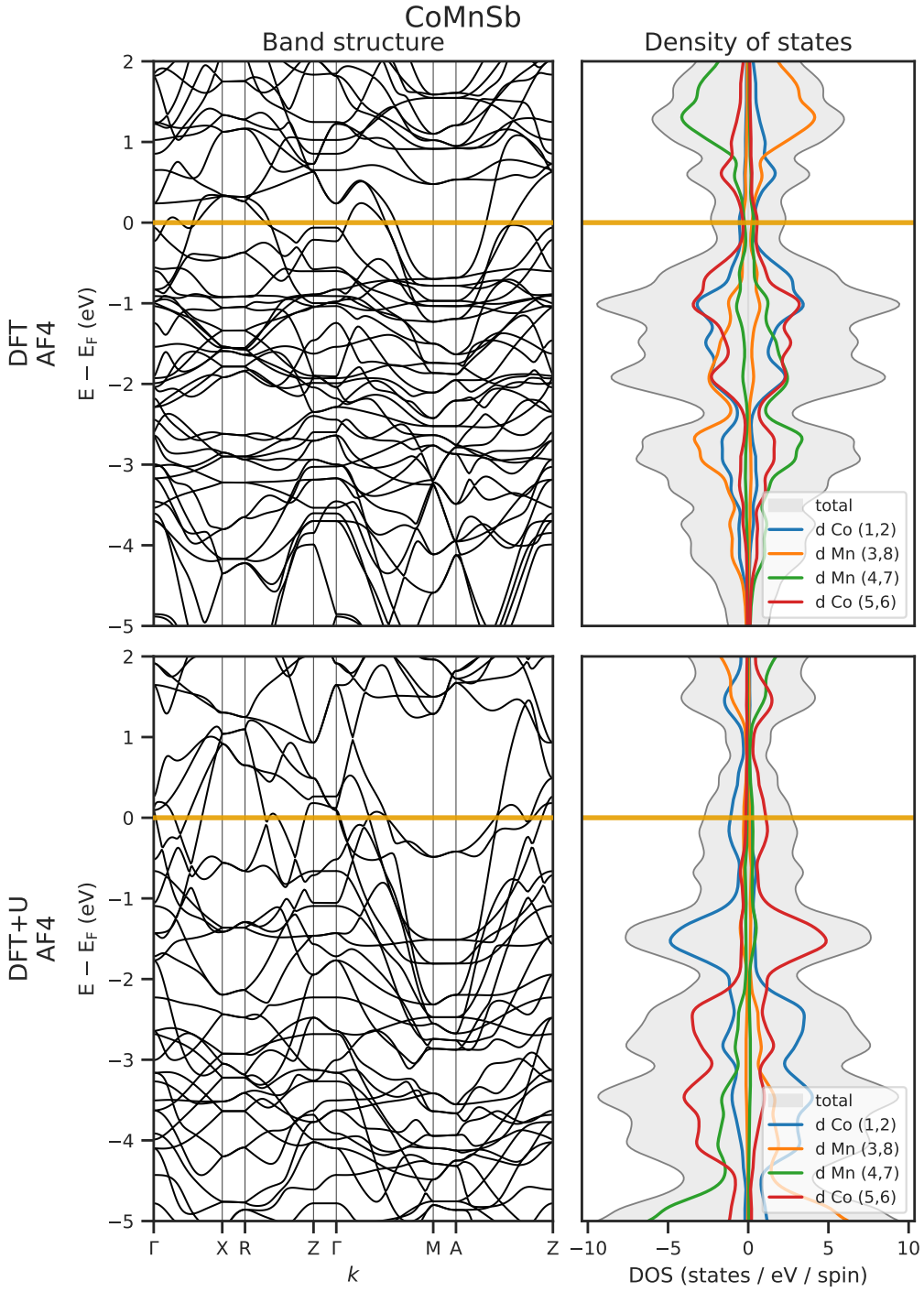


Figure 63: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnCoSb ■ higher-energy

Structure

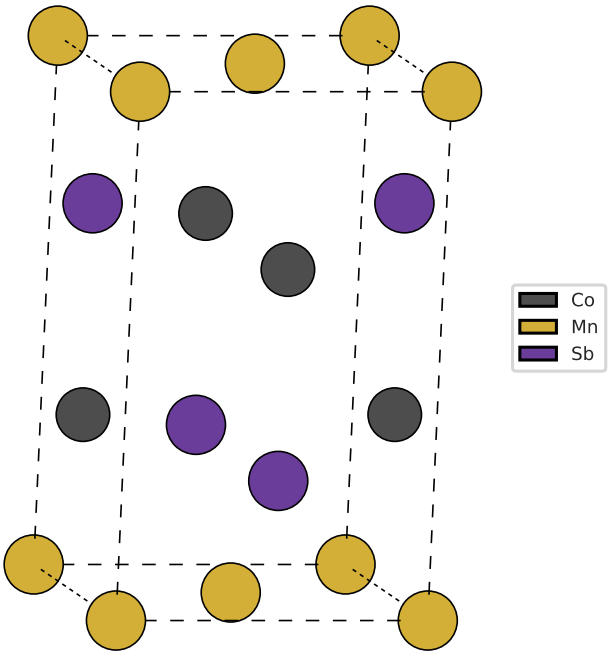


Figure 64: Structure of MnCoSb

a (Å)	c (Å)	z_1	z_2
3.7861	6.5954	0.2622	0.3298

Table 68: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

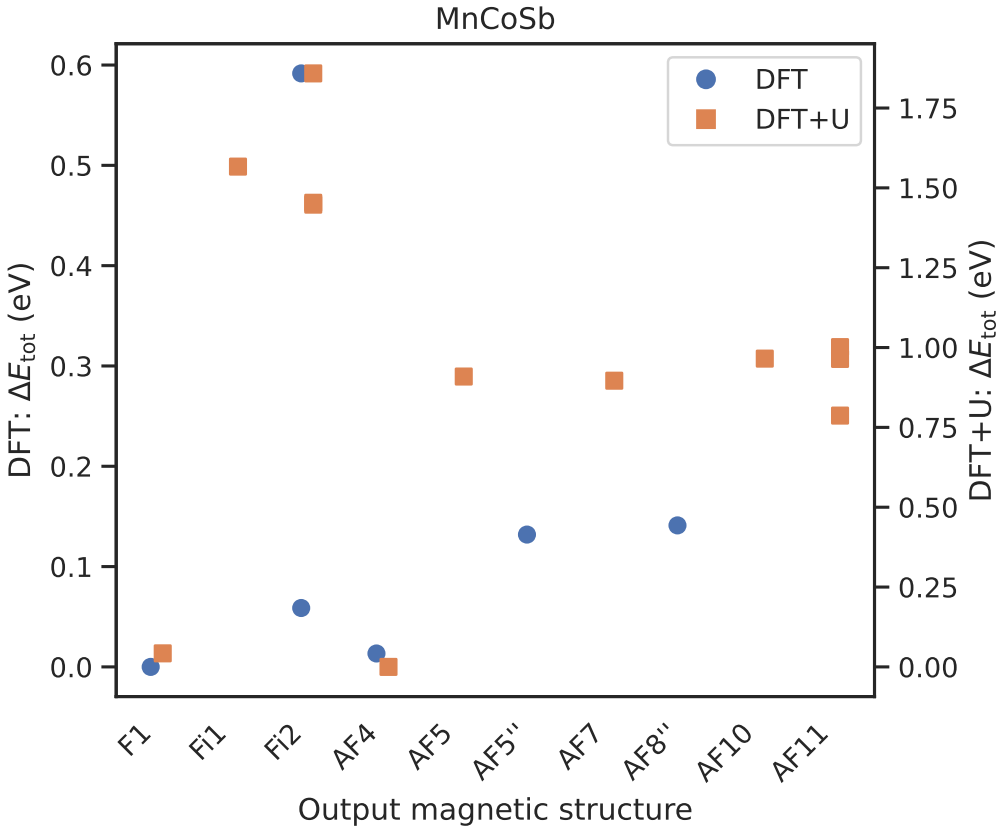


Figure 65: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-36807.339668	0.000000	3.39, 3.39, 0.94, 0.94, 3.39, 3.39, 0.94, 0.94
AF4	-36807.326294	0.013374	3.32, 3.32, 1.00, -1.00, -3.32, -3.32, -1.00, 1.00
Fi2	-36807.280953	0.058715	3.51, -3.52, 0.13, -0.92, -3.30, -3.33, -0.92, 0.13
AF5″	-36807.207748	0.131920	3.52, -3.52, 0.00, 0.00, 3.52, -3.52, 0.00, 0.00
AF8″	-36807.198603	0.141065	3.50, -3.50, 0.00, 0.00, -3.50, 3.50, 0.00, 0.00
Fi2	-36806.748002	0.591666	3.33, 3.34, 1.01, -0.56, -3.42, -0.28, -0.56, 1.01

Table 69: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-36792.889638	0.000000	4.30, 4.30, 1.62, -1.62, -4.30, -4.30, -1.62, 1.62
F1	-36792.847217	0.042420	4.27, 4.27, 1.52, 1.52, 4.27, 4.27, 1.52, 1.52
AF11	-36792.102684	0.786954	4.39, 4.39, 1.61, 1.81, -4.39, -4.39, -1.61, -1.81
AF7	-36791.993440	0.896197	4.59, -4.59, 1.77, 1.77, 4.59, -4.59, -1.77, -1.77
AF5	-36791.980413	0.909225	4.59, -4.59, -1.76, 1.76, 4.59, -4.59, -1.76, 1.76
AF11	-36791.925281	0.964356	4.70, -4.49, -1.76, 1.76, 4.49, -4.70, 1.76, -1.76
AF10	-36791.924280	0.965358	4.60, -4.60, 1.74, 1.74, -4.60, 4.60, -1.74, -1.74
AF11	-36791.888258	1.001379	4.71, -4.49, -1.76, 1.76, -4.71, 4.49, 1.76, -1.76
Fi2	-36791.442162	1.447475	4.69, -4.54, -0.12, 1.76, 4.51, -4.68, 1.77, -1.76
Fi2	-36791.436267	1.453371	4.58, -4.61, -1.75, 0.14, -4.57, 4.64, -1.75, 1.76
Fi1	-36791.323048	1.566590	4.47, 4.47, -1.83, -1.83, 4.47, 4.47, -1.83, -1.83
Fi2	-36791.031193	1.858444	-4.56, 4.65, 0.08, -1.72, -4.57, 4.65, 0.07, -1.72

Table 70: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

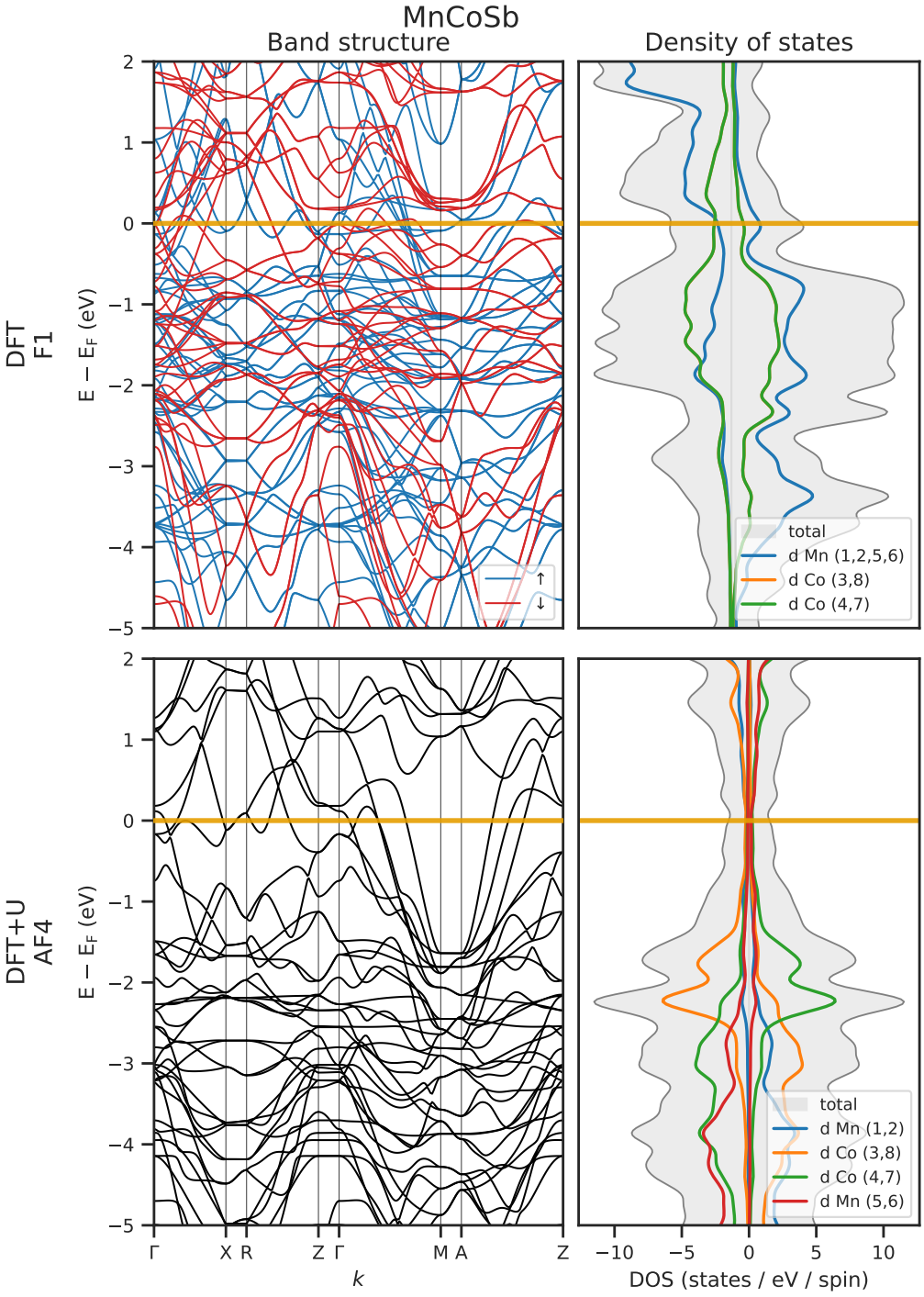


Figure 66: Band structure and Density of states of the lowest in energy calculations.

Material: CoNiAs

Configuration: CoNiAs ■ lower-energy

Structure

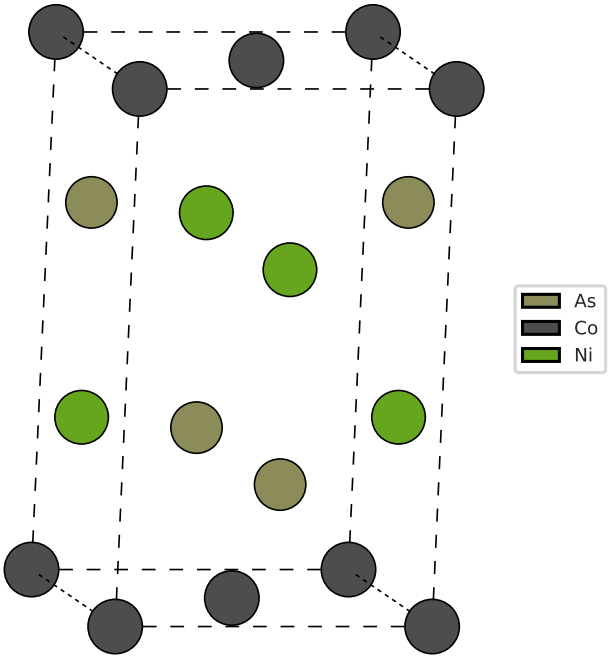


Figure 67: Structure of CoNiAs

a (Å)	c (Å)	z_1	z_2
3.6217	5.8371	0.3444	0.2582

Table 71: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-45754.757481	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 72: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

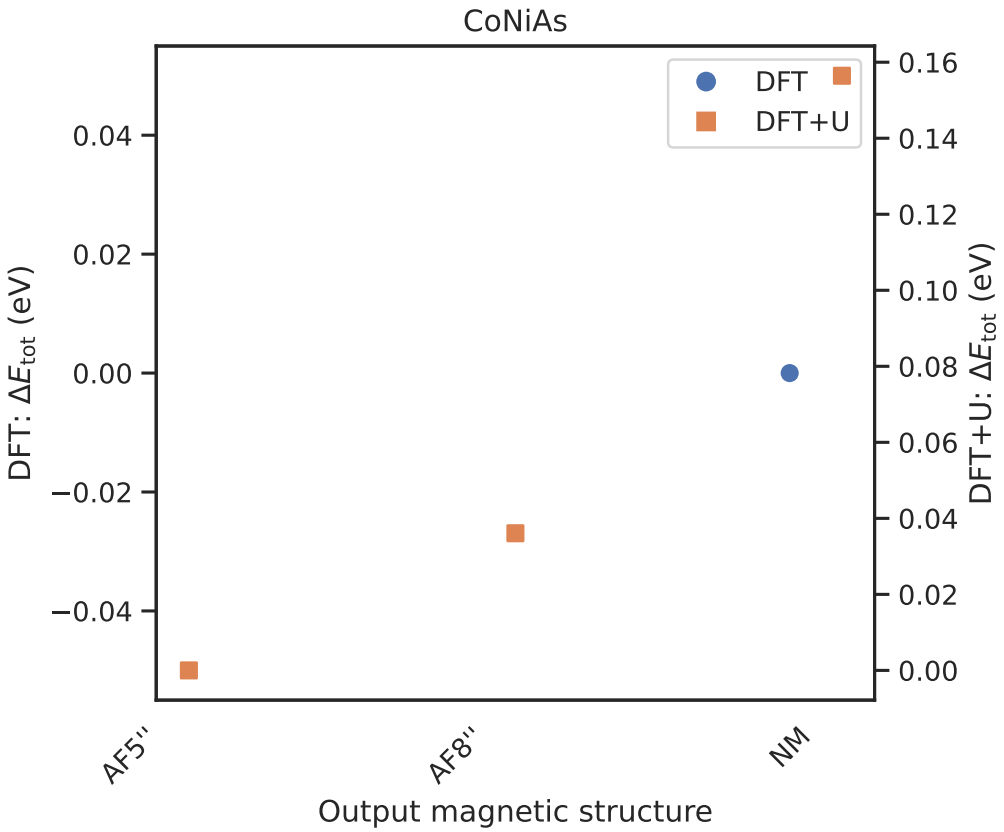


Figure 68: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-45736.503911	0.000000	1.20, -1.20, 0.00, 0.00, 1.20, -1.20, 0.00, 0.00
AF5″	-45736.503911	0.000000	1.20, -1.20, 0.00, 0.00, 1.20, -1.20, 0.00, 0.00
AF5″	-45736.503911	0.000000	1.20, -1.20, 0.00, 0.00, 1.20, -1.20, 0.00, 0.00
AF8″	-45736.467832	0.036079	1.13, -1.13, 0.00, 0.00, -1.13, 1.13, 0.00, 0.00
AF8″	-45736.467831	0.036081	1.13, -1.13, 0.00, 0.00, -1.13, 1.13, 0.00, 0.00
AF8″	-45736.467830	0.036081	1.13, -1.13, 0.00, 0.00, -1.13, 1.13, 0.00, 0.00
NM	-45736.347471	0.156441	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45736.347470	0.156441	0.00, -0.00, -0.00, -0.00, 0.00, 0.00, -0.00, -0.00
NM	-45736.347470	0.156442	-0.00, 0.00, 0.00, 0.00, -0.00, 0.00, 0.00, 0.00
NM	-45736.347469	0.156442	0.00, -0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45736.347469	0.156443	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45736.347469	0.156443	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 73: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

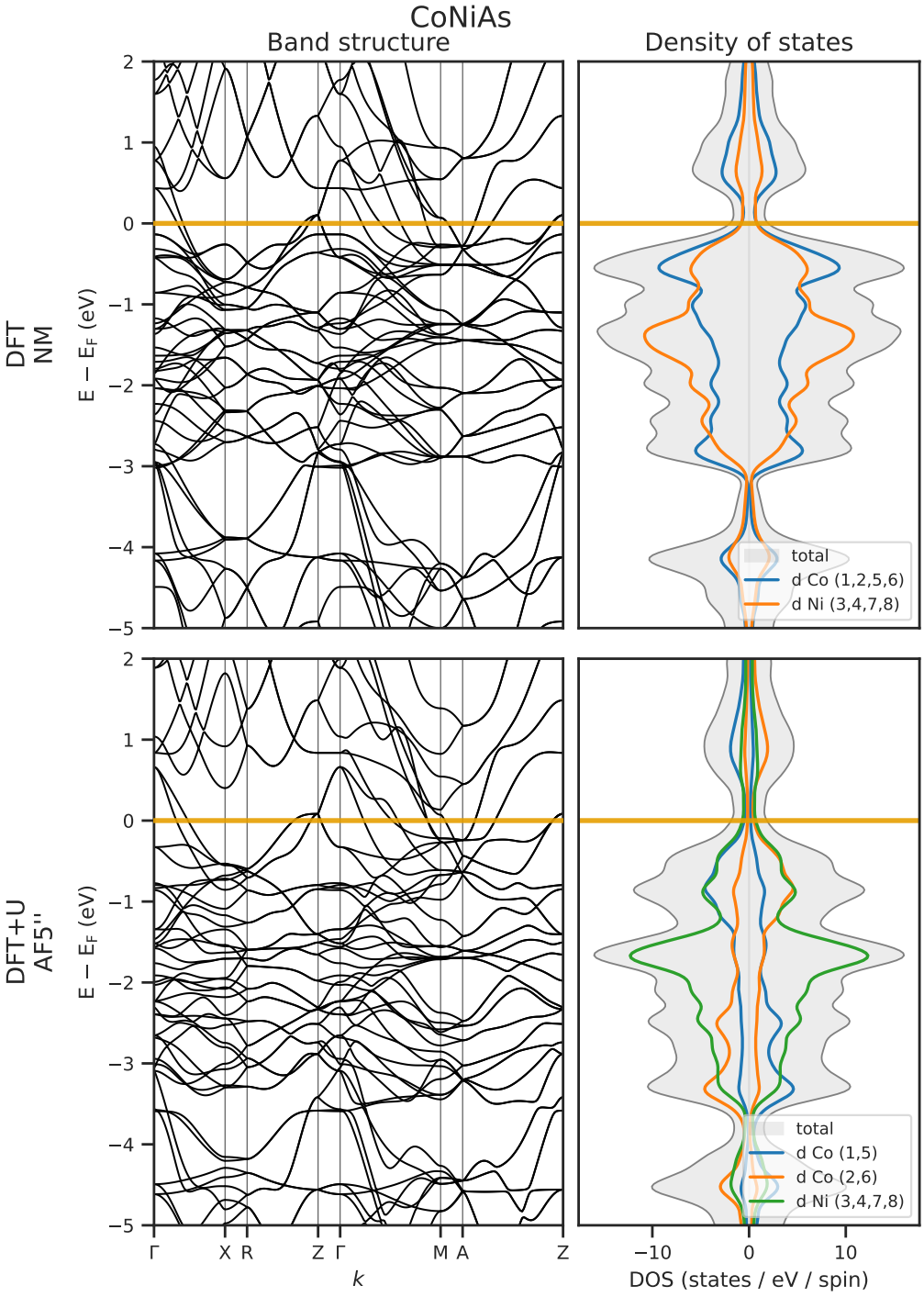


Figure 69: Band structure and Density of states of the lowest in energy calculations.

Configuration: NiCoAs ■ higher-energy

Structure

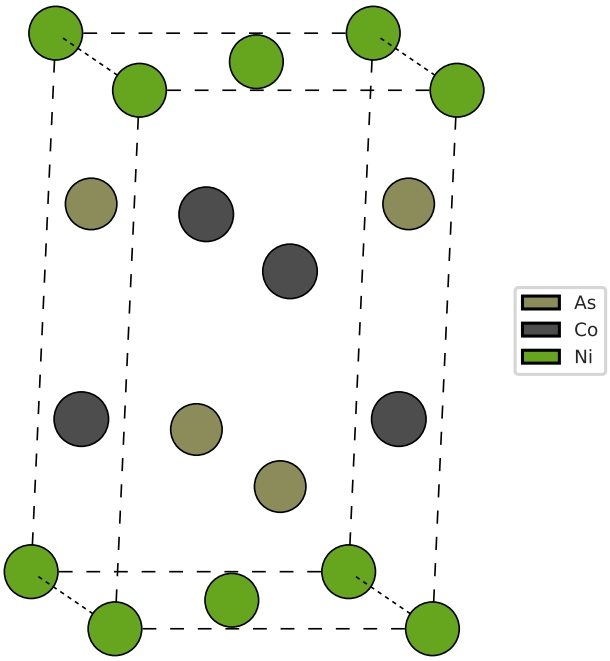


Figure 70: Structure of NiCoAs

a (Å)	c (Å)	z_1	z_2
3.5129	6.0804	0.3563	0.2690

Table 74: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-45753.931150	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45753.926592	0.004558	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 75: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

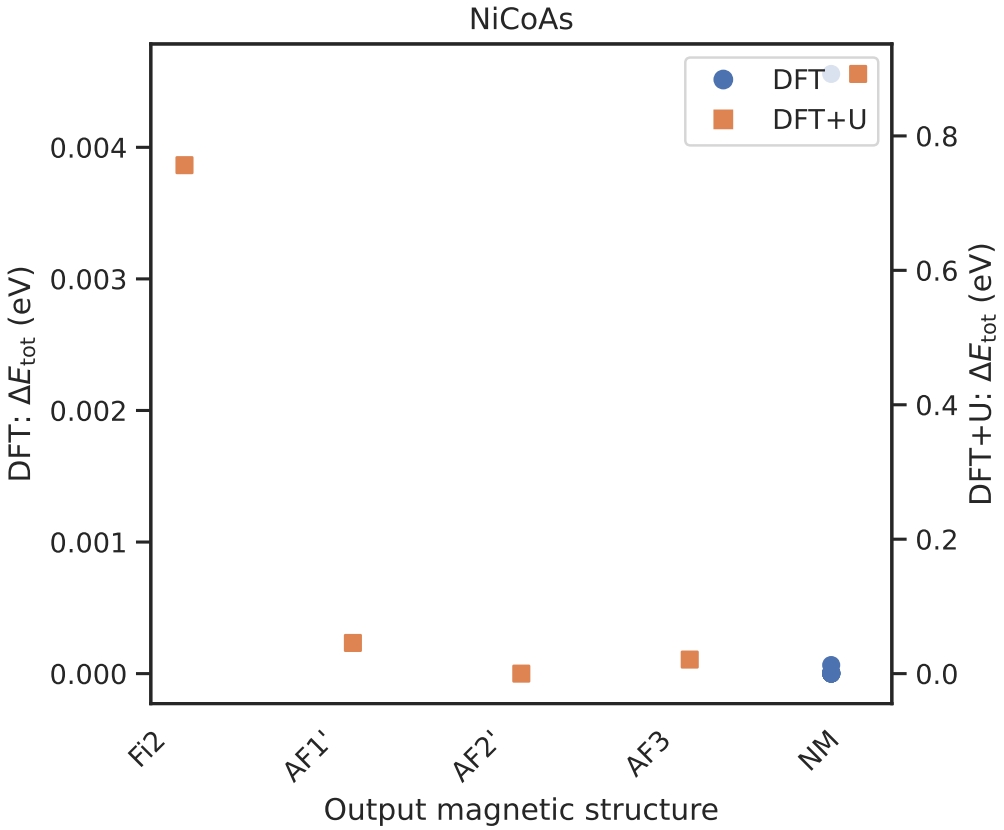


Figure 71: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-45736.592640	0.000000	0.00, 0.00, -1.64, 1.64, 0.00, 0.00, -1.64, 1.64
AF2′	-45736.592638	0.000002	0.00, 0.00, -1.64, 1.64, 0.00, 0.00, -1.64, 1.64
AF2′	-45736.592638	0.000002	0.00, 0.00, -1.64, 1.64, 0.00, 0.00, -1.64, 1.64
AF3	-45736.571729	0.020911	-0.21, -0.21, 1.61, -1.61, 0.21, 0.21, -1.61, 1.61
AF3	-45736.571728	0.020912	0.21, 0.21, -1.61, 1.61, -0.21, -0.21, 1.61, -1.61
AF3	-45736.571725	0.020915	0.21, 0.21, -1.61, 1.61, -0.21, -0.21, 1.61, -1.61
AF3	-45736.571724	0.020916	0.21, 0.21, -1.61, 1.61, -0.21, -0.21, 1.61, -1.61
AF1′	-45736.547014	0.045626	0.00, 0.00, 1.77, 1.77, 0.00, 0.00, -1.77, -1.77
AF1′	-45736.547010	0.045630	0.00, 0.00, 1.77, 1.77, 0.00, 0.00, -1.77, -1.77
Fi2	-45735.836162	0.756478	0.08, 0.08, -0.15, -1.45, 0.19, 0.19, -0.09, -0.08
NM	-45735.700413	0.892227	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45735.700349	0.892291	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 76: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

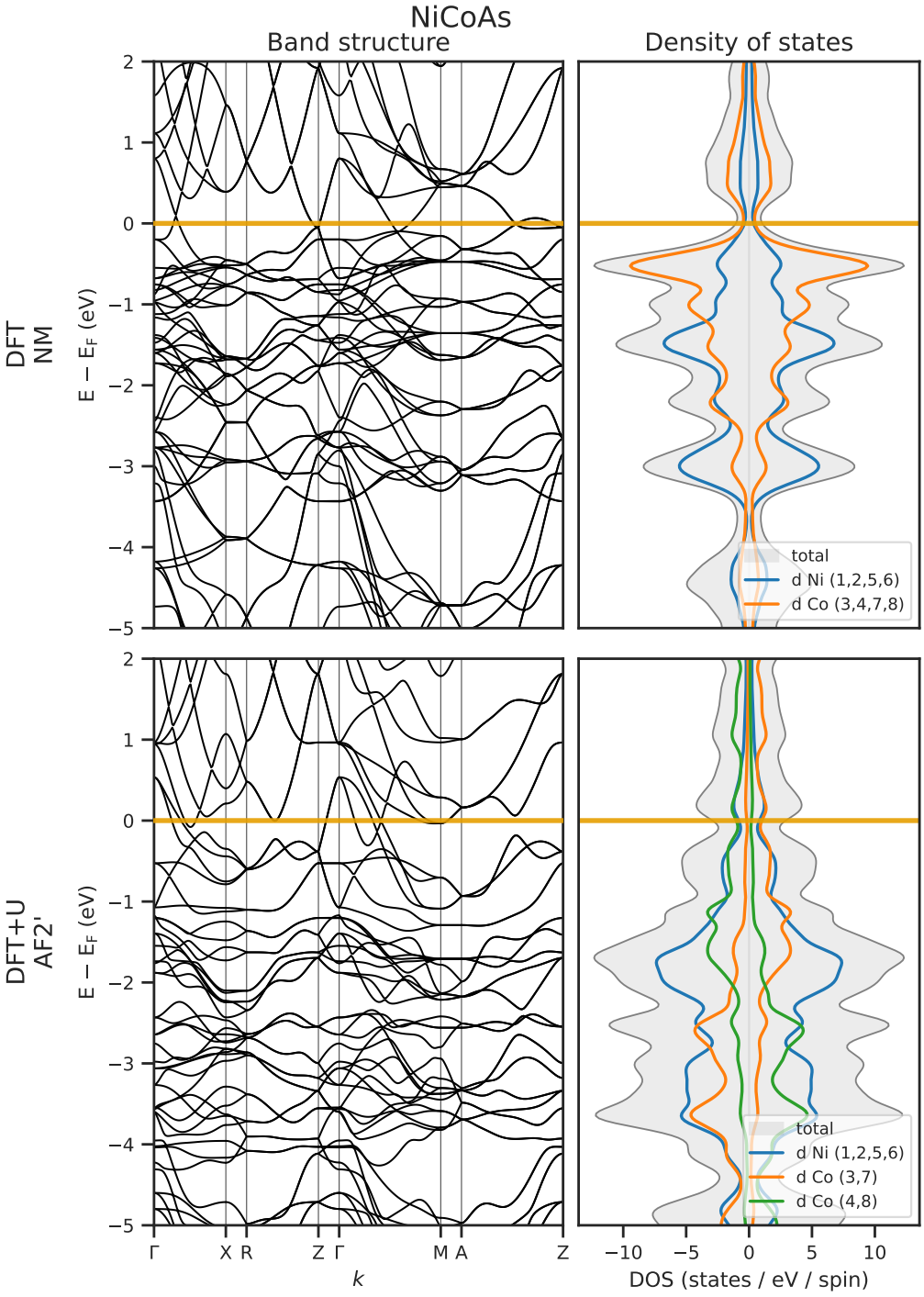


Figure 72: Band structure and Density of states of the lowest in energy calculations.

Material: CoNiSb

Configuration: CoNiSb ■ lower-energy

Structure

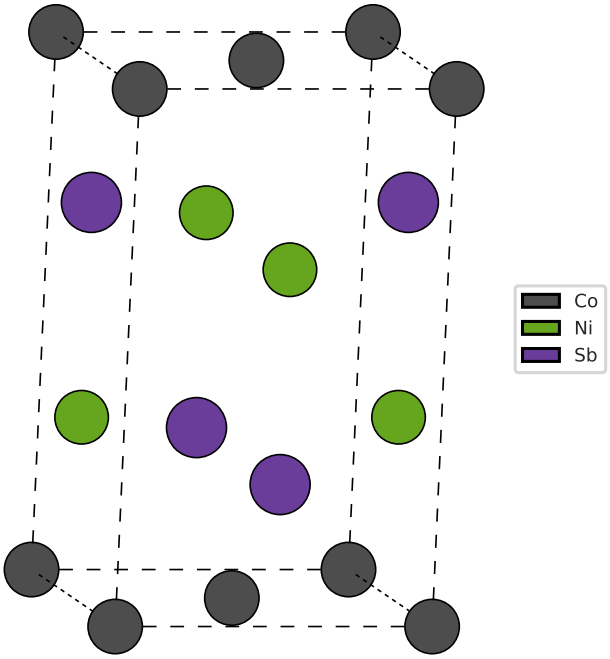


Figure 73: Structure of CoNiSb

a (Å)	c (Å)	z_1	z_2
3.8436	6.0580	0.2778	0.2915

Table 77: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Co atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-43639.702698	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 78: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

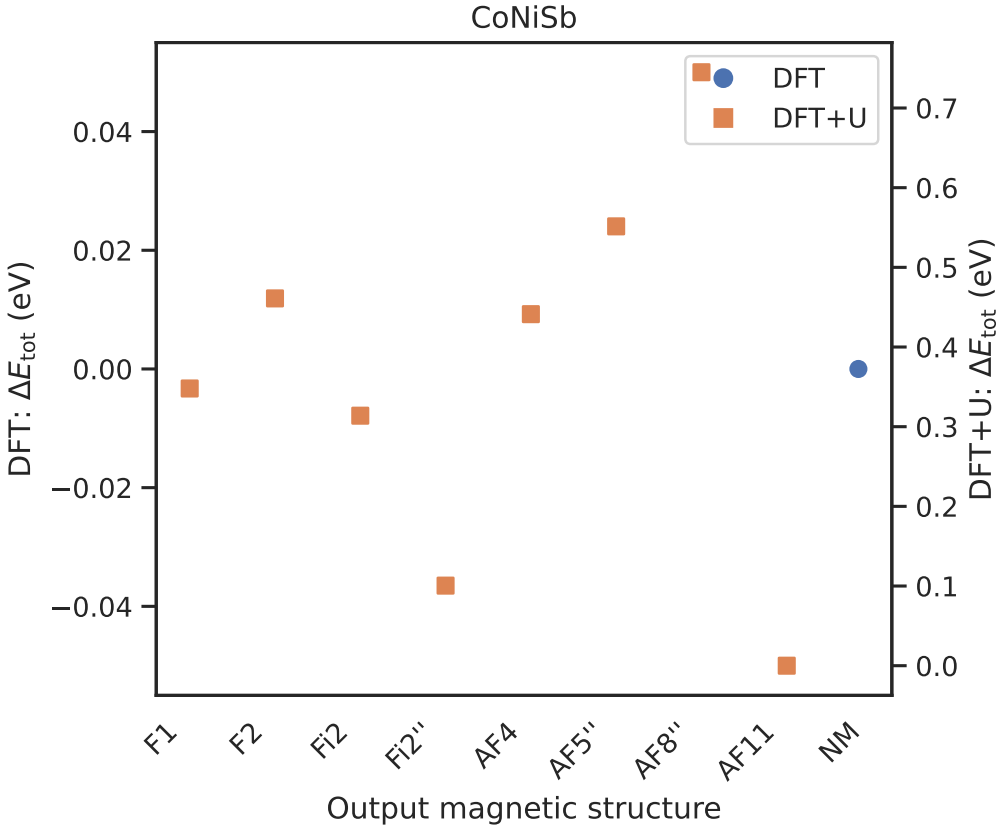


Figure 74: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF11	-43623.509300	0.000000	1.90, 1.89, -0.01, -0.27, -1.84, -1.84, 0.09, 0.19
Fi2″	-43623.408792	0.100509	1.94, -1.62, 0.04, 0.00, -2.04, 2.04, 0.00, 0.04
Fi2	-43623.195488	0.313812	1.97, 1.97, 0.11, 0.03, -1.84, -1.84, 0.03, 0.11
F1	-43623.161352	0.347949	1.93, 1.93, 0.10, 0.10, 1.93, 1.93, 0.10, 0.10
AF4	-43623.068063	0.441237	1.98, 1.98, 0.17, -0.17, -1.98, -1.98, -0.17, 0.17
F2	-43623.048273	0.461028	1.90, 1.90, 0.16, -0.02, 1.84, 1.84, -0.02, 0.16
AF5″	-43622.957847	0.551454	1.77, -1.77, 0.00, 0.00, 1.77, -1.77, 0.00, 0.00
AF5″	-43622.957847	0.551454	1.77, -1.77, 0.00, 0.00, 1.77, -1.77, 0.00, 0.00
AF5″	-43622.957847	0.551454	1.77, -1.77, 0.00, 0.00, 1.77, -1.77, 0.00, 0.00
AF8″	-43622.764399	0.744901	1.75, -1.75, 0.00, 0.00, -1.75, 1.75, 0.00, 0.00
AF8″	-43622.764399	0.744901	1.75, -1.75, 0.00, 0.00, -1.75, 1.75, 0.00, 0.00

Table 79: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

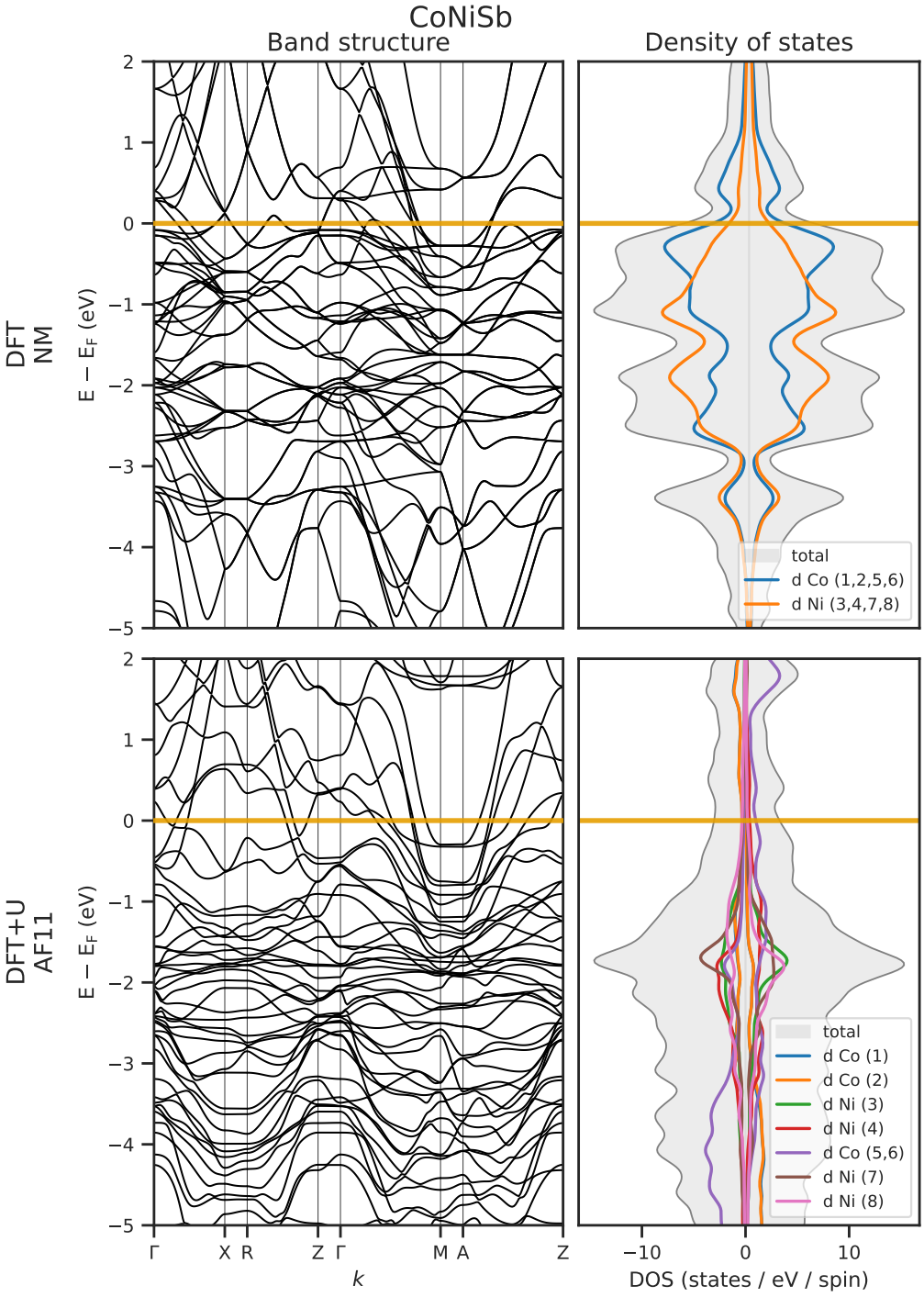


Figure 75: Band structure and Density of states of the lowest in energy calculations.

Configuration: NiCoSb ■ higher-energy

Structure

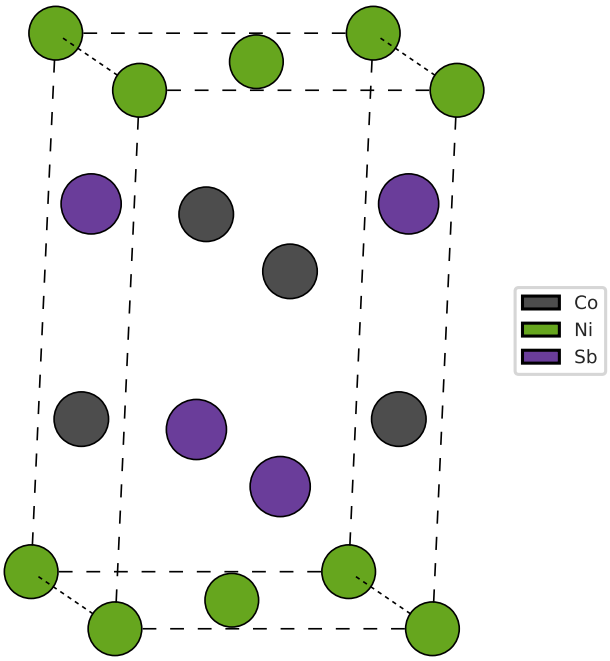


Figure 76: Structure of NiCoSb

a (Å)	c (Å)	z_1	z_2
3.7475	6.3768	0.3308	0.2763

Table 80: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Co atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-43638.325181	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 81: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

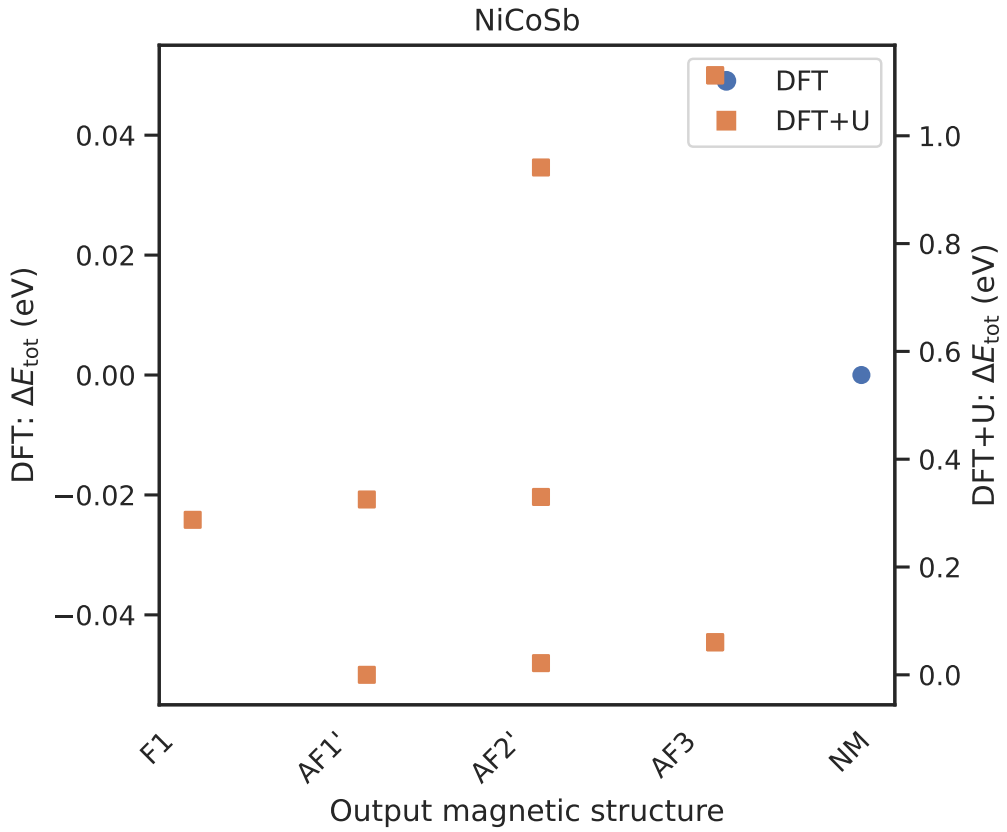


Figure 77: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1′	-43622.498549	0.000000	0.06, -0.06, 1.87, 1.87, -0.06, 0.06, -1.87, -1.87
AF2′	-43622.476857	0.021692	0.00, 0.00, -1.79, 1.79, 0.00, 0.00, -1.79, 1.79
AF3	-43622.438141	0.060408	0.28, 0.28, -1.78, 1.78, -0.28, -0.28, 1.78, -1.78
AF3	-43622.438141	0.060408	0.28, 0.28, -1.78, 1.78, -0.28, -0.28, 1.78, -1.78
F1	-43622.211016	0.287533	0.24, 0.24, 2.00, 2.00, 0.24, 0.24, 2.00, 2.00
AF1′	-43622.173276	0.325273	0.00, -0.00, 2.04, 2.03, 0.00, 0.00, -2.03, -2.04
AF2′	-43622.168561	0.329988	0.01, -0.07, -1.82, 1.83, 0.09, -0.07, -1.81, 1.86
AF2′	-43621.557357	0.941192	0.00, 0.00, -1.75, 1.74, 0.00, 0.00, -1.74, 1.75
AF3	-43621.386530	1.112019	0.21, 0.21, -1.67, 1.66, -0.21, -0.21, 1.66, -1.67
AF3	-43621.386204	1.112345	-0.21, -0.21, 1.67, -1.66, 0.21, 0.21, -1.66, 1.67

Table 82: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

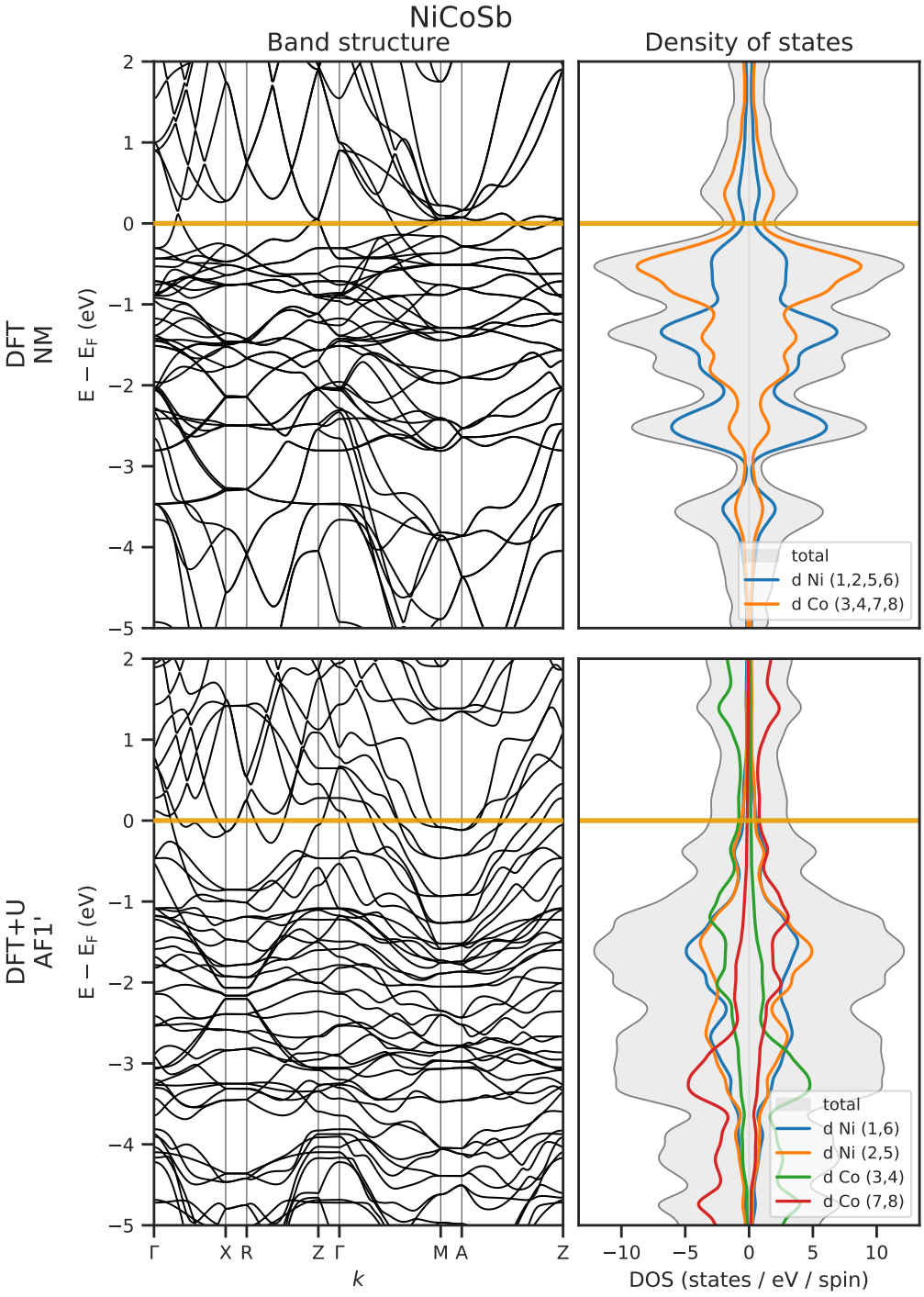


Figure 78: Band structure and Density of states of the lowest in energy calculations.

Material: Cr_2As

Configuration: Cr_2As

Structure

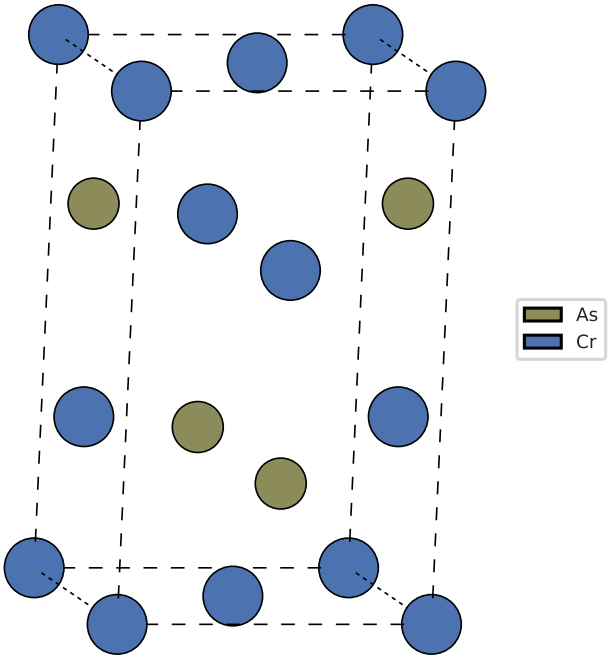


Figure 79: Structure of Cr_2As

a (Å)	c (Å)	z_1	z_2
3.6448	6.4074	0.3381	0.2707

Table 83: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

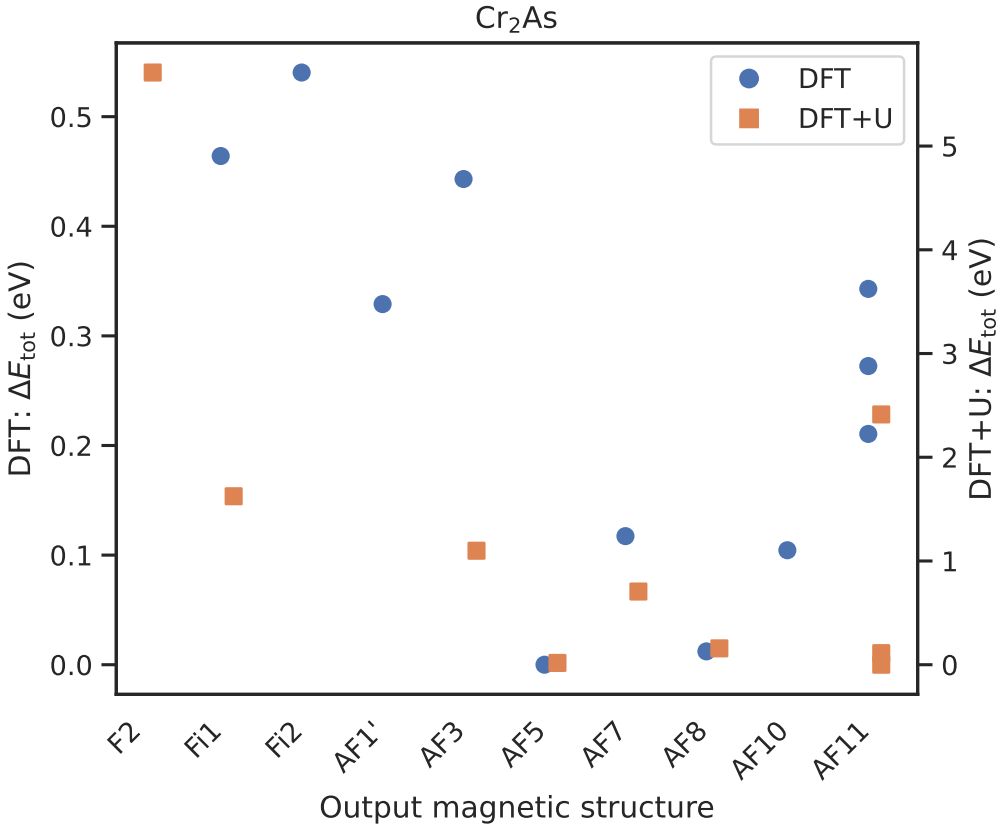


Figure 80: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5	-30593.047933	0.000000	1.93, -1.93, -3.19, 3.19, 1.93, -1.93, -3.19, 3.19
AF8	-30593.035777	0.012155	1.80, -1.80, -3.18, 3.18, -1.80, 1.80, -3.18, 3.18
AF10	-30592.943491	0.104442	1.76, -1.76, 2.70, 2.70, -1.76, 1.76, -2.70, -2.70
AF7	-30592.930620	0.117313	1.76, -1.76, 2.72, 2.72, 1.76, -1.76, -2.72, -2.72
AF11	-30592.837377	0.210555	2.91, -2.16, -3.16, 3.16, 2.16, -2.91, 3.16, -3.16
AF11	-30592.775463	0.272470	0.63, 0.63, -3.29, 3.29, -0.63, -0.63, -3.14, 3.14
AF1′	-30592.718923	0.329010	0.00, 0.00, 2.92, 2.92, 0.00, 0.00, -2.92, -2.92
AF11	-30592.705041	0.342892	2.79, -1.85, -3.07, 3.07, -2.79, 1.85, 3.07, -3.07
AF3	-30592.604823	0.443109	1.62, 1.62, -2.94, 2.94, -1.63, -1.63, 2.94, -2.94
Fi1	-30592.583846	0.464087	1.83, 1.83, -2.47, -2.47, 1.83, 1.83, -2.47, -2.47
Fi2	-30592.507662	0.540271	-0.19, -2.30, 2.38, 2.50, -1.86, -1.83, 2.50, 2.38

Table 84: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF11	-30576.889542	0.000000	4.63, -4.27, -4.51, 4.51, 4.27, -4.63, 4.51, -4.51
AF5	-30576.872235	0.017307	4.46, -4.46, -4.53, 4.53, 4.46, -4.46, -4.53, 4.53
AF11	-30576.778104	0.111438	4.63, -4.28, -4.51, 4.51, -4.63, 4.28, 4.51, -4.51
AF8	-30576.731887	0.157655	4.45, -4.45, -4.54, 4.54, -4.45, 4.45, -4.54, 4.54
AF7	-30576.183980	0.705561	4.50, -4.50, 4.50, 4.50, 4.50, -4.50, -4.50, -4.50
AF3	-30575.790578	1.098964	4.33, 4.33, -4.59, 4.59, -4.33, -4.33, 4.59, -4.59
Fi1	-30575.265420	1.624122	4.43, 4.43, -4.39, -4.39, 4.43, 4.43, -4.39, -4.39
AF11	-30574.476646	2.412896	4.22, 4.22, -4.60, 4.60, -4.22, -4.22, -4.41, 4.40
F2	-30571.180585	5.708957	3.93, 3.93, 4.32, 4.52, 0.52, -0.03, 4.47, 4.34

Table 85: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

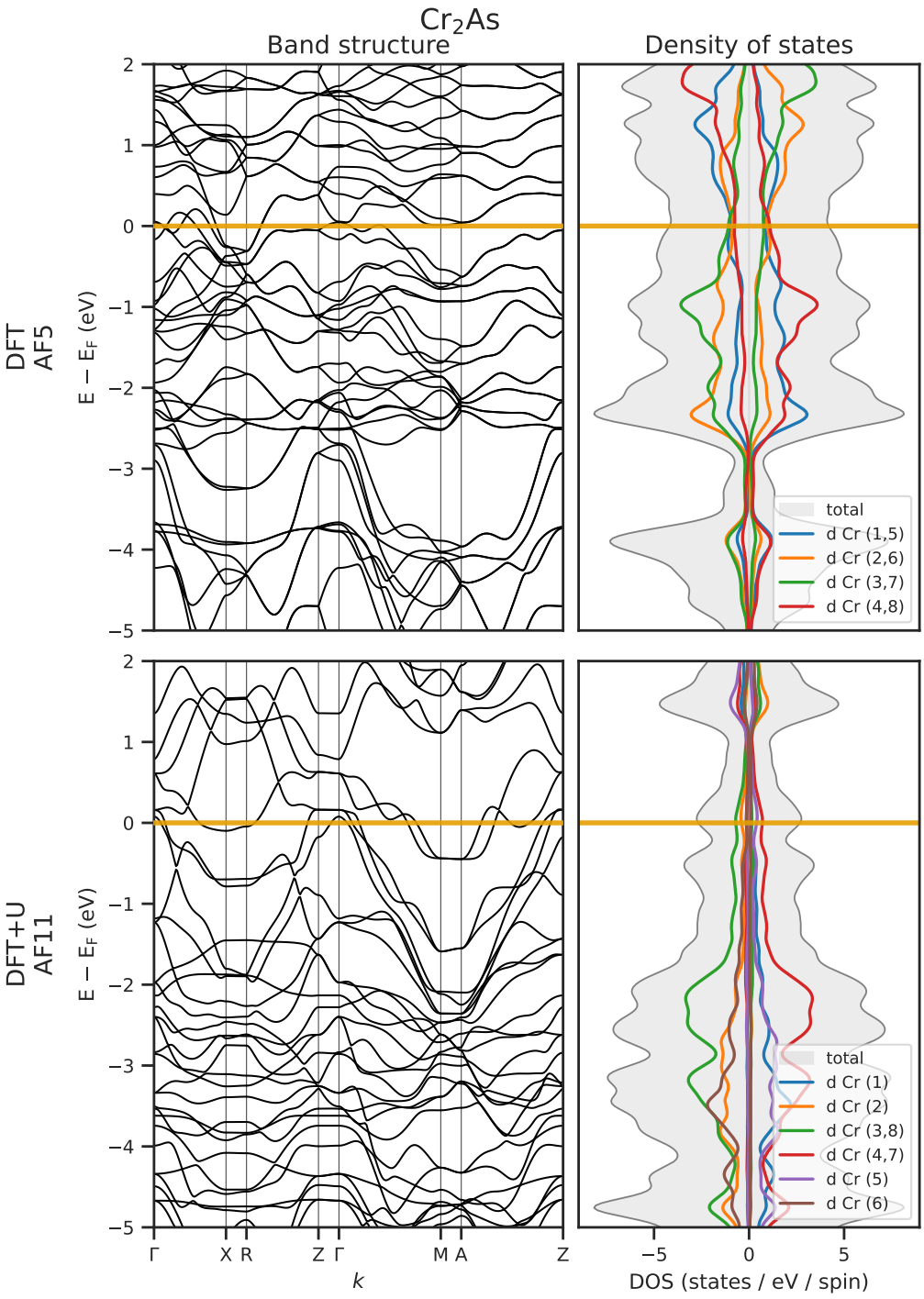


Figure 81: Band structure and Density of states of the lowest in energy calculations.

Material: Cr_2Sb

Configuration: Cr_2Sb

Structure

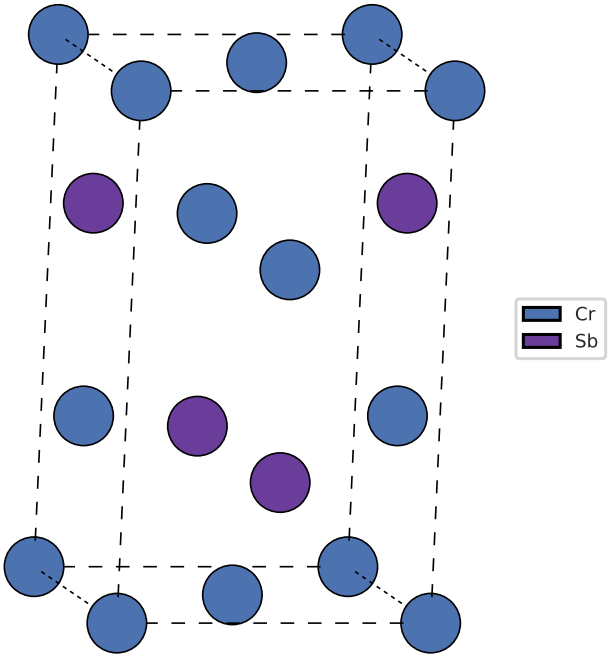


Figure 82: Structure of Cr_2Sb

a (Å)	c (Å)	z_1	z_2
4.0666	6.7363	0.2944	0.2902

Table 86: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of an Sb atom in the unit cell.

Magnetic structure and energy

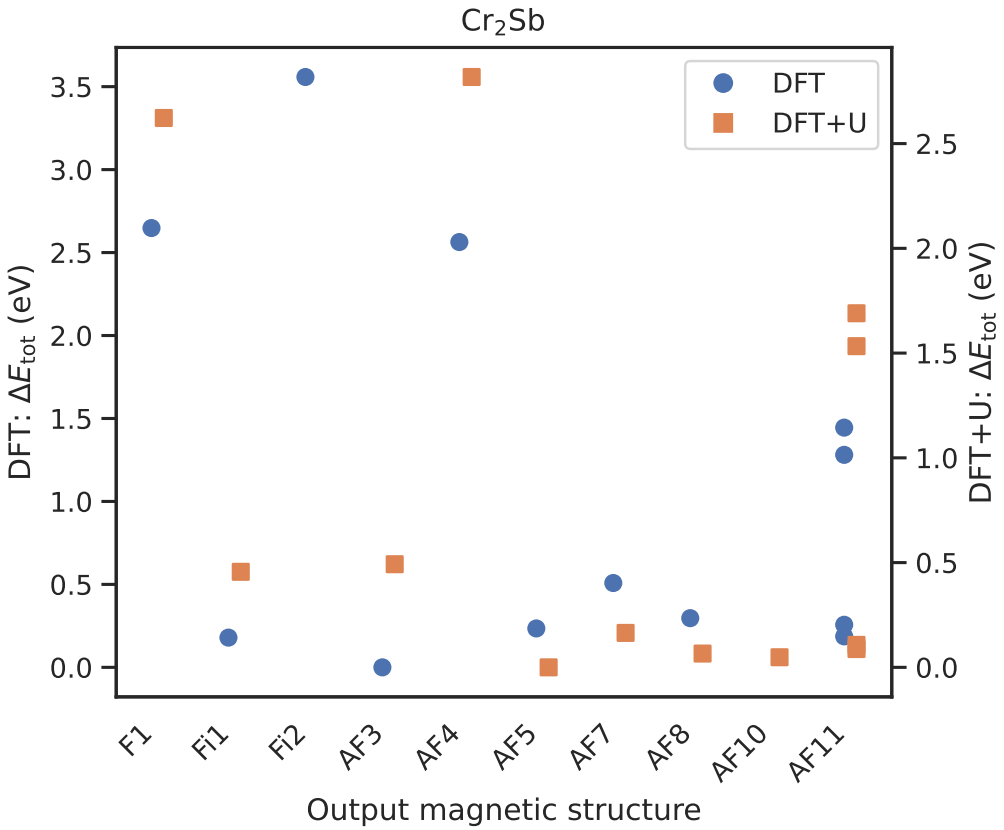


Figure 83: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-28476.949811	0.000000	3.62, 3.62, -3.87, 3.87, -3.62, -3.62, 3.87, -3.87
Fi1	-28476.770566	0.179244	3.67, 3.67, -3.88, -3.88, 3.67, 3.67, -3.88, -3.88
AF11	-28476.763142	0.186669	3.80, -3.55, -3.98, 3.98, 3.55, -3.80, 3.98, -3.98
AF5	-28476.715306	0.234505	3.68, -3.68, -3.99, 3.99, 3.68, -3.68, -3.99, 3.99
AF11	-28476.693112	0.256698	3.80, -3.58, -4.01, 4.01, -3.80, 3.58, 4.01, -4.01
AF8	-28476.653344	0.296467	3.66, -3.66, -3.99, 3.99, -3.66, 3.66, -3.99, 3.99
AF7	-28476.441565	0.508245	3.65, -3.65, 3.98, 3.98, 3.65, -3.65, -3.98, -3.98
AF11	-28475.669012	1.280799	2.64, 2.64, -3.95, 3.95, -2.64, -2.64, -3.60, 3.60
AF11	-28475.505007	1.444804	2.74, 2.74, 3.58, 3.95, -2.74, -2.74, -3.58, -3.95
AF4	-28474.386444	2.563366	2.20, 2.20, 3.83, -3.83, -2.20, -2.20, -3.83, 3.83
F1	-28474.302019	2.647792	1.90, 1.96, 3.81, 3.81, 1.96, 1.90, 3.81, 3.81
Fi2	-28473.391616	3.558194	-3.22, -3.22, -0.44, 0.05, -0.16, -0.16, -0.07, 3.93

Table 87: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5	-28465.692086	0.000000	4.77, -4.77, -4.74, 4.74, 4.77, -4.77, -4.74, 4.74
AF10	-28465.643858	0.048228	4.77, -4.77, 4.77, 4.77, -4.77, 4.77, -4.77, -4.77
AF8	-28465.626268	0.065819	4.77, -4.77, -4.73, 4.73, -4.77, 4.77, -4.73, 4.73
AF11	-28465.604728	0.087358	4.90, -4.65, -4.72, 4.72, -4.90, 4.65, 4.72, -4.72
AF11	-28465.584866	0.107220	4.90, -4.65, -4.72, 4.72, 4.65, -4.90, 4.72, -4.72
AF7	-28465.527716	0.164371	4.78, -4.78, 4.77, 4.77, 4.78, -4.78, -4.77, -4.77
Fi1	-28465.236036	0.456050	4.71, 4.71, -4.86, -4.86, 4.71, 4.71, -4.86, -4.86
AF3	-28465.199853	0.492233	4.68, 4.68, -4.84, 4.84, -4.68, -4.68, 4.84, -4.84
AF11	-28464.158985	1.533102	4.67, 4.67, -4.86, 4.86, -4.67, -4.67, -4.73, 4.73
AF11	-28464.001951	1.690136	4.66, 4.66, 4.75, 4.87, -4.66, -4.66, -4.75, -4.87
F1	-28463.069814	2.622273	4.70, 4.70, 4.82, 4.82, 4.70, 4.70, 4.82, 4.82
AF4	-28462.874214	2.817872	4.65, 4.65, 4.74, -4.74, -4.65, -4.65, -4.74, 4.74

Table 88: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

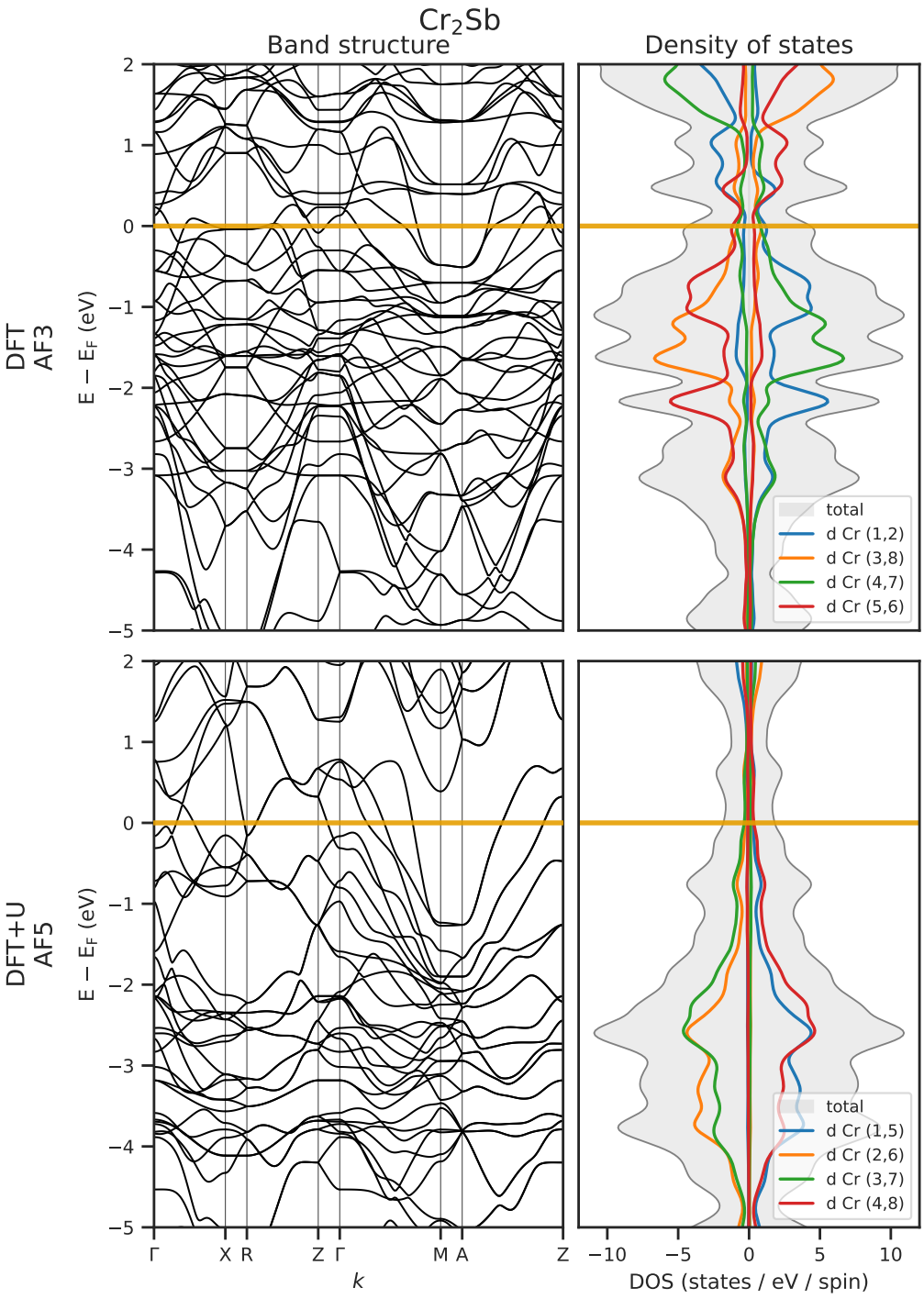


Figure 84: Band structure and Density of states of the lowest in energy calculations.

Material: CrCuAs

Configuration: CrCuAs ■ lower-energy

Structure

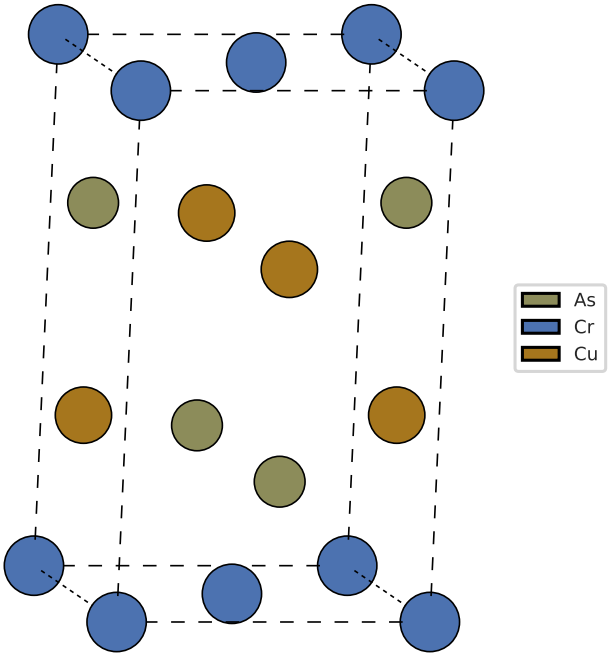


Figure 85: Structure of CrCuAs

a (Å)	c (Å)	z_1	z_2
3.7998	6.1013	0.3101	0.2811

Table 89: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-42589.157279	0.000000	2.56, -2.56, 0.00, 0.00, -2.56, 2.56, 0.00, 0.00
AF5″	-42589.154002	0.003277	2.54, -2.54, 0.00, 0.00, 2.54, -2.54, 0.00, 0.00
F1″	-42588.533482	0.623797	0.92, 0.92, -0.04, -0.04, 0.92, 0.92, -0.04, -0.04
AF1″	-42588.533043	0.624236	0.84, 0.84, -0.03, 0.03, -0.84, -0.84, 0.03, -0.03

Table 90: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

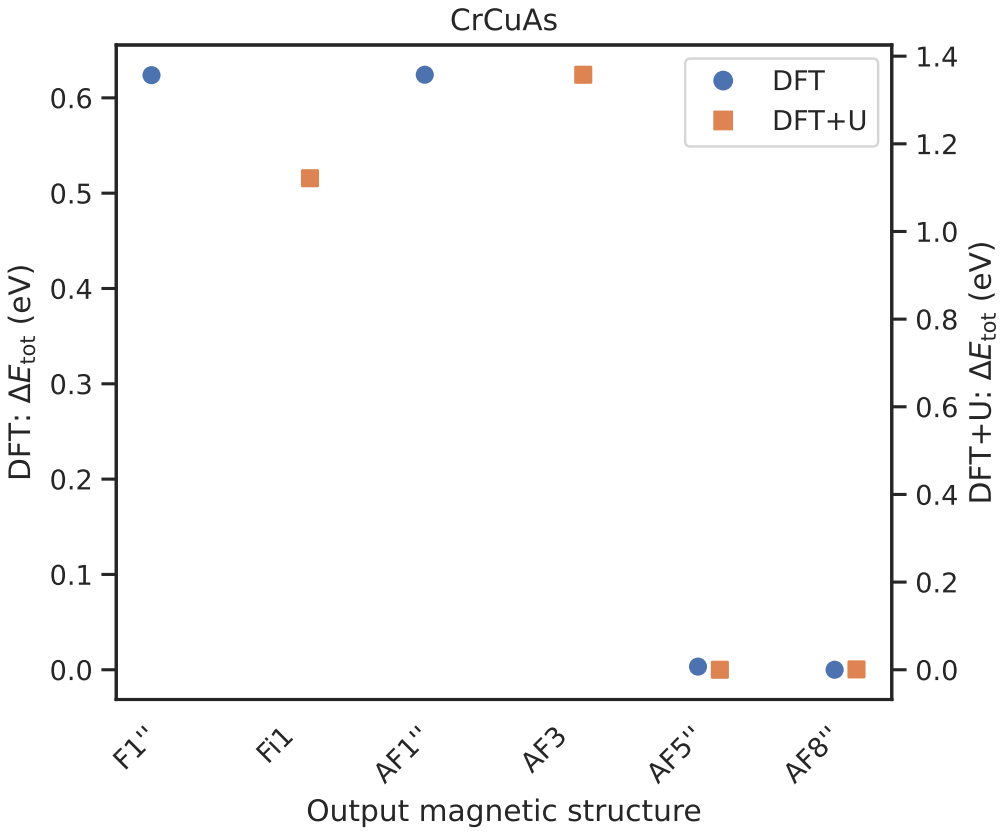


Figure 86: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-42580.618776	0.000000	4.46, -4.46, 0.00, 0.00, 4.46, -4.46, 0.00, 0.00
AF8″	-42580.617994	0.000782	4.47, -4.47, 0.00, 0.00, -4.47, 4.47, 0.00, 0.00
Fi1	-42579.497298	1.121478	4.27, 4.27, -0.14, -0.14, 4.27, 4.27, -0.14, -0.14
AF3	-42579.261162	1.357614	4.28, 4.28, -0.15, 0.15, -4.28, -4.28, 0.15, -0.15

Table 91: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

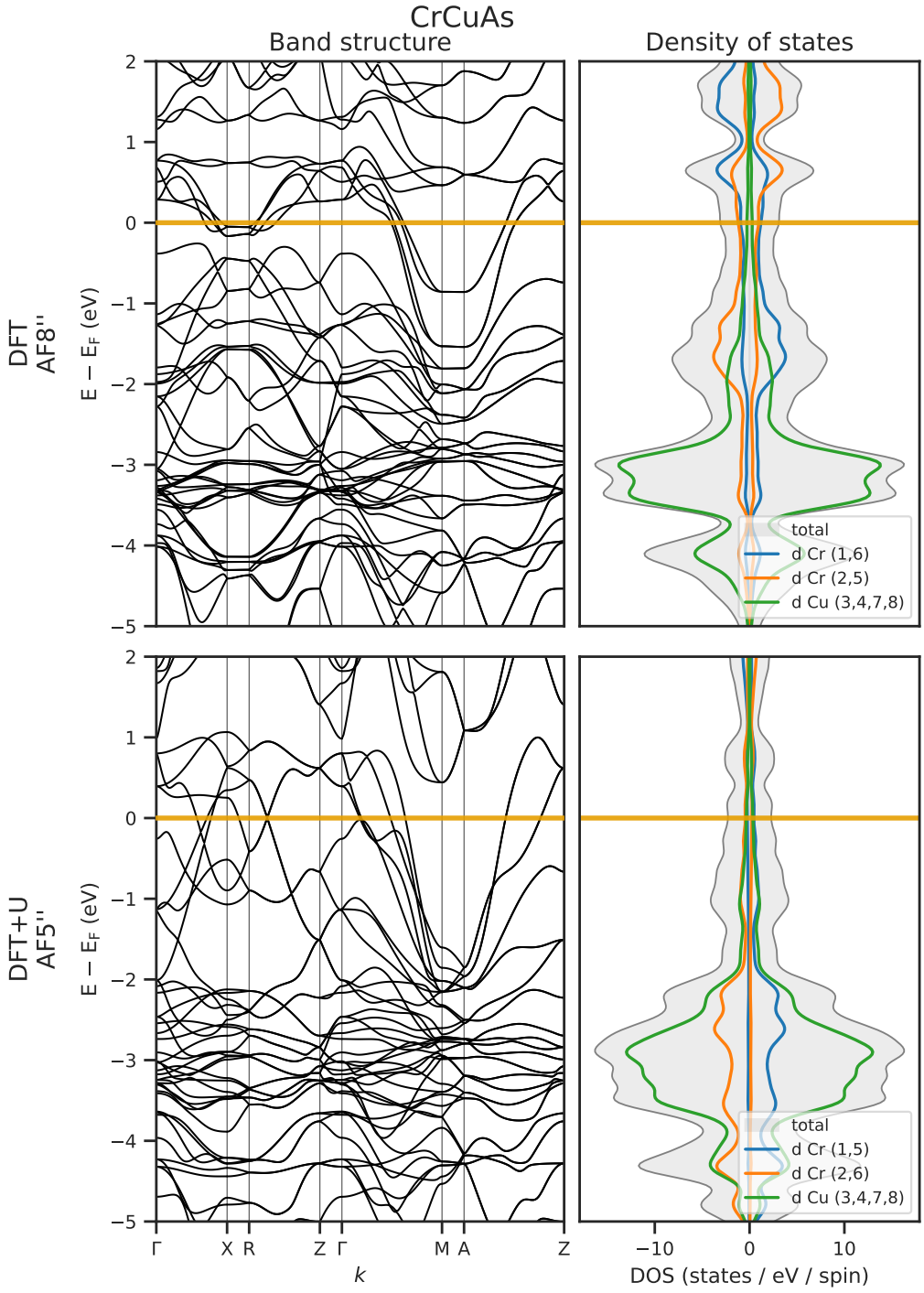


Figure 87: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuCrAs ■ higher-energy

Structure

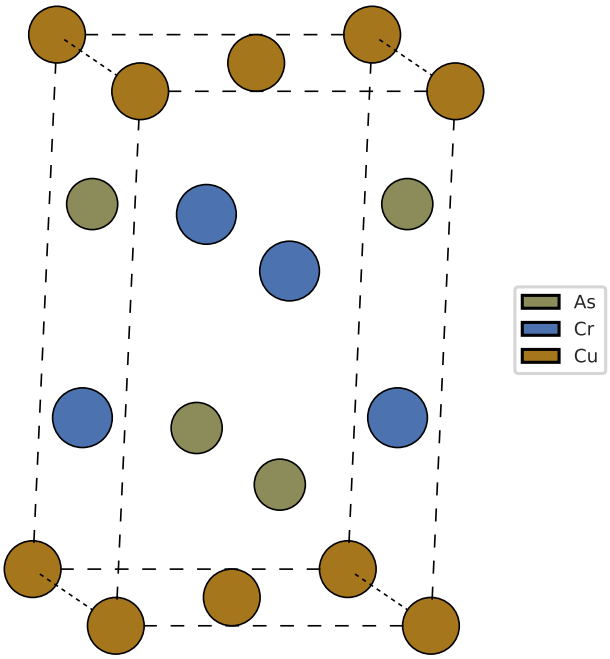


Figure 88: Structure of CuCrAs

a (Å)	c (Å)	z_1	z_2
3.6342	6.6712	0.3482	0.2708

Table 92: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-42588.855574	0.000000	0.00, 0.00, -3.60, 3.60, 0.00, 0.00, -3.60, 3.60
AF3′	-42588.768241	0.087333	0.04, 0.04, -3.61, 3.61, -0.04, -0.04, 3.61, -3.61
AF1′	-42588.611922	0.243652	0.00, 0.00, 3.41, 3.41, 0.00, 0.00, -3.41, -3.41
F1′	-42588.328693	0.526881	-0.04, -0.04, 3.37, 3.37, -0.04, -0.04, 3.37, 3.37

Table 93: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

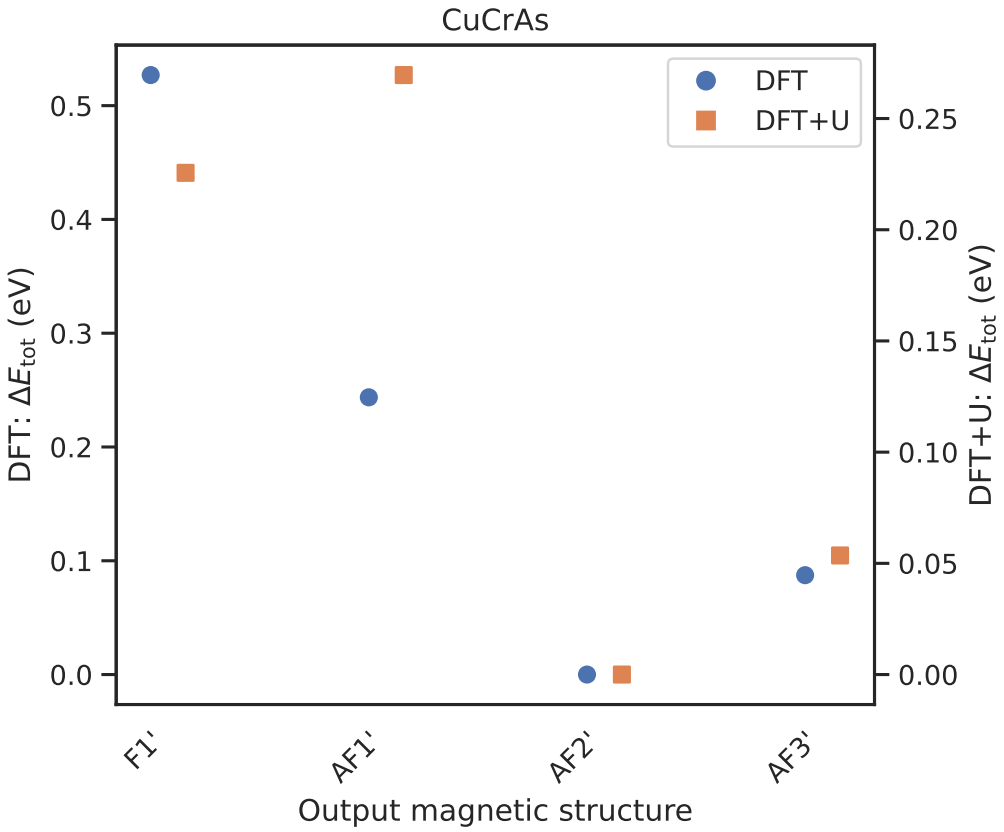


Figure 89: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-42582.474532	0.000000	0.00, 0.00, -4.48, 4.48, 0.00, 0.00, -4.48, 4.48
AF3′	-42582.420984	0.053548	0.10, 0.10, -4.50, 4.50, -0.10, -0.10, 4.50, -4.50
F1′	-42582.248947	0.225585	-0.05, -0.05, 4.53, 4.53, -0.05, -0.05, 4.53, 4.53
AF1′	-42582.204984	0.269548	0.00, 0.00, 4.46, 4.46, 0.00, 0.00, -4.46, -4.46

Table 94: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

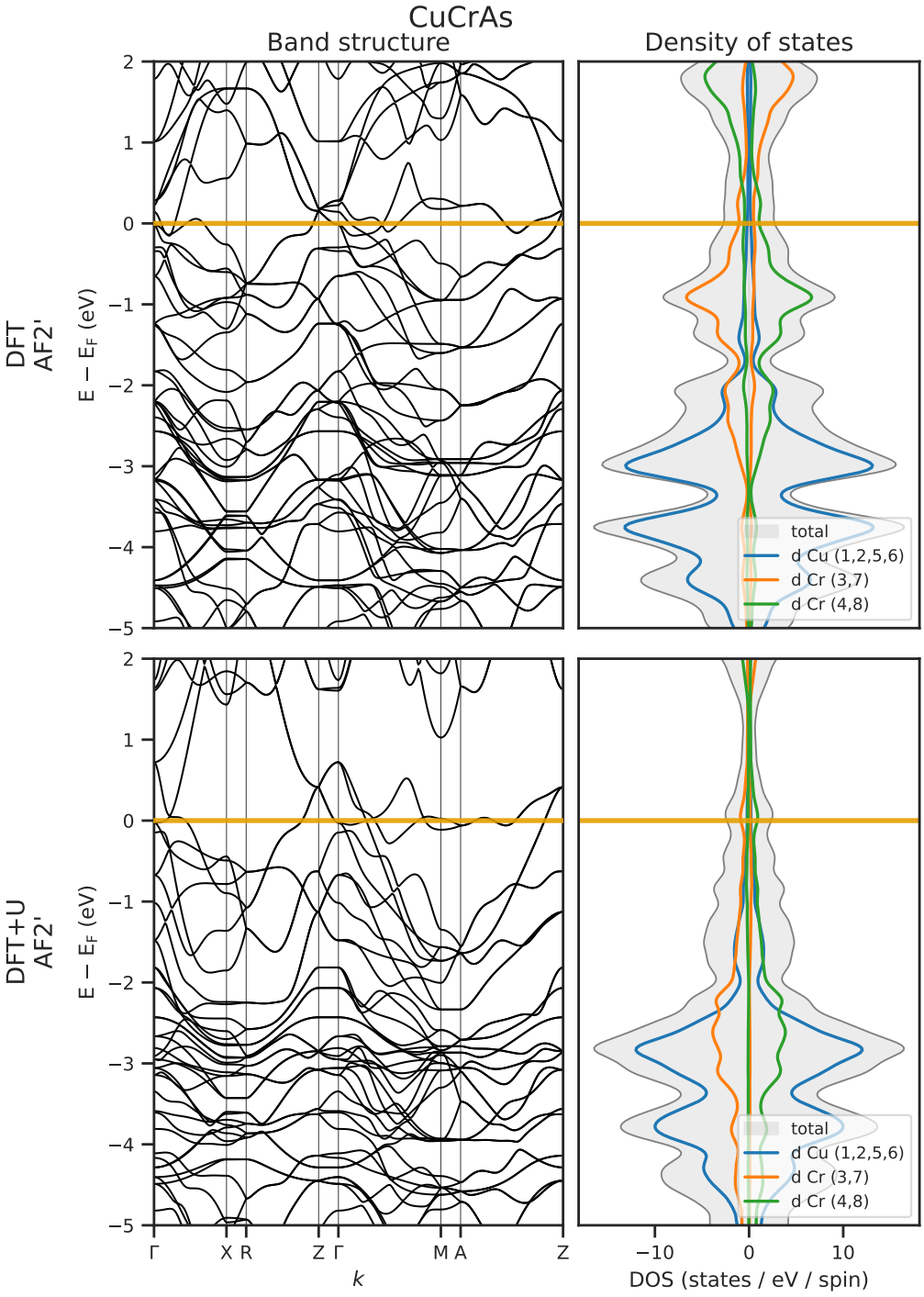


Figure 90: Band structure and Density of states of the lowest in energy calculations.

Material: CrCuSb

Configuration: CrCuSb ■ lower-energy

Structure

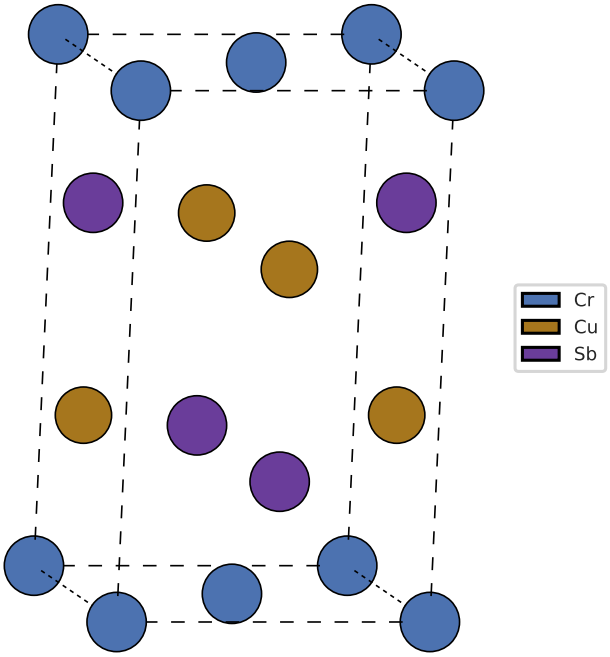


Figure 91: Structure of CrCuSb

a (Å)	c (Å)	z_1	z_2
4.0135	6.5678	0.2731	0.3026

Table 95: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-40474.690603	0.000000	3.56, -3.56, 0.00, 0.00, 3.56, -3.56, 0.00, 0.00
AF8″	-40474.649694	0.040909	3.53, -3.53, 0.00, 0.00, -3.53, 3.53, 0.00, 0.00
AF1″	-40473.688671	1.001932	3.54, 3.54, -0.08, 0.08, -3.54, -3.54, 0.08, -0.08
F1″	-40473.646590	1.044013	3.54, 3.54, -0.08, -0.08, 3.54, 3.54, -0.08, -0.08

Table 96: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

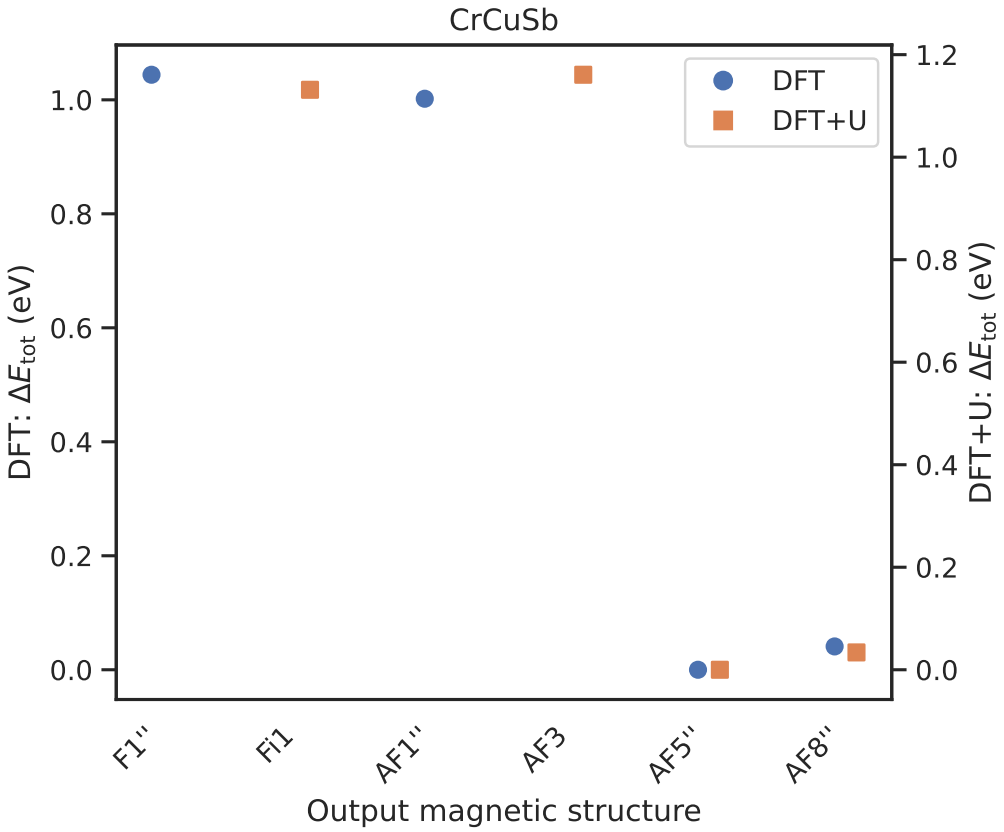


Figure 92: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF5″	-40468.383671	0.000000	4.71, -4.71, 0.00, 0.00, 4.71, -4.71, 0.00, 0.00
AF8″	-40468.349854	0.033817	4.72, -4.72, 0.00, 0.00, -4.72, 4.72, 0.00, 0.00
Fi1	-40467.252198	1.131473	4.49, 4.49, -0.16, -0.16, 4.49, 4.49, -0.16, -0.16
AF3	-40467.222862	1.160809	4.55, 4.55, -0.13, 0.13, -4.55, -4.55, 0.13, -0.13

Table 97: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

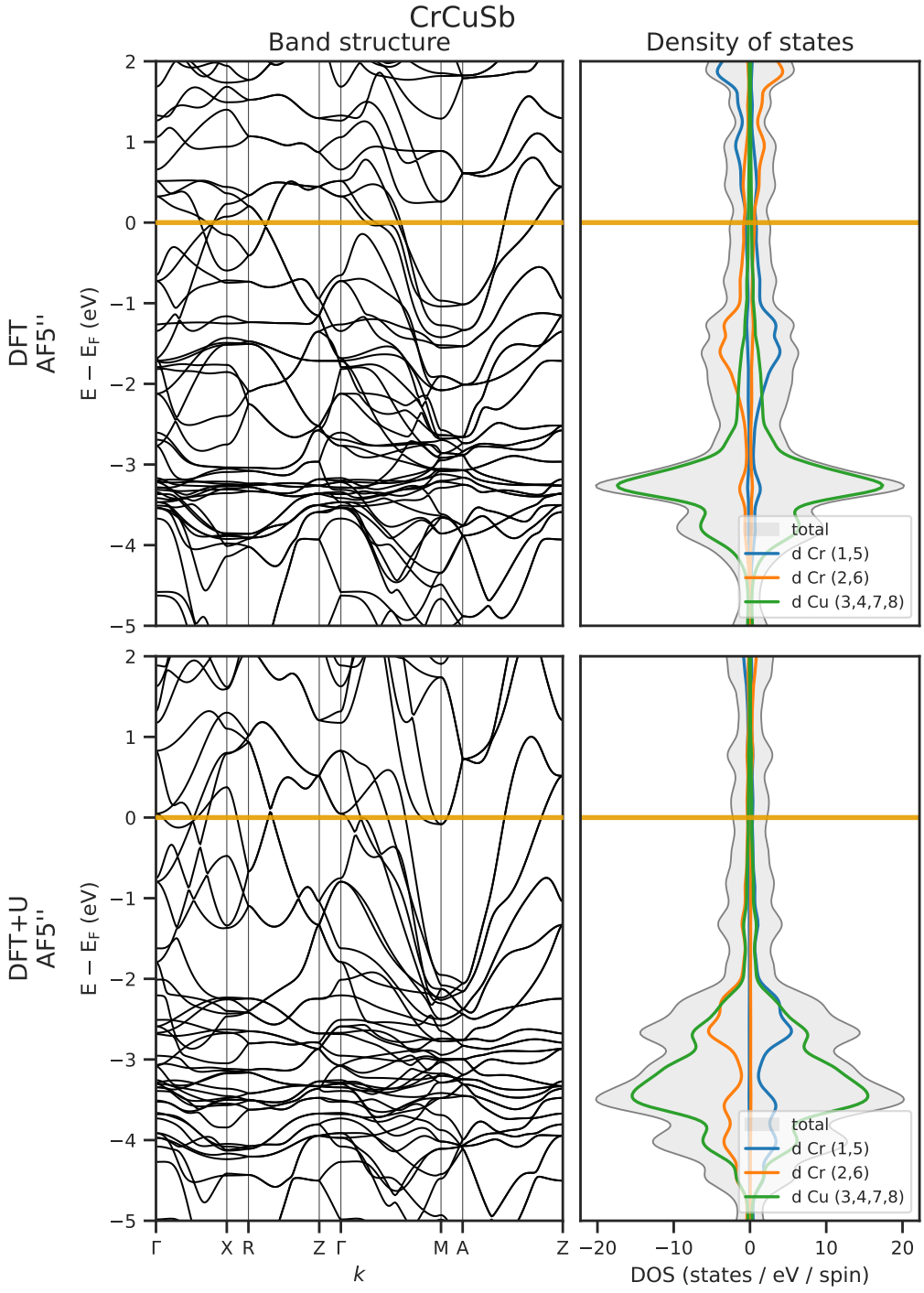


Figure 93: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuCrSb ■ higher-energy

Structure

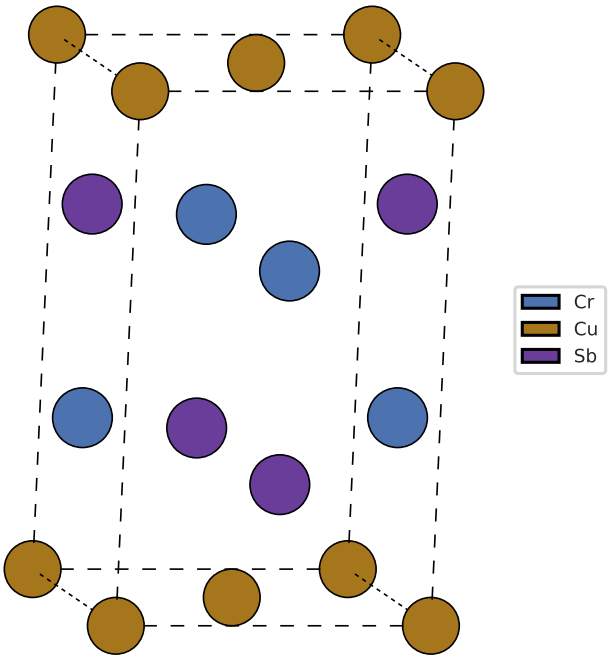


Figure 94: Structure of CuCrSb

a (Å)	c (Å)	z_1	z_2
4.1435	6.4632	0.2906	0.2789

Table 98: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1′	-40473.794095	0.000000	-0.04, -0.04, 4.28, 4.28, -0.04, -0.04, 4.28, 4.28
AF3′	-40473.631092	0.163003	0.05, 0.05, -4.19, 4.19, -0.05, -0.05, 4.19, -4.19
AF2′	-40473.604125	0.189970	0.00, 0.00, -4.21, 4.21, 0.00, 0.00, -4.21, 4.21
AF1′	-40473.276621	0.517474	0.00, 0.00, 4.26, 4.26, 0.00, 0.00, -4.26, -4.26

Table 99: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

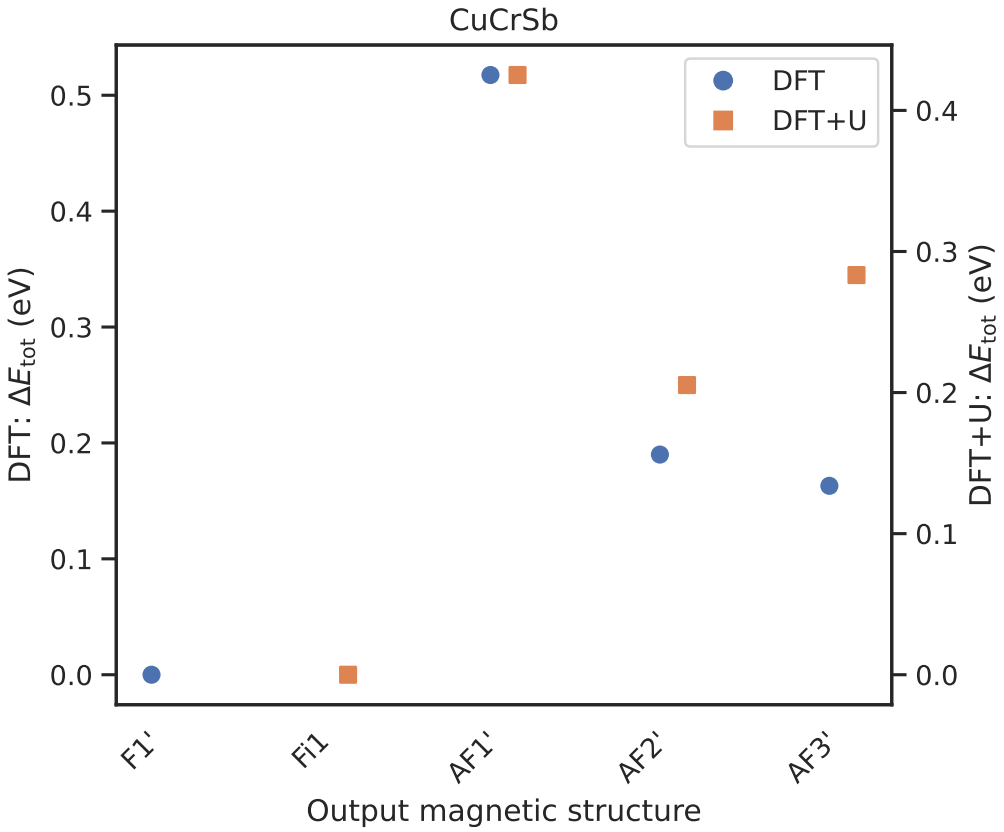


Figure 95: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-40469.440462	0.000000	-0.13, -0.13, 4.79, 4.79, -0.13, -0.13, 4.79, 4.79
AF2′	-40469.235131	0.205331	0.00, 0.00, -4.77, 4.77, 0.00, 0.00, -4.77, 4.77
AF3′	-40469.157178	0.283284	0.10, 0.10, -4.77, 4.77, -0.10, -0.10, 4.77, -4.77
AF1′	-40469.015370	0.425092	0.00, 0.00, 4.80, 4.80, 0.00, 0.00, -4.80, -4.80

Table 100: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

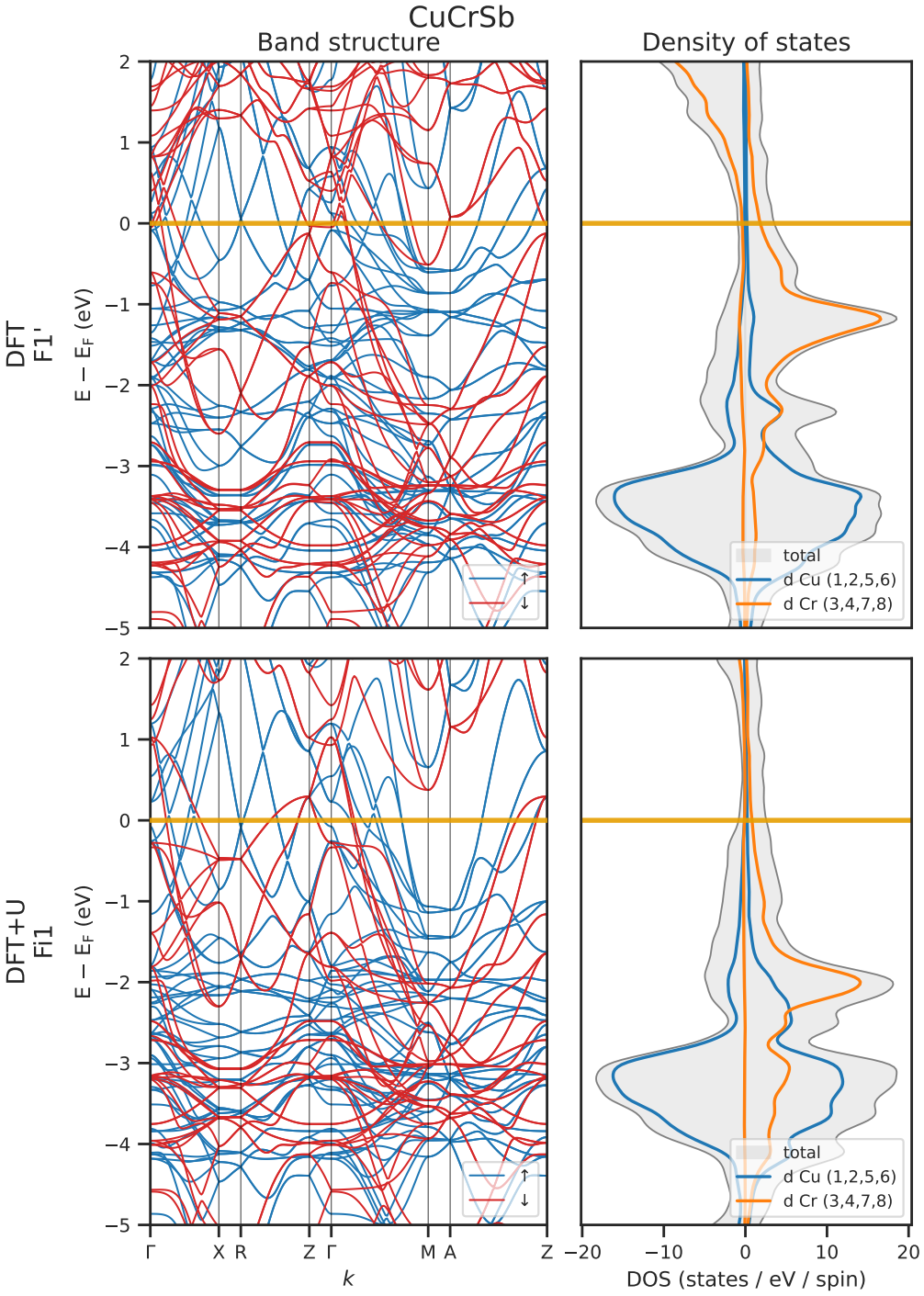


Figure 96: Band structure and Density of states of the lowest in energy calculations.

Material: FeCrAs

Configuration: FeCrAs ■ lower-energy

Structure

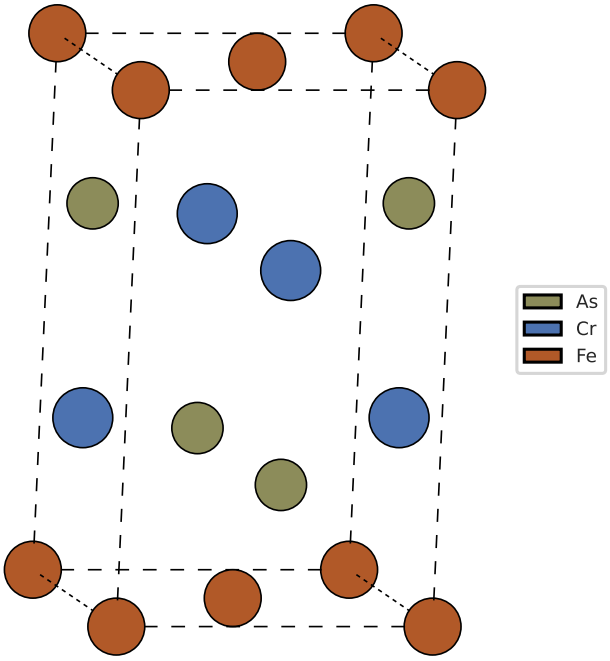


Figure 97: Structure of FeCrAs

a (Å)	c (Å)	z_1	z_2
3.7113	5.9448	0.3243	0.2542

Table 101: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-34624.293965	0.000000	0.00, 0.00, -3.40, 3.41, 0.00, 0.00, -3.41, 3.41
AF3	-34623.879960	0.414005	1.18, 1.18, -3.25, 3.25, -1.18, -1.18, 3.25, -3.25
AF1′	-34623.870337	0.423628	0.00, 0.00, 3.07, 3.07, 0.00, 0.00, -3.07, -3.07
Fi1	-34623.822761	0.471204	1.78, 1.78, -3.00, -3.00, 1.78, 1.78, -3.00, -3.00

Table 102: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

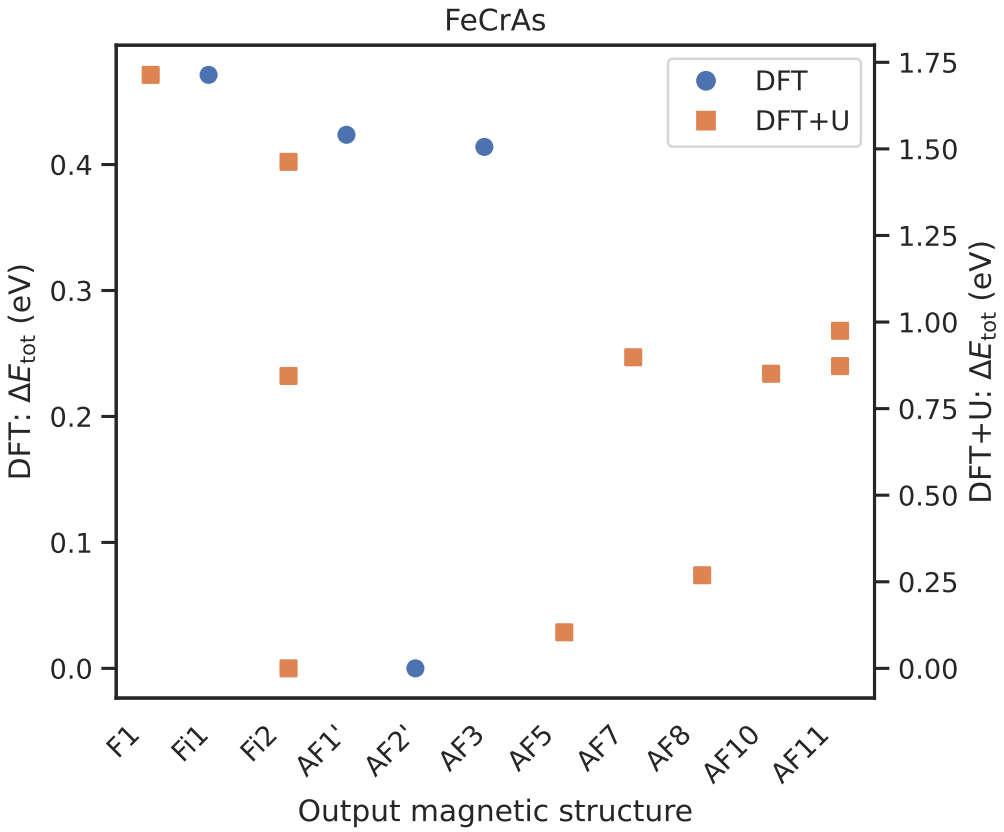


Figure 98: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
Fi2	-34607.633786	0.000000	3.15, 2.95, -4.53, -4.53, 2.96, 3.15, -4.53, -4.53
AF5	-34607.529681	0.104106	2.54, -2.54, -4.55, 4.55, 2.54, -2.54, -4.55, 4.55
AF8	-34607.364873	0.268913	2.50, -2.50, -4.56, 4.56, -2.50, 2.50, -4.56, 4.56
Fi2	-34606.789439	0.844348	2.50, -2.57, 4.55, -4.58, -2.81, 2.85, -4.53, -4.53
AF10	-34606.783047	0.850739	2.53, -2.53, 4.51, 4.51, -2.53, 2.53, -4.51, -4.51
AF11	-34606.761038	0.872748	2.67, 2.67, 4.37, 4.59, -2.67, -2.67, -4.37, -4.59
AF7	-34606.735540	0.898247	2.54, -2.54, 4.49, 4.49, 2.54, -2.54, -4.49, -4.49
AF11	-34606.659081	0.974705	3.04, -2.64, -4.57, 4.59, 2.61, -2.94, 4.59, -4.57
Fi2	-34606.171237	1.462550	3.04, -2.66, -4.56, 4.53, -2.82, 0.85, 4.53, -4.56
F1	-34605.920047	1.713739	2.73, 2.73, 4.52, 4.52, 2.73, 2.73, 4.52, 4.52

Table 103: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

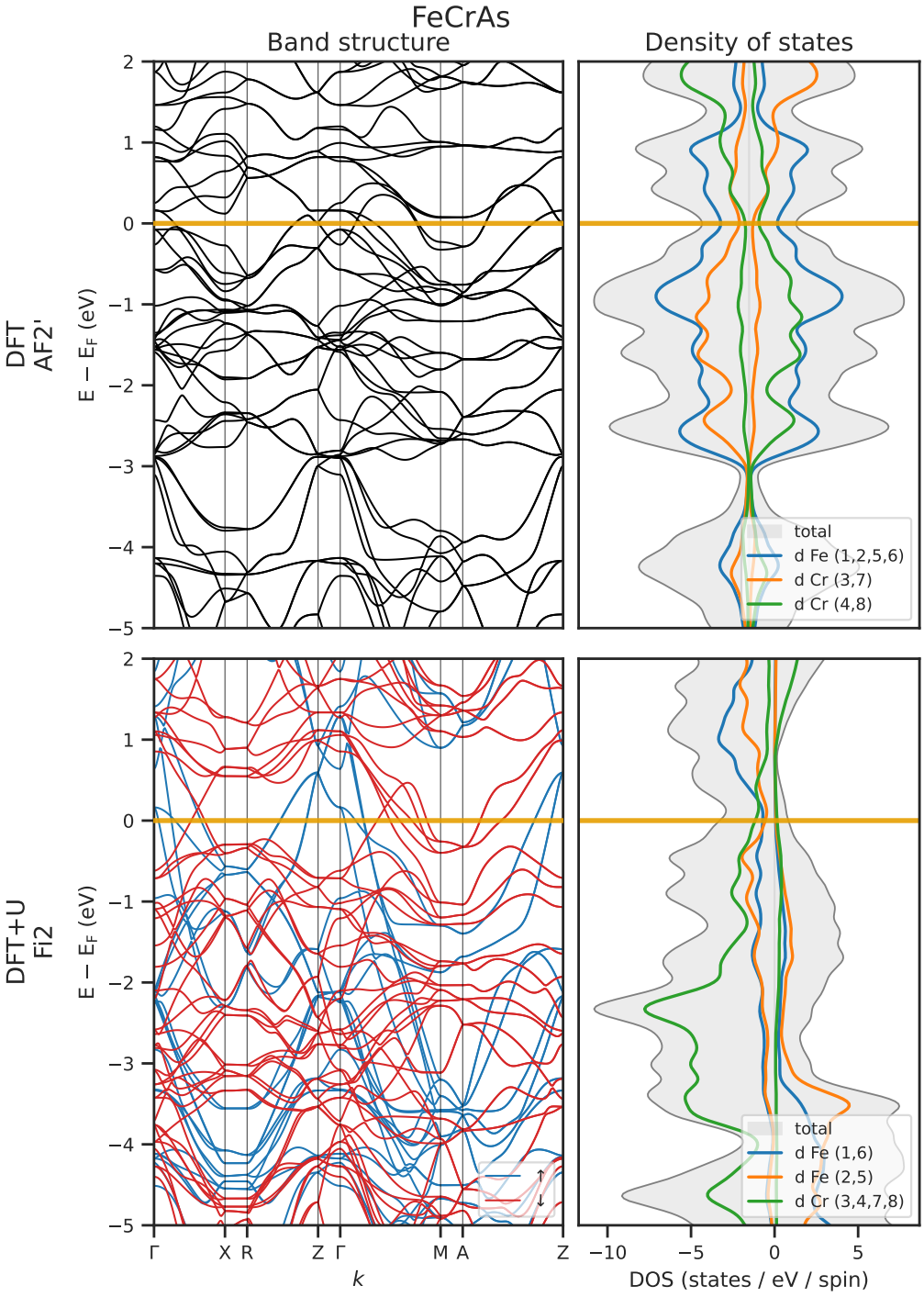


Figure 99: Band structure and Density of states of the lowest in energy calculations.

Configuration: CrFeAs ■ higher-energy

Structure

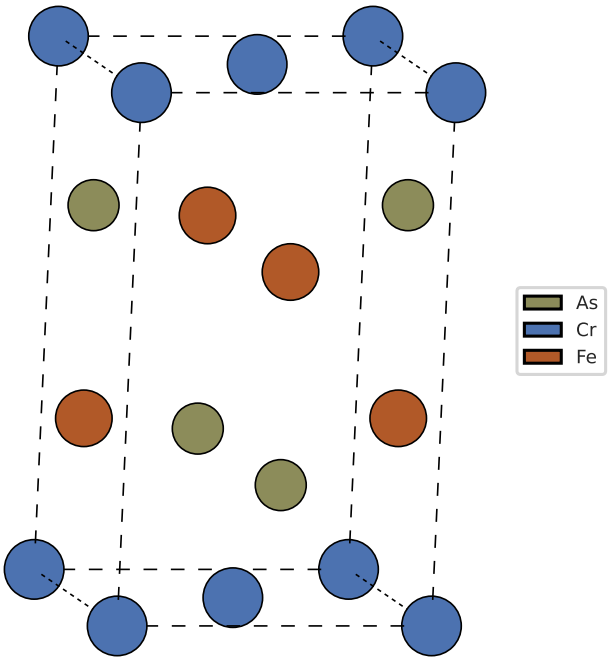


Figure 100: Structure of CrFeAs

a (Å)	c (Å)	z_1	z_2
3.7011	6.0157	0.2939	0.2883

Table 104: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

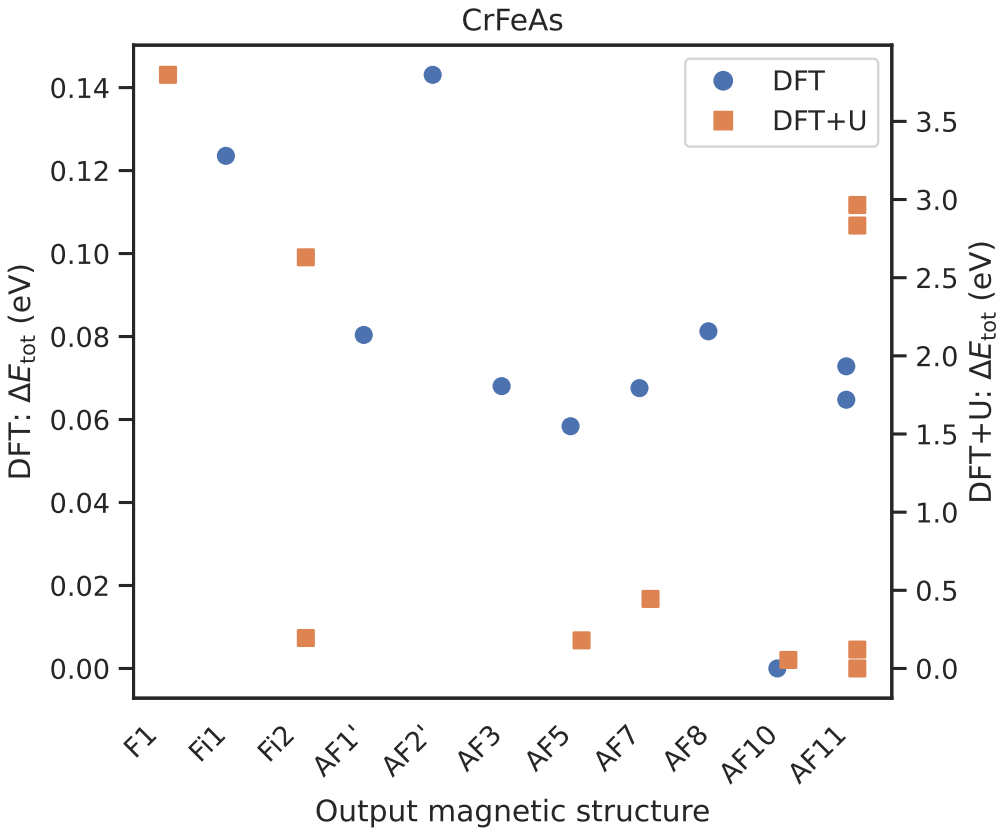


Figure 101: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF10	-34623.575885	0.000000	1.38, -1.38, 2.45, 2.45, -1.39, 1.39, -2.45, -2.45
AF5	-34623.517505	0.058380	1.44, -1.44, -2.36, 2.36, 1.44, -1.44, -2.36, 2.36
AF11	-34623.511111	0.064774	1.56, -0.65, -2.56, 2.55, 0.65, -1.56, 2.55, -2.56
AF7	-34623.508319	0.067567	1.07, -1.07, 2.45, 2.45, 1.07, -1.07, -2.45, -2.45
AF3	-34623.507837	0.068048	0.42, 0.42, -2.62, 2.62, -0.42, -0.42, 2.62, -2.62
AF11	-34623.503064	0.072822	1.52, -0.57, -2.56, 2.56, -1.53, 0.58, 2.56, -2.56
AF1′	-34623.495498	0.080388	0.00, 0.00, 2.49, 2.49, 0.00, 0.00, -2.49, -2.49
AF8	-34623.494620	0.081266	1.38, -1.38, -2.38, 2.38, -1.38, 1.38, -2.38, 2.38
Fi1	-34623.452334	0.123552	0.59, 0.59, -2.69, -2.68, 0.59, 0.59, -2.68, -2.69
AF2′	-34623.432810	0.143076	-0.00, 0.00, -2.46, 2.45, -0.00, 0.00, -2.45, 2.46

Table 105: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF11	-34605.770337	0.000000	4.50, -3.81, -2.70, 2.69, -4.50, 3.81, 2.69, -2.70
AF10	-34605.715940	0.054396	4.19, -4.19, 2.77, 2.77, -4.19, 4.19, -2.77, -2.77
AF11	-34605.649430	0.120907	4.49, -3.81, -2.67, 2.67, 3.81, -4.49, 2.67, -2.67
AF5	-34605.590559	0.179778	4.19, -4.19, -2.69, 2.69, 4.19, -4.19, -2.69, 2.69
Fi2	-34605.575491	0.194846	4.20, -4.21, -2.71, 2.72, -4.34, 4.13, -3.21, 2.71
AF7	-34605.325326	0.445011	4.19, -4.19, 2.74, 2.74, 4.19, -4.19, -2.74, -2.74
Fi2	-34603.139942	2.630395	4.02, 2.49, -3.36, -3.36, 2.49, 4.01, -3.36, -3.36
AF11	-34602.936619	2.833718	4.05, 3.12, -3.37, 3.37, -4.05, -3.12, 3.37, -3.37
AF11	-34602.805287	2.965050	3.86, 3.86, 2.99, 3.36, -3.86, -3.86, -2.99, -3.37
F1	-34601.972587	3.797750	3.65, 3.65, 2.94, 2.95, 3.58, 3.58, 2.85, 2.99

Table 106: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

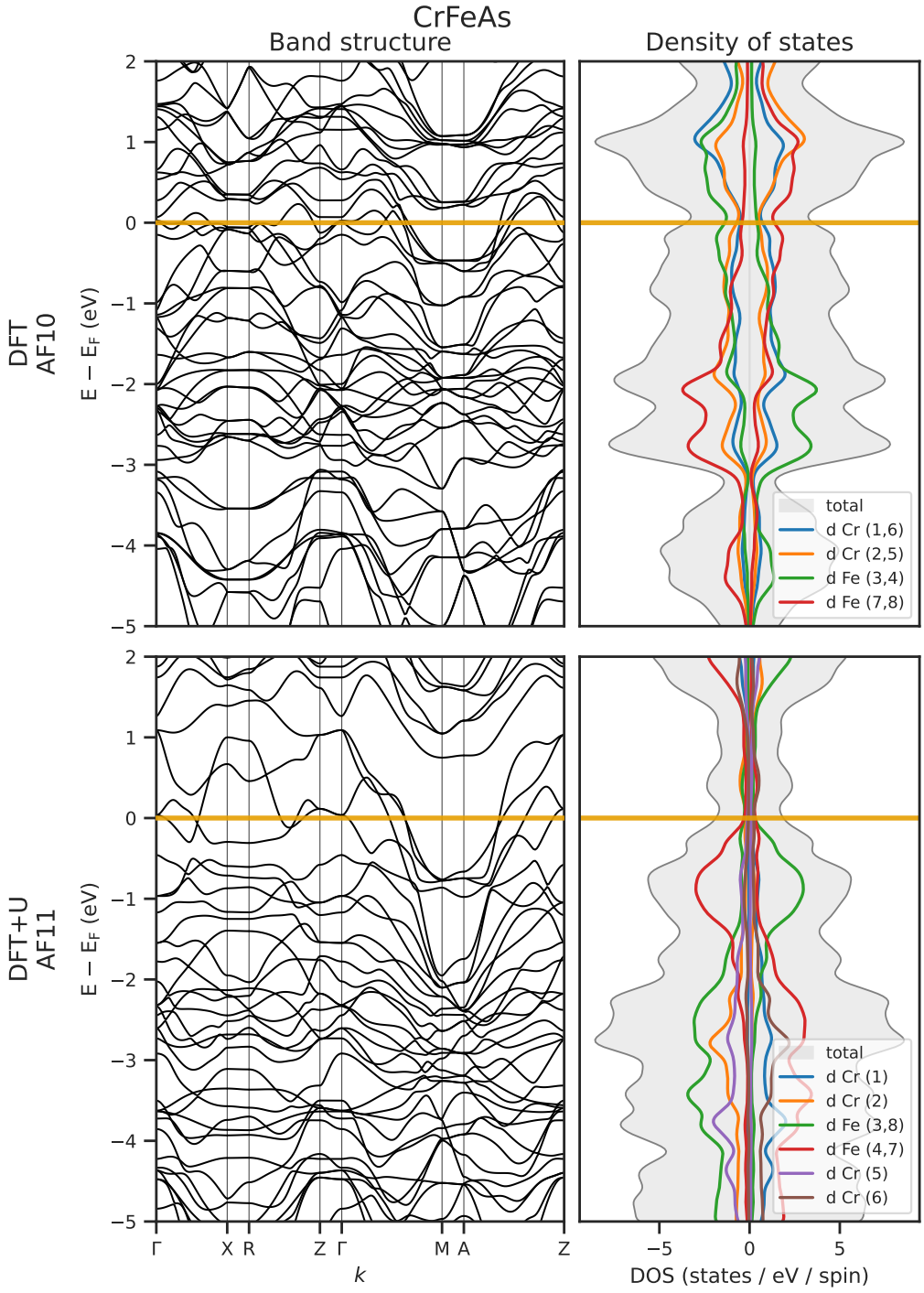


Figure 102: Band structure and Density of states of the lowest in energy calculations.

Material: CrFeSb

Configuration: CrFeSb ■ lower-energy

Structure

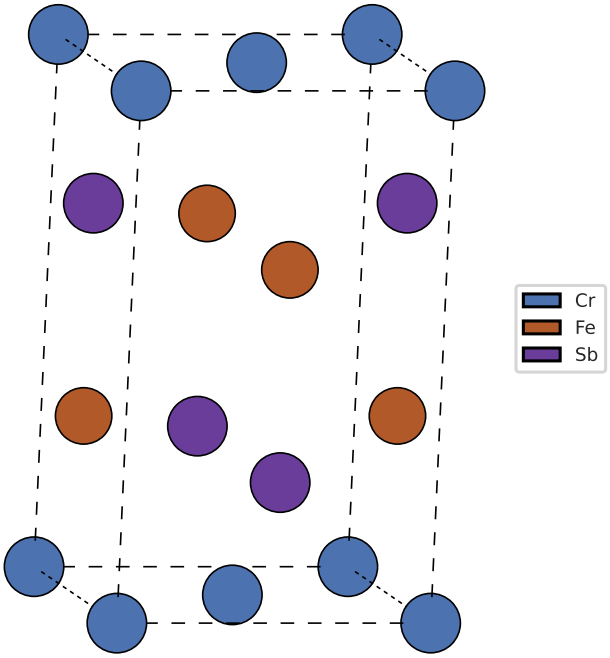


Figure 103: Structure of CrFeSb

a (Å)	c (Å)	z_1	z_2
3.8788	6.3417	0.2461	0.3163

Table 107: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

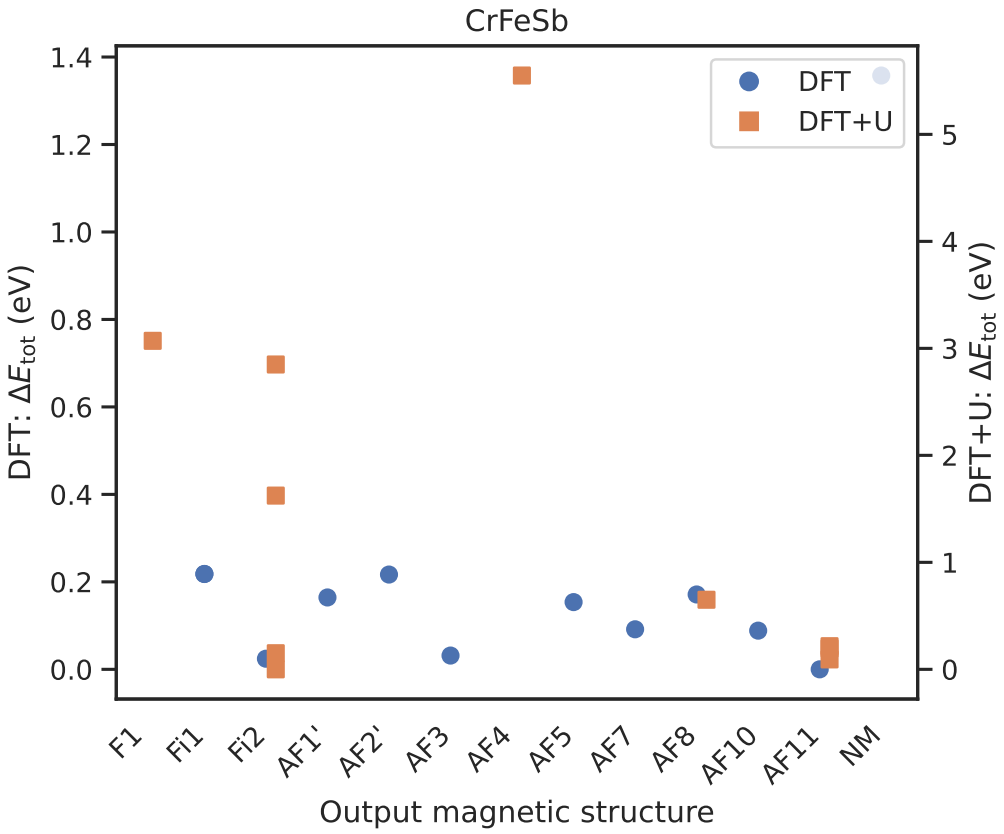


Figure 104: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF11	-32508.693033	0.000000	2.07, -0.58, -2.37, 2.37, 0.58, -2.07, 2.37, -2.37
Fi2	-32508.668744	0.024289	1.52, -0.11, -2.43, 2.38, -1.90, 0.44, 2.38, -2.43
AF3	-32508.661531	0.031502	0.69, 0.69, -2.45, 2.45, -0.69, -0.69, 2.45, -2.45
AF10	-32508.604557	0.088476	1.49, -1.49, 2.22, 2.22, -1.49, 1.49, -2.22, -2.22
AF7	-32508.601460	0.091573	1.39, -1.39, 2.20, 2.20, 1.39, -1.39, -2.20, -2.20
AF5	-32508.539302	0.153731	1.45, -1.45, -2.15, 2.15, 1.45, -1.45, -2.15, 2.15
AF1′	-32508.528690	0.164343	-0.00, 0.00, 2.28, 2.27, 0.00, -0.00, -2.27, -2.28
AF8	-32508.521859	0.171174	1.35, -1.35, -2.17, 2.17, -1.35, 1.35, -2.17, 2.17
AF2′	-32508.476306	0.216727	0.00, 0.00, -2.25, 2.25, 0.00, 0.00, -2.25, 2.25
Fi1	-32508.475083	0.217949	-0.45, -0.45, 2.42, 2.42, -0.45, -0.45, 2.42, 2.42
Fi1	-32508.474923	0.218110	0.45, 0.44, -2.42, -2.42, 0.45, 0.45, -2.42, -2.42
NM	-32507.335327	1.357706	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 108: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi2	-32491.178701	0.000000	4.59, -4.24, -3.11, 2.68, 4.09, -4.62, 2.68, -2.70
AF11	-32491.085829	0.092872	4.49, -4.49, -3.04, 2.68, 4.38, -4.38, -2.68, 3.04
Fi2	-32491.028012	0.150689	4.35, -4.48, 2.70, 3.07, 4.46, -4.48, -3.10, -3.08
AF11	-32490.982967	0.195734	4.59, -4.30, -3.05, 3.04, -4.59, 4.38, 3.04, -3.07
AF11	-32490.962286	0.216415	4.48, -4.41, 3.05, 2.68, -4.38, 4.37, -2.70, -3.06
AF8	-32490.528264	0.650437	4.40, -4.40, -3.03, 3.03, -4.40, 4.40, -3.03, 3.03
Fi2	-32489.554783	1.623918	2.45, 4.28, -3.21, 3.10, -4.34, -4.34, 3.10, -3.21
Fi2	-32488.329450	2.849251	4.09, 4.09, -3.13, 3.13, -3.96, -3.96, -2.69, 0.93
F1	-32488.108292	3.070409	3.93, 3.93, 2.70, 2.70, 3.93, 3.93, 2.70, 2.70
AF4	-32485.628659	5.550042	2.71, 2.71, 2.32, -2.32, -2.71, -2.71, -2.35, 2.35

Table 109: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

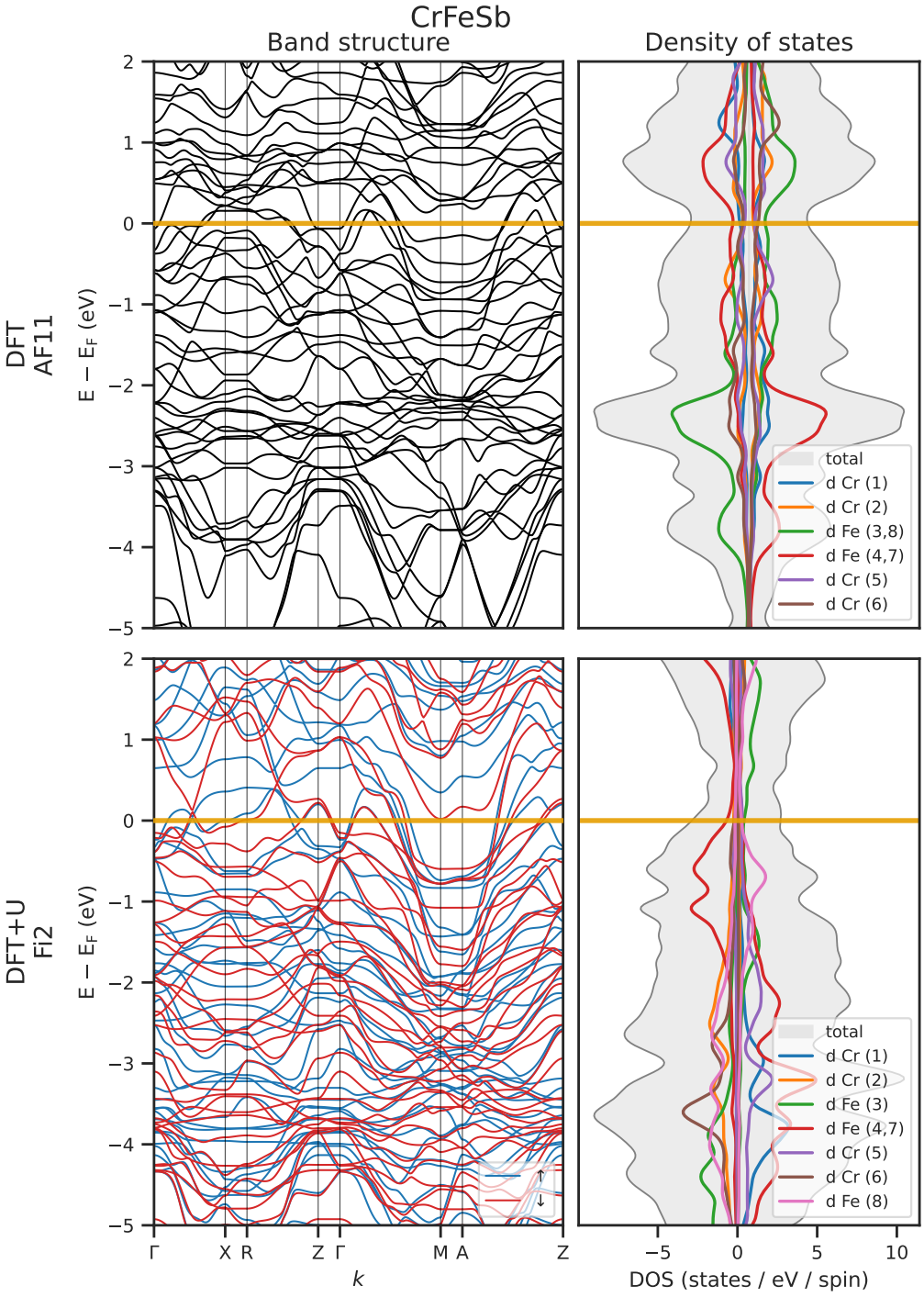


Figure 105: Band structure and Density of states of the lowest in energy calculations.

Configuration: FeCrSb ■ higher-energy

Structure

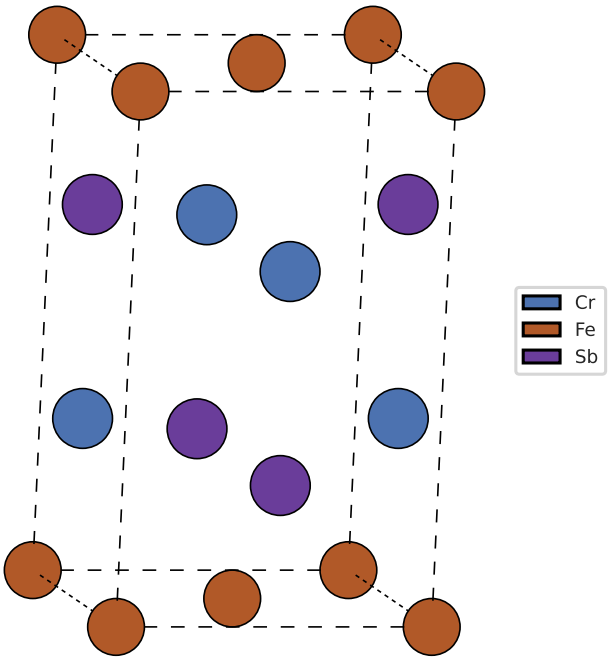


Figure 106: Structure of FeCrSb

a (Å)	c (Å)	z_1	z_2
3.9803	6.2467	0.2811	0.2702

Table 110: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

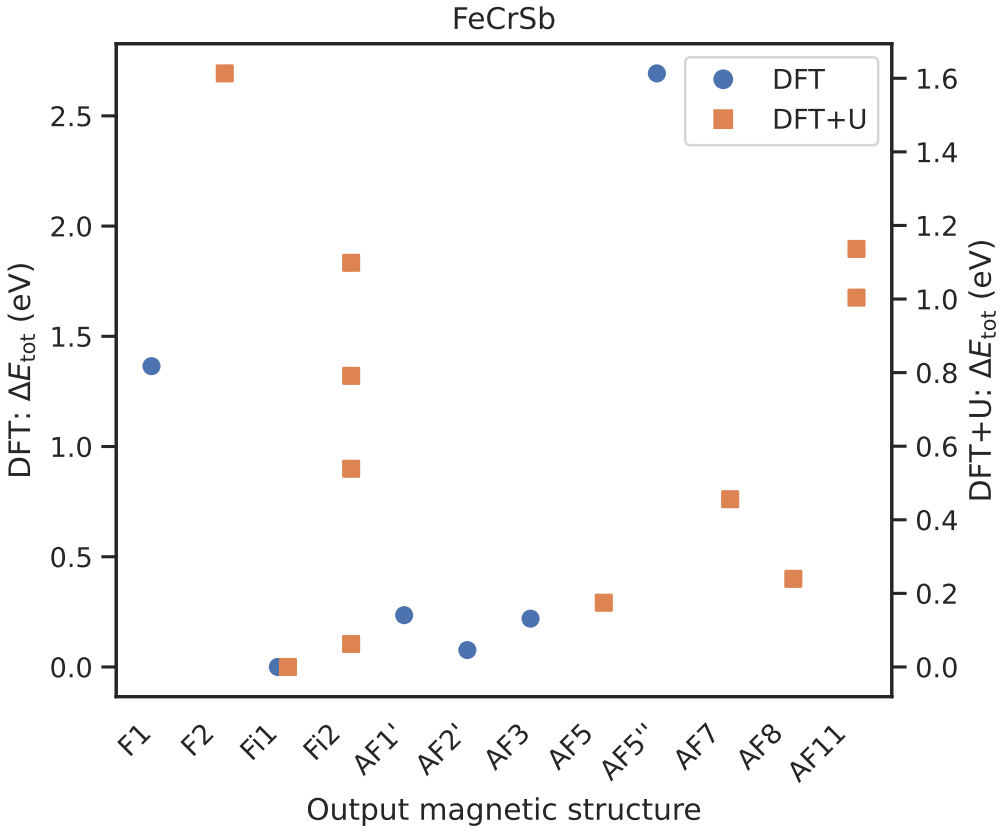


Figure 107: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-32508.280689	0.000000	2.39, 2.39, -3.64, -3.64, 2.39, 2.39, -3.64, -3.64
AF2′	-32508.204034	0.076655	-0.00, -0.00, -3.61, 3.61, -0.00, -0.00, -3.61, 3.61
AF3	-32508.061484	0.219206	2.36, 2.36, -3.64, 3.64, -2.36, -2.36, 3.64, -3.64
AF1′	-32508.045681	0.235009	0.00, 0.00, 3.63, 3.63, 0.00, 0.00, -3.63, -3.63
F1	-32506.916154	1.364536	1.73, 1.73, 3.30, 3.30, 1.72, 1.72, 3.30, 3.30
AF5″	-32505.587981	2.692708	1.92, -1.92, 0.00, 0.00, 1.92, -1.92, -0.00, 0.00

Table 111: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-32493.702646	0.000000	3.21, 3.21, -4.73, -4.73, 3.21, 3.21, -4.73, -4.73
Fi2	-32493.640172	0.062474	3.00, 3.00, -4.74, 4.69, -3.21, -3.21, 4.69, -4.74
AF5	-32493.528035	0.174610	2.73, -2.73, -4.62, 4.62, 2.73, -2.73, -4.62, 4.62
AF8	-32493.463131	0.239515	2.72, -2.72, -4.62, 4.62, -2.72, 2.72, -4.62, 4.62
AF7	-32493.246725	0.455921	2.71, -2.71, 4.63, 4.63, 2.71, -2.71, -4.63, -4.63
Fi2	-32493.163871	0.538775	2.69, -2.69, 4.64, 4.67, -2.74, 2.95, -4.64, -4.64
Fi2	-32492.911491	0.791155	3.02, 3.02, -4.72, 4.72, -3.01, -3.01, -4.50, 4.60
AF11	-32492.698727	1.003919	3.19, -2.85, -4.65, 4.65, 2.85, -3.19, 4.65, -4.65
Fi2	-32492.604177	1.098468	2.74, 2.77, 4.51, 4.74, -2.83, -2.91, -4.57, -4.70
AF11	-32492.566461	1.136185	3.18, -2.81, -4.64, 4.64, -3.18, 2.81, 4.64, -4.64
F2	-32492.089352	1.613293	2.59, 2.59, 4.56, 4.64, 2.89, 2.89, 4.64, 4.56

Table 112: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

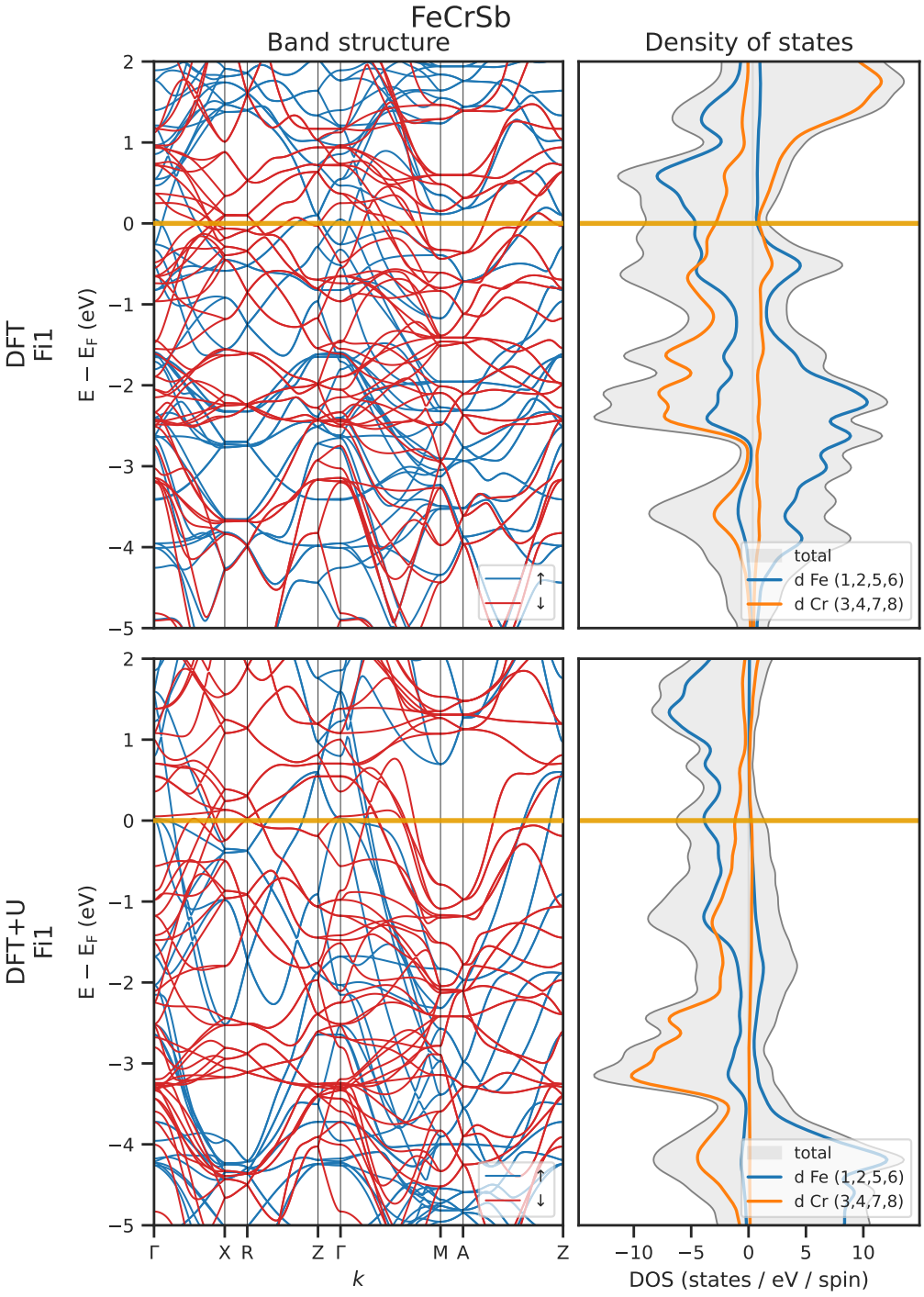


Figure 108: Band structure and Density of states of the lowest in energy calculations.

Material: CrGaAs

Configuration: CrGaAs ■ lower-energy

Structure

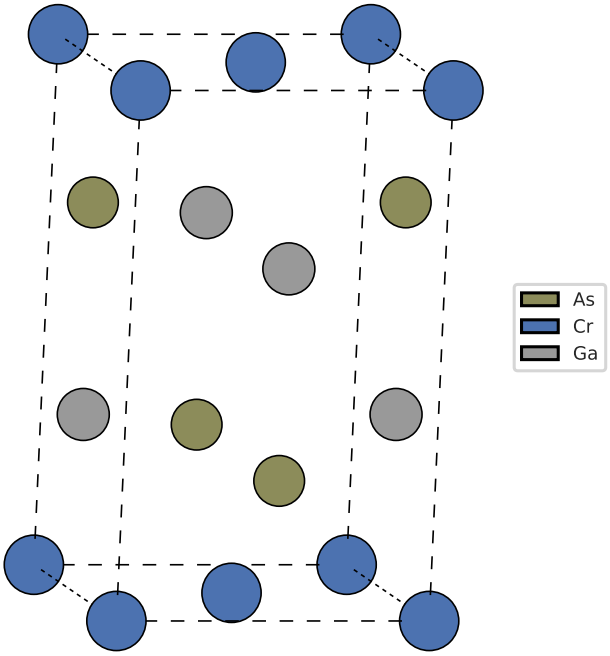


Figure 109: Structure of CrGaAs

a (Å)	c (Å)	z_1	z_2
4.1941	5.9123	0.2952	0.2674

Table 113: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-29431.053943	0.000000	3.40, -3.40, 0.00, 0.00, -3.40, 3.40, 0.00, 0.00
AF5″	-29431.016827	0.037116	3.41, -3.41, 0.00, 0.00, 3.41, -3.41, 0.00, 0.00
F1″	-29430.843195	0.210748	2.41, 2.42, -0.09, -0.09, 2.41, 2.42, -0.09, -0.09
AF1″	-29430.834982	0.218960	2.44, 2.44, -0.07, 0.07, -2.44, -2.44, 0.07, -0.07

Table 114: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

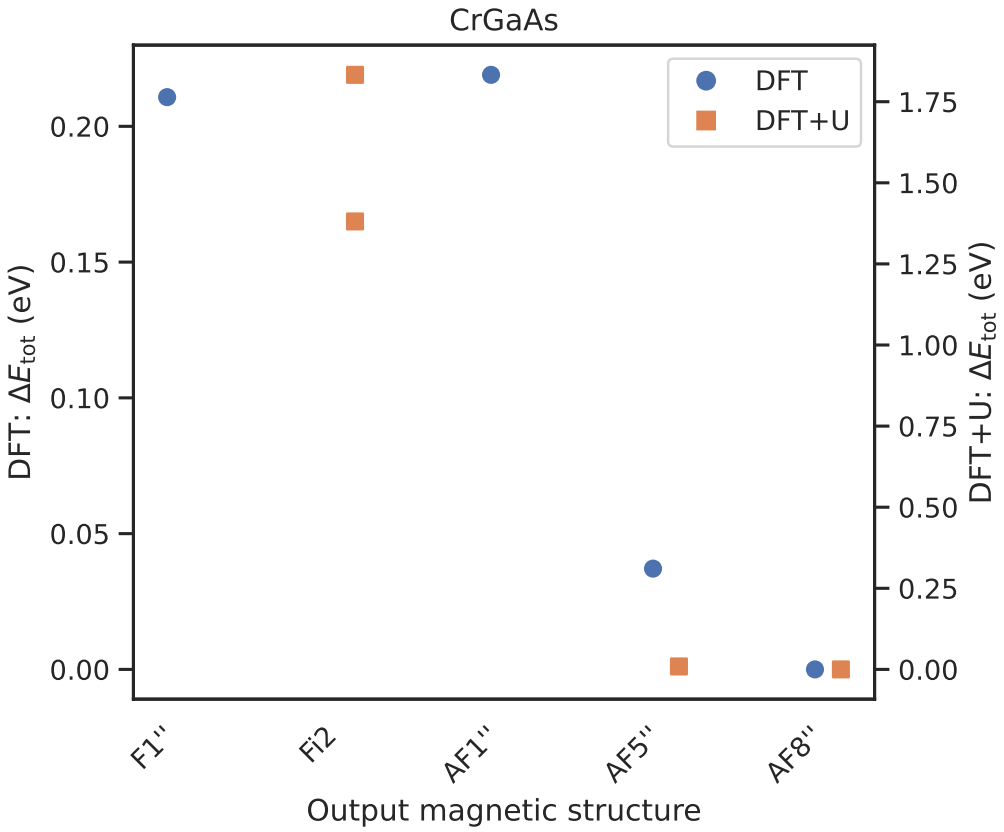


Figure 110: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-29423.867612	0.000000	4.57, -4.57, 0.00, 0.00, -4.57, 4.56, 0.00, 0.00
AF5″	-29423.858512	0.009100	4.56, -4.56, 0.00, 0.00, 4.56, -4.56, 0.00, 0.00
Fi2	-29422.486682	1.380929	4.53, 4.53, -0.17, 0.23, -4.37, -3.37, 0.23, -0.17
Fi2	-29422.034786	1.832825	4.48, 2.72, -0.17, -0.17, 4.48, 2.72, -0.17, -0.17

Table 115: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

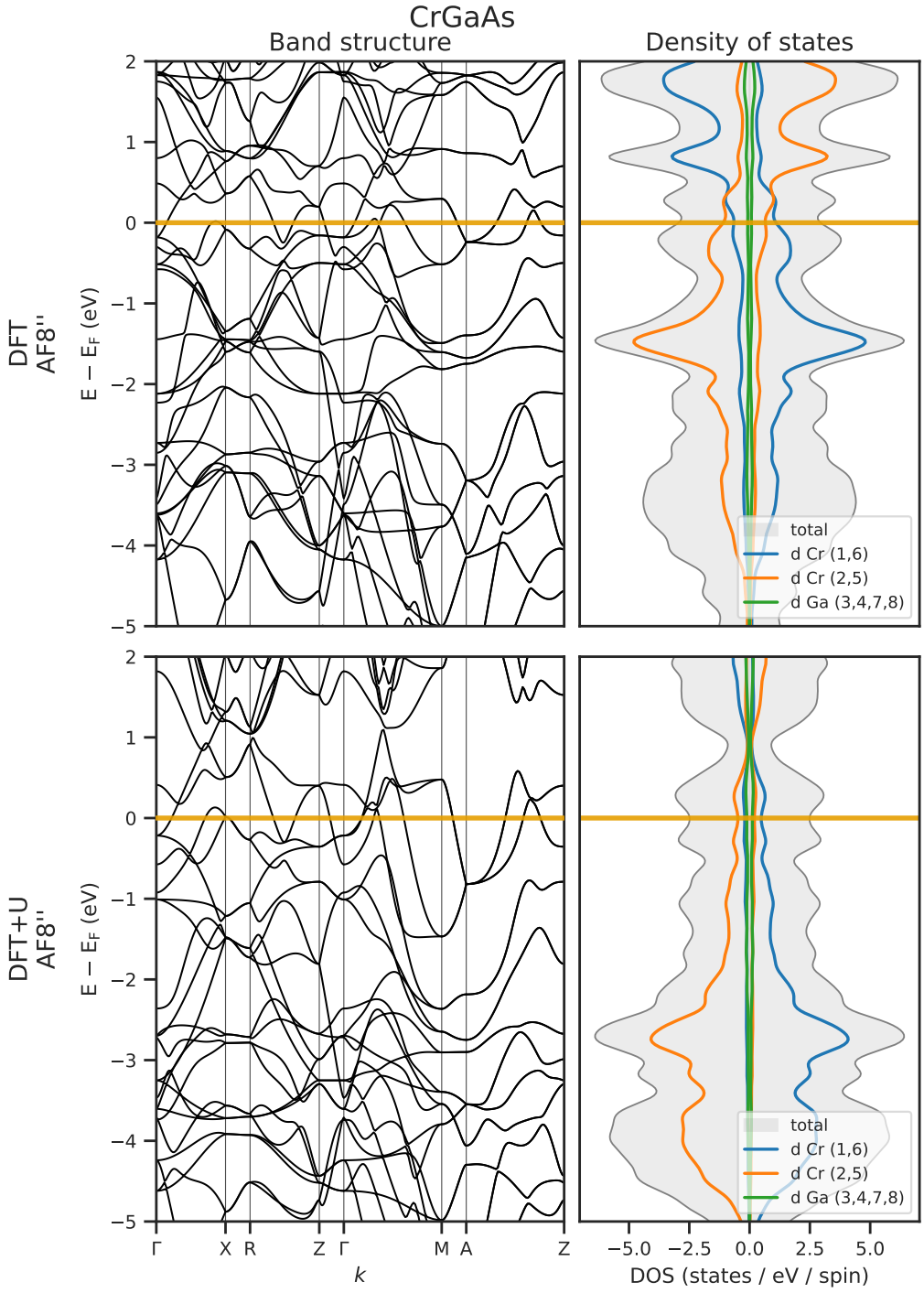


Figure 111: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaCrAs ■ higher-energy

Structure

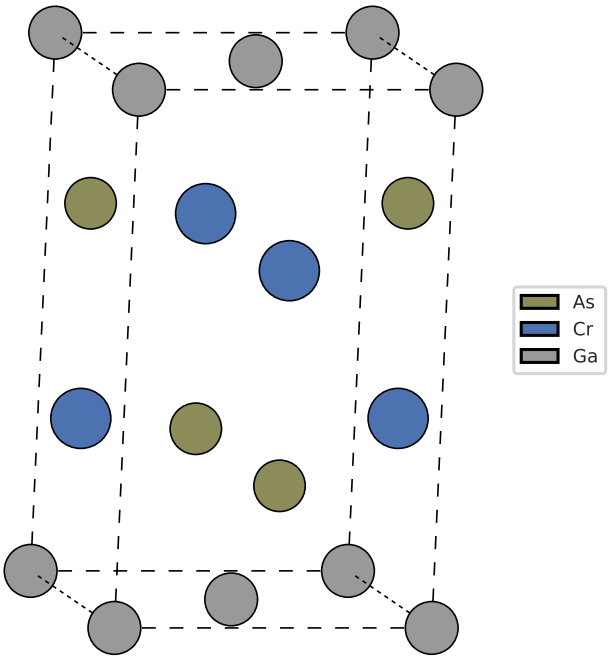


Figure 112: Structure of GaCrAs

a (Å)	c (Å)	z_1	z_2
3.6203	7.3770	0.2779	0.3671

Table 116: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-29430.601682	0.000000	0.00, 0.00, -2.96, 2.96, 0.00, 0.00, -2.96, 2.96
AF1′	-29430.463251	0.138431	0.00, 0.00, 2.97, 2.97, 0.00, 0.00, -2.97, -2.97
Fi1	-29430.264695	0.336986	-0.24, -0.24, 2.84, 2.84, -0.24, -0.24, 2.84, 2.84
AF3	-29430.233421	0.368261	0.26, 0.26, -2.59, 2.59, -0.26, -0.26, 2.59, -2.59

Table 117: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

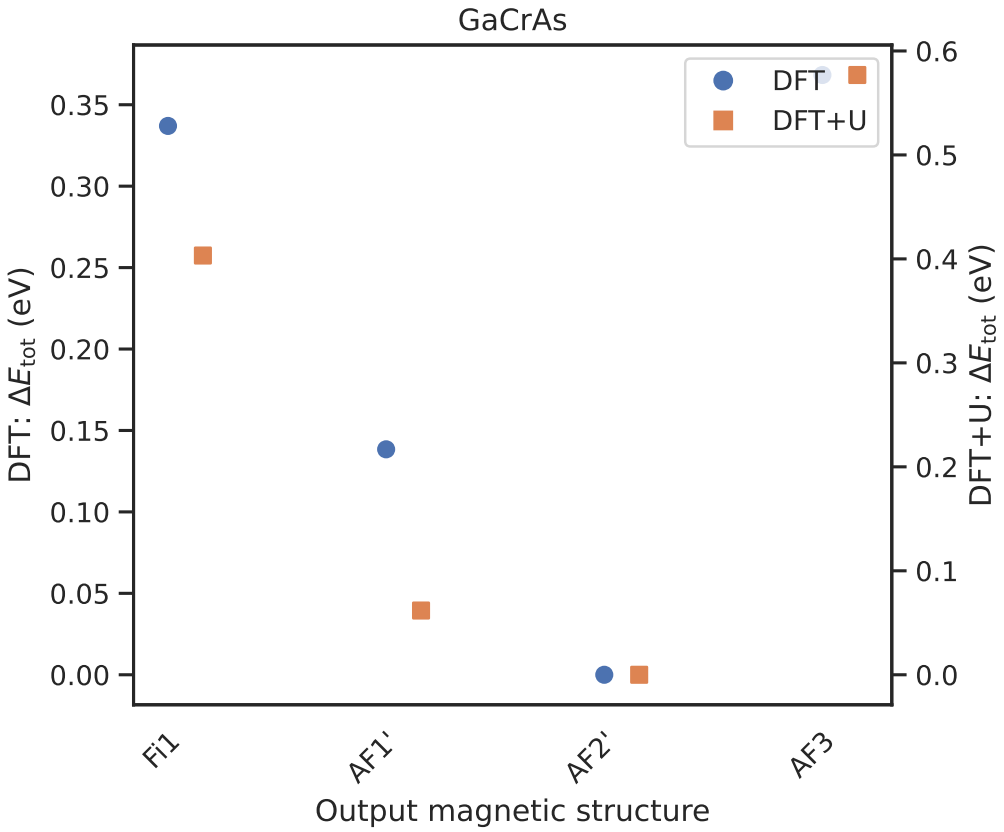


Figure 113: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-29422.591457	0.000000	0.00, 0.00, -4.36, 4.36, 0.00, 0.00, -4.36, 4.36
AF1′	-29422.529663	0.061794	0.00, 0.00, 4.37, 4.37, 0.00, 0.00, -4.37, -4.37
Fi1	-29422.188213	0.403244	-0.29, -0.29, 4.36, 4.36, -0.29, -0.29, 4.36, 4.36
AF3	-29422.014571	0.576886	0.30, 0.30, -4.36, 4.36, -0.30, -0.30, 4.36, -4.36

Table 118: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

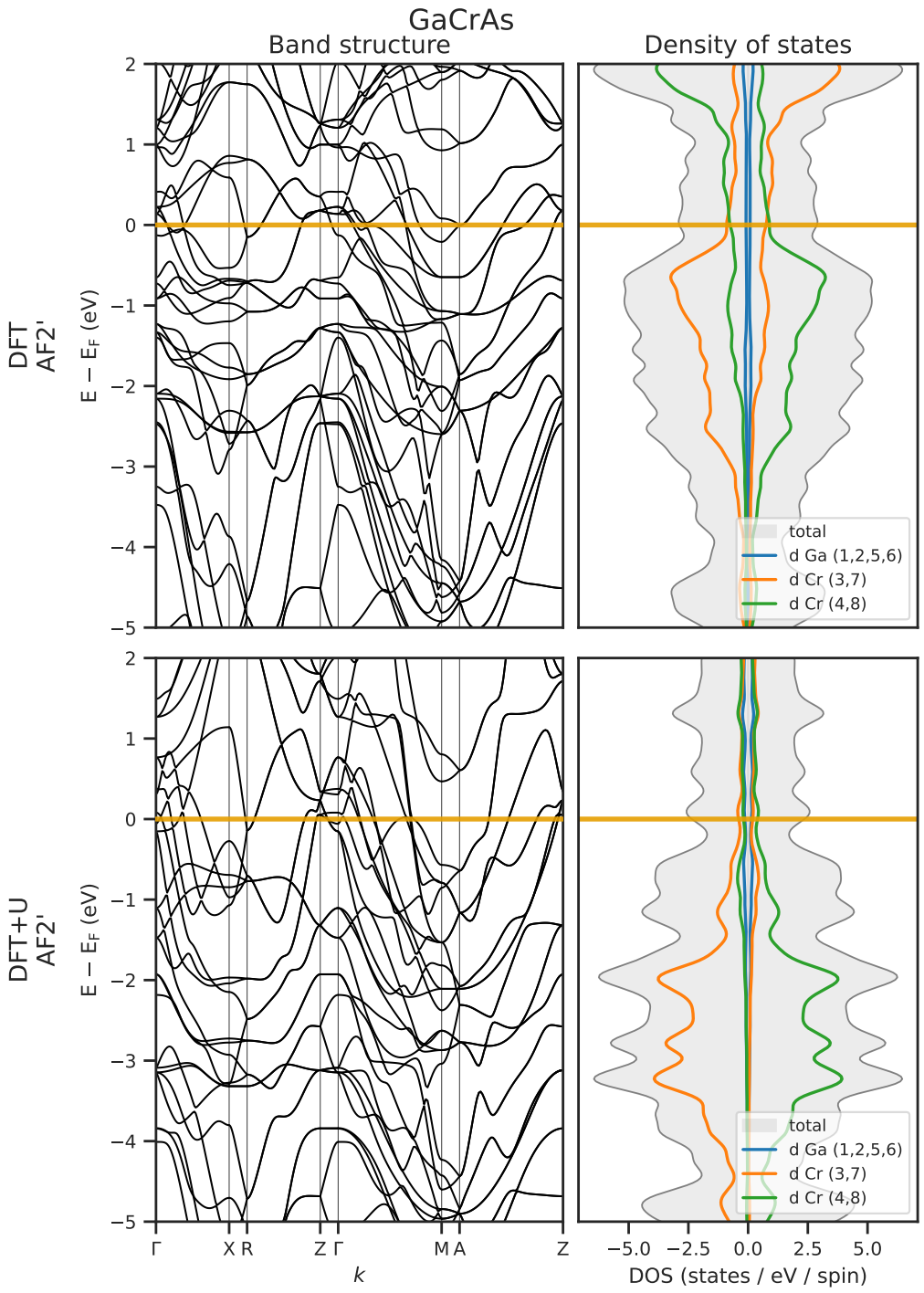


Figure 114: Band structure and Density of states of the lowest in energy calculations.

Material: GaCrSb

Configuration: GaCrSb ■ lower-energy

Structure

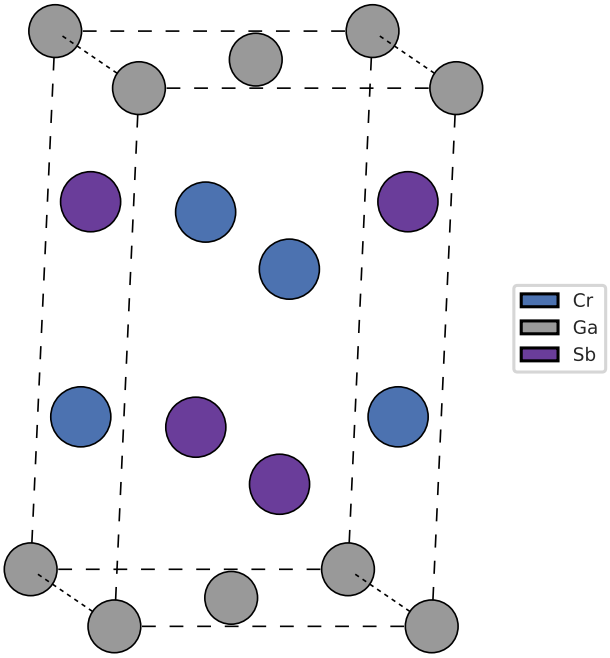


Figure 115: Structure of GaCrSb

a (Å)	c (Å)	z_1	z_2
3.8025	7.7348	0.2591	0.3658

Table 119: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-27317.074397	0.000000	0.00, 0.00, -3.25, 3.25, 0.00, 0.00, -3.25, 3.25
AF1′	-27316.905977	0.168420	0.00, 0.00, 3.27, 3.27, 0.00, 0.00, -3.27, -3.27
Fi1	-27316.740315	0.334082	-0.23, -0.23, 3.18, 3.18, -0.23, -0.23, 3.18, 3.18
AF3	-27316.677639	0.396758	0.27, 0.27, -2.99, 2.99, -0.27, -0.27, 2.99, -2.99

Table 120: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

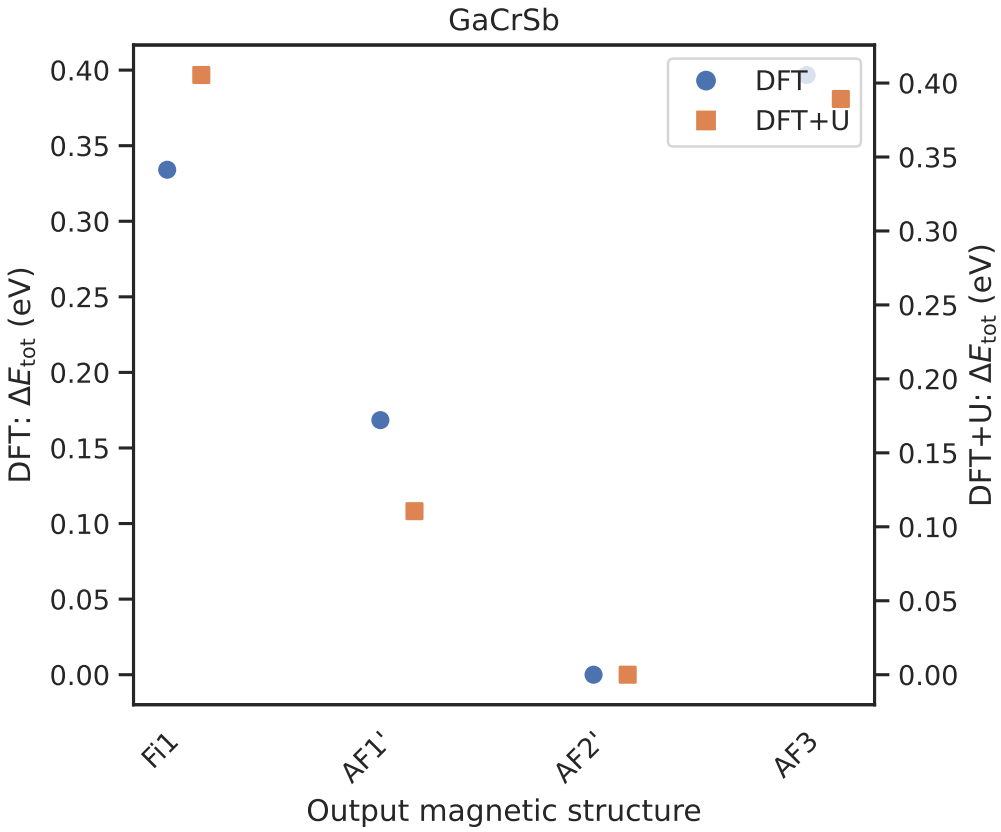


Figure 116: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-27309.974864	0.000000	0.00, 0.00, -4.54, 4.54, 0.00, 0.00, -4.54, 4.54
AF1′	-27309.864312	0.110551	0.00, 0.00, 4.54, 4.54, 0.00, 0.00, -4.54, -4.54
AF3	-27309.585628	0.389236	0.28, 0.28, -4.55, 4.55, -0.28, -0.28, 4.55, -4.55
Fi1	-27309.569426	0.405437	-0.28, -0.28, 4.56, 4.56, -0.28, -0.28, 4.56, 4.56

Table 121: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

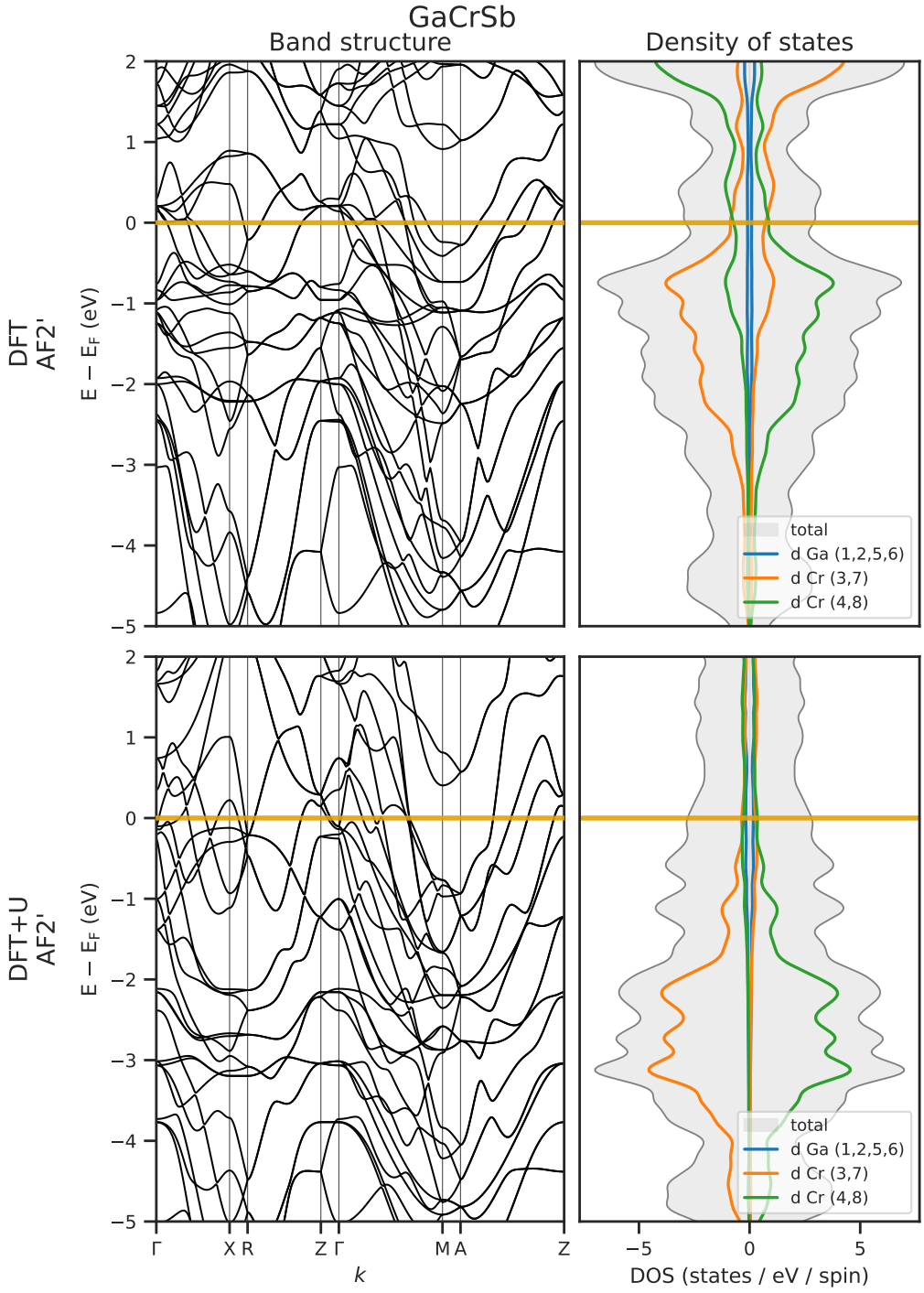


Figure 117: Band structure and Density of states of the lowest in energy calculations.

Configuration: CrGaSb ■ higher-energy

Structure

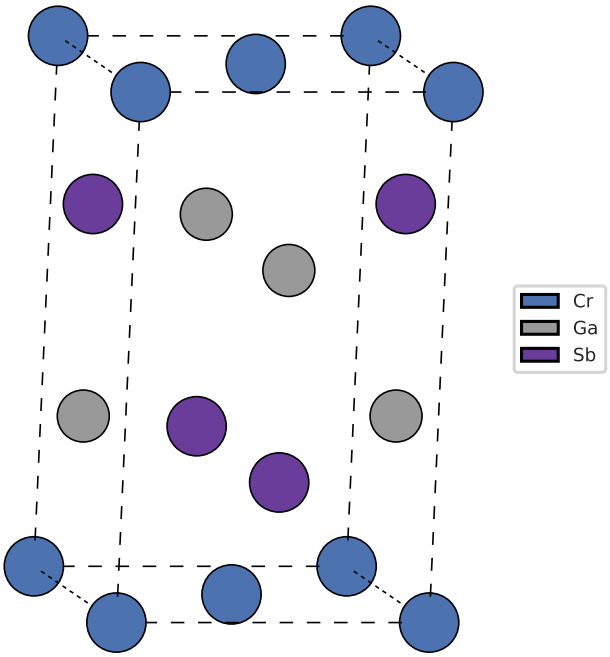


Figure 118: Structure of CrGaSb

a (Å)	c (Å)	z_1	z_2
4.3968	6.2862	0.2641	0.2845

Table 122: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-27316.974853	0.000000	3.65, -3.65, 0.00, 0.00, -3.65, 3.65, 0.00, 0.00
AF5″	-27316.970718	0.004135	3.64, -3.64, 0.00, 0.00, 3.64, -3.64, 0.00, 0.00
AF3	-27316.497136	0.477716	2.67, 2.67, -0.13, 0.13, -2.67, -2.67, 0.13, -0.13
Fi2	-27316.378612	0.596241	2.73, 2.73, -0.17, -0.19, 3.29, 3.29, -0.19, -0.17

Table 123: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

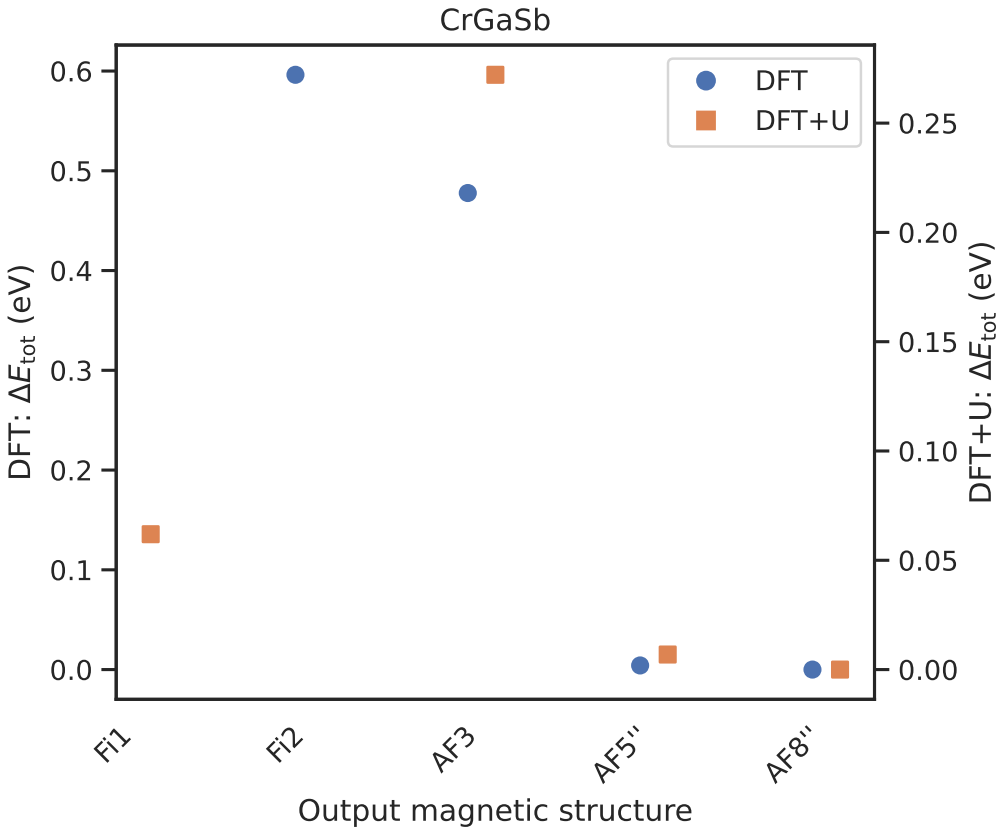


Figure 119: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-27310.678538	0.000000	4.66, -4.66, 0.00, 0.00, -4.66, 4.66, 0.00, 0.00
AF5″	-27310.671650	0.006888	4.66, -4.66, 0.00, 0.00, 4.66, -4.66, 0.00, 0.00
Fi1	-27310.616611	0.061927	4.62, 4.62, -0.22, -0.22, 4.62, 4.62, -0.22, -0.22
AF3	-27310.406431	0.272107	4.63, 4.63, -0.21, 0.21, -4.63, -4.63, 0.21, -0.21

Table 124: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

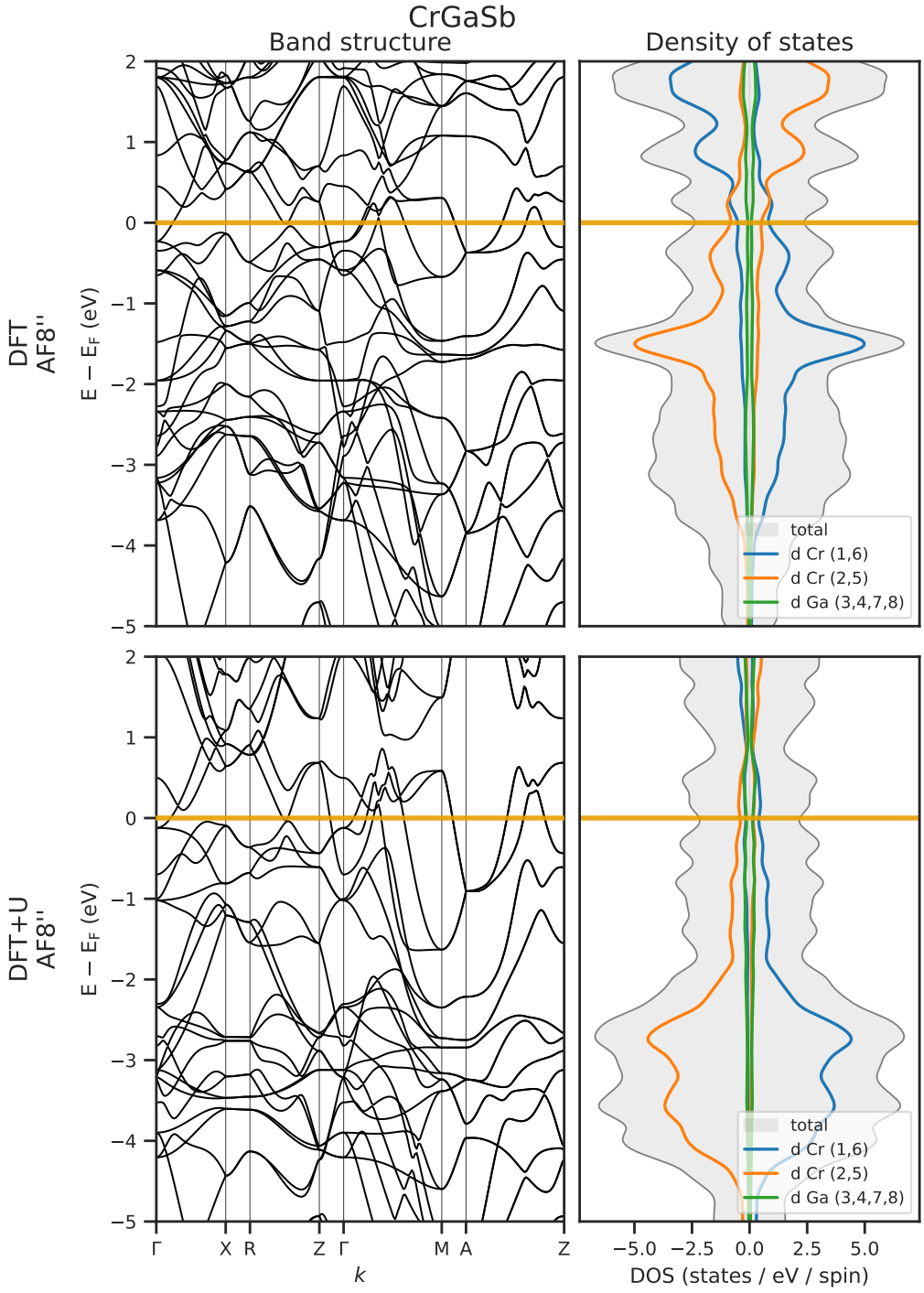


Figure 120: Band structure and Density of states of the lowest in energy calculations.

Material: CrMnAs

Configuration: CrMnAs ■ lower-energy

Structure

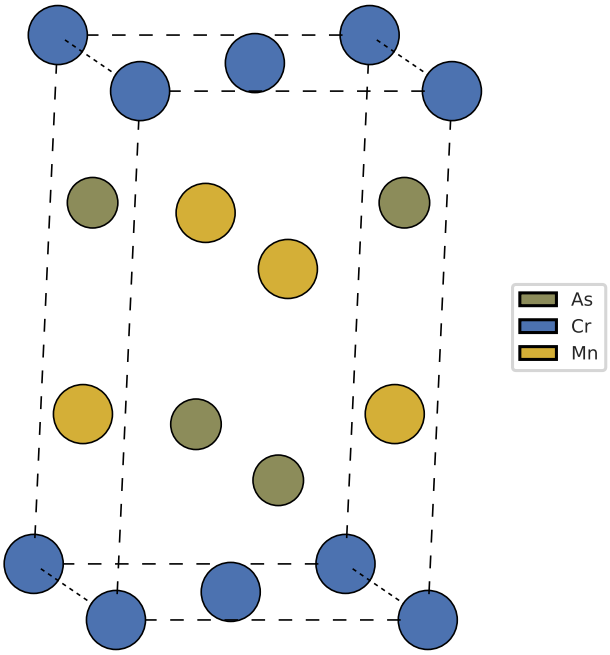


Figure 121: Structure of CrMnAs

a (Å)	c (Å)	z_1	z_2
3.7187	6.2503	0.3364	0.2679

Table 125: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

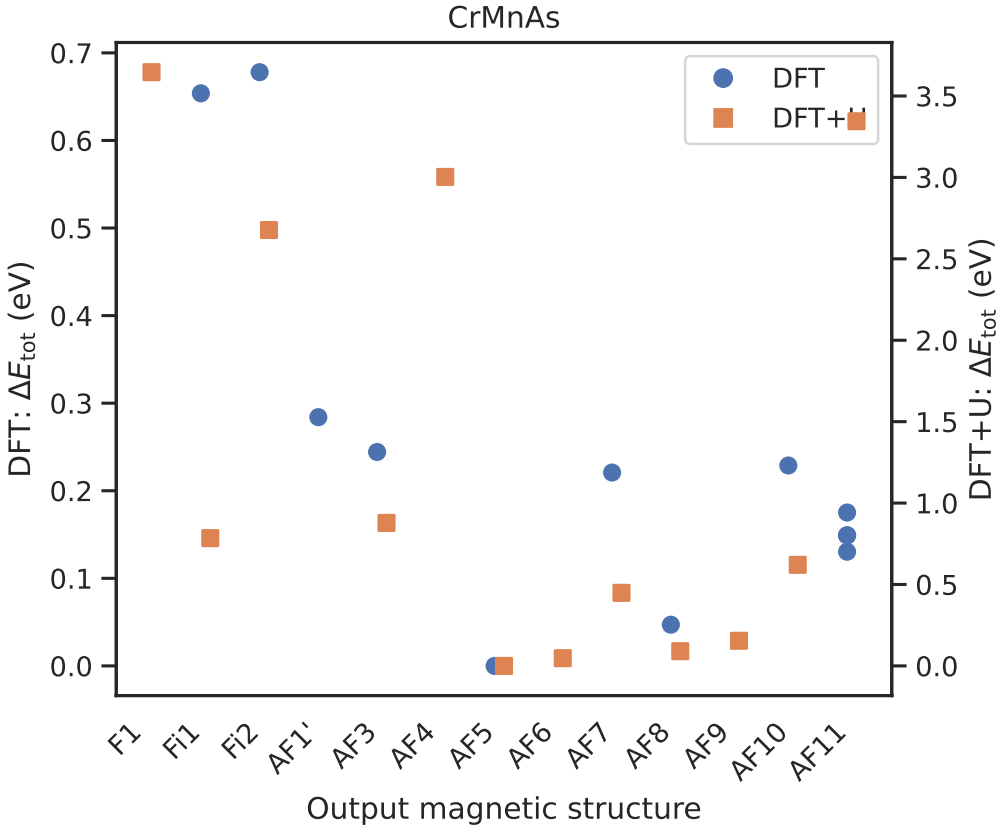


Figure 122: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF5	-32495.797627	0.000000	1.88, -1.88, -3.67, 3.67, 1.88, -1.88, -3.67, 3.67
AF8	-32495.750580	0.047047	1.73, -1.73, -3.68, 3.68, -1.73, 1.73, -3.68, 3.68
AF11	-32495.667229	0.130398	1.00, 1.00, -3.82, 3.82, -1.00, -1.00, -3.55, 3.55
AF11	-32495.648531	0.149096	2.63, -1.59, -3.67, 3.67, 1.59, -2.64, 3.67, -3.67
AF11	-32495.622497	0.175129	2.59, -1.50, -3.67, 3.67, -2.59, 1.50, 3.67, -3.67
AF7	-32495.576826	0.220801	1.51, -1.51, 3.65, 3.65, 1.51, -1.51, -3.65, -3.65
AF10	-32495.568792	0.228834	1.54, -1.54, 3.64, 3.64, -1.54, 1.54, -3.64, -3.64
AF3	-32495.553359	0.244267	2.02, 2.02, -3.66, 3.66, -2.01, -2.01, 3.66, -3.66
AF1′	-32495.513601	0.284025	0.00, -0.00, 3.64, 3.64, -0.00, 0.00, -3.64, -3.64
Fi1	-32495.143785	0.653842	1.62, 1.62, -3.68, -3.68, 1.62, 1.62, -3.68, -3.68
Fi2	-32495.119655	0.677972	-1.69, -1.59, 3.68, 3.69, -0.46, -1.90, 3.69, 3.68

Table 126: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5	-32480.812001	0.000000	4.48, -4.48, -4.66, 4.66, 4.48, -4.48, -4.66, 4.66
AF6	-32480.764538	0.047462	4.49, -4.46, -4.67, 4.67, 4.46, -4.49, 4.67, -4.67
AF8	-32480.721581	0.090420	4.49, -4.49, -4.66, 4.66, -4.49, 4.49, -4.66, 4.66
AF9	-32480.657710	0.154291	4.47, -4.47, -4.67, 4.67, -4.47, 4.47, 4.67, -4.67
AF7	-32480.363286	0.448715	4.48, -4.48, 4.66, 4.66, 4.48, -4.48, -4.66, -4.66
AF10	-32480.191422	0.620579	4.47, -4.47, 4.64, 4.64, -4.47, 4.47, -4.64, -4.64
Fi1	-32480.027319	0.784682	4.38, 4.38, -4.66, -4.66, 4.38, 4.38, -4.66, -4.66
AF3	-32479.933841	0.878160	4.43, 4.43, -4.68, 4.68, -4.43, -4.43, 4.68, -4.68
Fi2	-32478.135117	2.676884	4.01, 2.97, -4.73, 4.68, -4.20, -4.20, -4.50, 4.48
AF4	-32477.808854	3.003147	4.06, 4.06, 4.48, -4.48, -4.06, -4.06, -4.48, 4.48
AF11	-32477.467176	3.344825	4.13, 2.78, 4.53, 4.68, -2.90, -4.11, -4.52, -4.67
F1	-32477.165722	3.646279	3.93, 3.93, 4.46, 4.46, 3.93, 3.93, 4.46, 4.46

Table 127: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

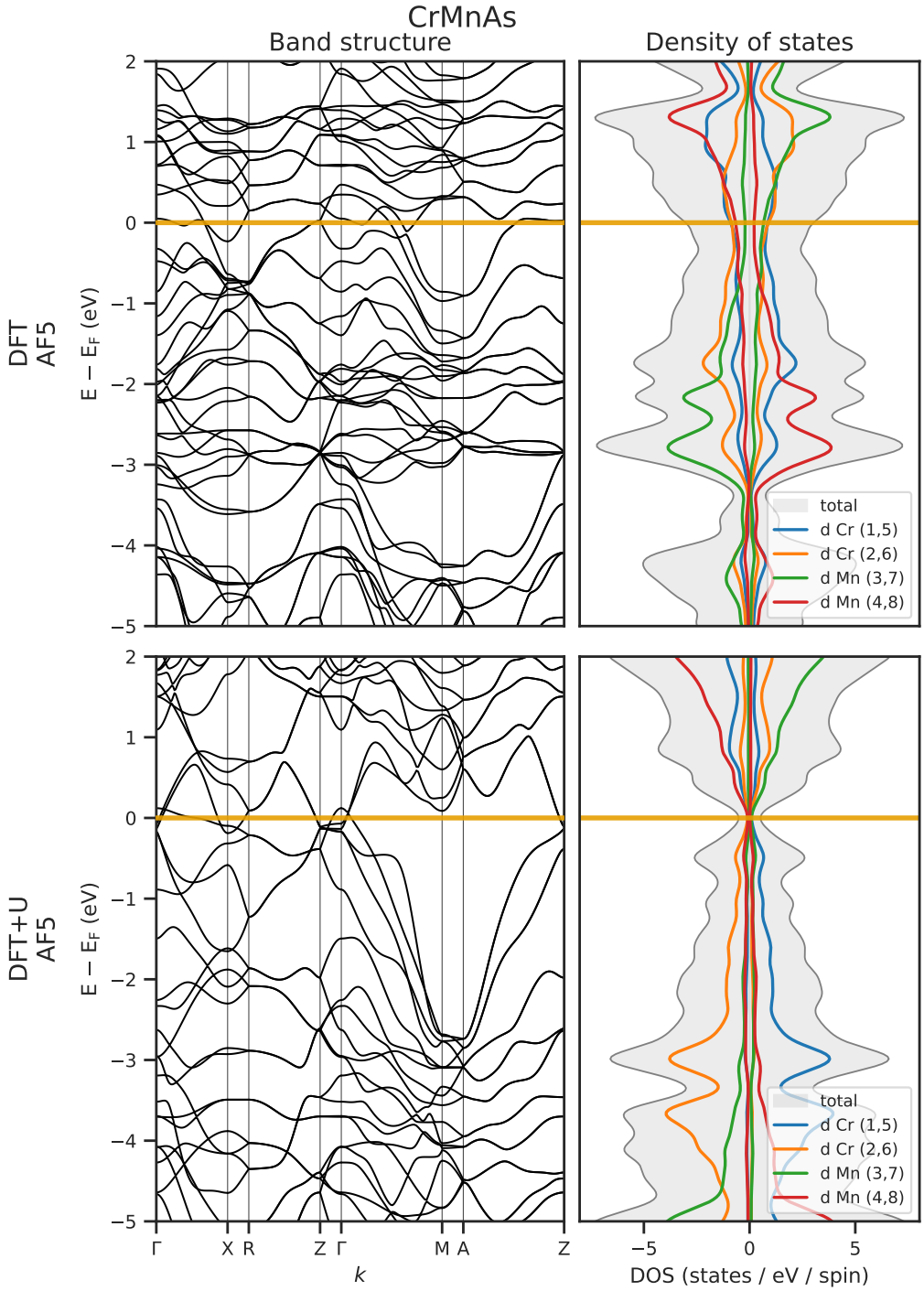


Figure 123: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnCrAs ■ higher-energy

Structure

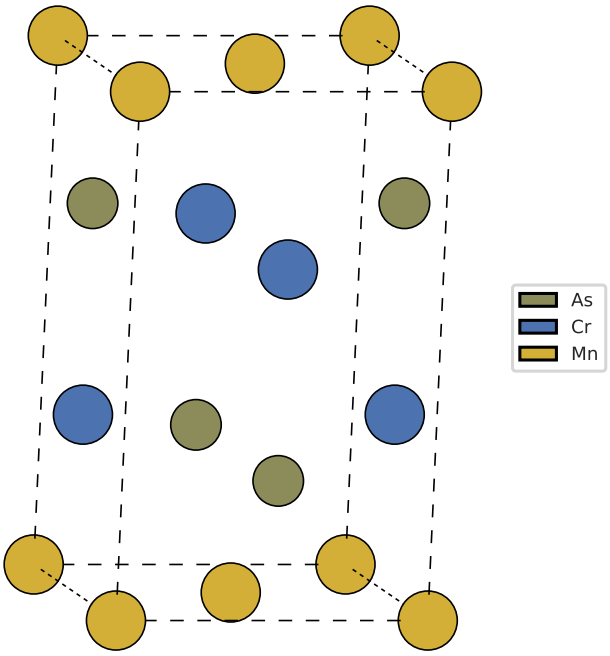


Figure 124: Structure of MnCrAs

a (Å)	c (Å)	z_1	z_2
3.6764	6.2228	0.3340	0.2664

Table 128: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

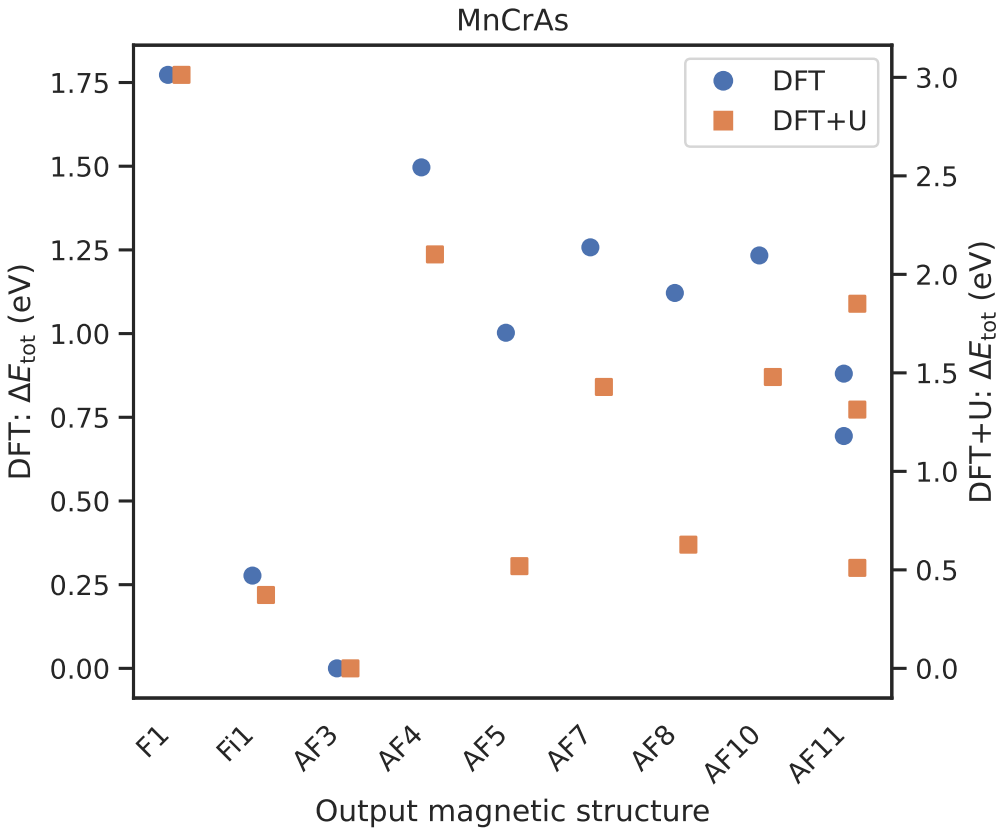


Figure 125: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-32495.658290	0.000000	2.50, 2.50, -3.16, 3.16, -2.50, -2.50, 3.16, -3.16
Fi1	-32495.381171	0.277119	2.50, 2.50, -2.88, -2.88, 2.50, 2.50, -2.88, -2.88
AF11	-32494.964256	0.694034	1.97, 1.96, -3.50, 3.50, -1.96, -1.97, -2.75, 2.75
AF11	-32494.777918	0.880373	2.03, 2.03, 1.95, 3.15, -2.03, -2.03, -1.95, -3.15
AF5	-32494.655773	1.002517	2.13, -2.13, -3.11, 3.11, 2.13, -2.13, -3.11, 3.11
AF8	-32494.536911	1.121379	1.87, -1.87, -3.15, 3.15, -1.87, 1.87, -3.15, 3.15
AF10	-32494.424807	1.233483	2.01, -2.01, 2.62, 2.62, -2.01, 2.01, -2.62, -2.62
AF7	-32494.400631	1.257659	1.87, -1.87, 2.65, 2.65, 1.87, -1.87, -2.65, -2.65
AF4	-32494.161761	1.496529	2.31, 2.31, 3.35, -3.35, -2.31, -2.31, -3.35, 3.35
F1	-32493.885416	1.772874	2.01, 2.01, 2.37, 2.37, 2.01, 2.01, 2.37, 2.37

Table 129: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-32479.173534	0.000000	4.37, 4.37, -4.62, 4.62, -4.37, -4.37, 4.62, -4.62
Fi1	-32478.801056	0.372478	4.31, 4.31, -4.58, -4.58, 4.31, 4.31, -4.58, -4.58
AF11	-32478.663436	0.510098	4.20, -4.44, -4.64, 4.64, 4.44, -4.20, 4.64, -4.64
AF5	-32478.654660	0.518875	4.36, -4.36, -4.64, 4.64, 4.36, -4.36, -4.64, 4.64
AF8	-32478.545547	0.627988	4.36, -4.36, -4.64, 4.64, -4.36, 4.36, -4.64, 4.64
AF11	-32477.859940	1.313594	4.25, 4.25, -4.60, 4.60, -4.25, -4.25, -4.40, 4.40
AF7	-32477.745056	1.428478	4.35, -4.35, 4.60, 4.60, 4.35, -4.35, -4.60, -4.60
AF10	-32477.694542	1.478992	4.34, -4.34, 4.59, 4.59, -4.34, 4.34, -4.59, -4.59
AF11	-32477.322629	1.850905	4.06, 4.06, 4.36, 4.56, -4.06, -4.06, -4.36, -4.56
AF4	-32477.072194	2.101341	3.94, 3.94, 4.36, -4.36, -3.94, -3.94, -4.36, 4.36
F1	-32476.160863	3.012671	3.92, 3.92, 4.30, 4.30, 3.92, 3.92, 4.30, 4.30

Table 130: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

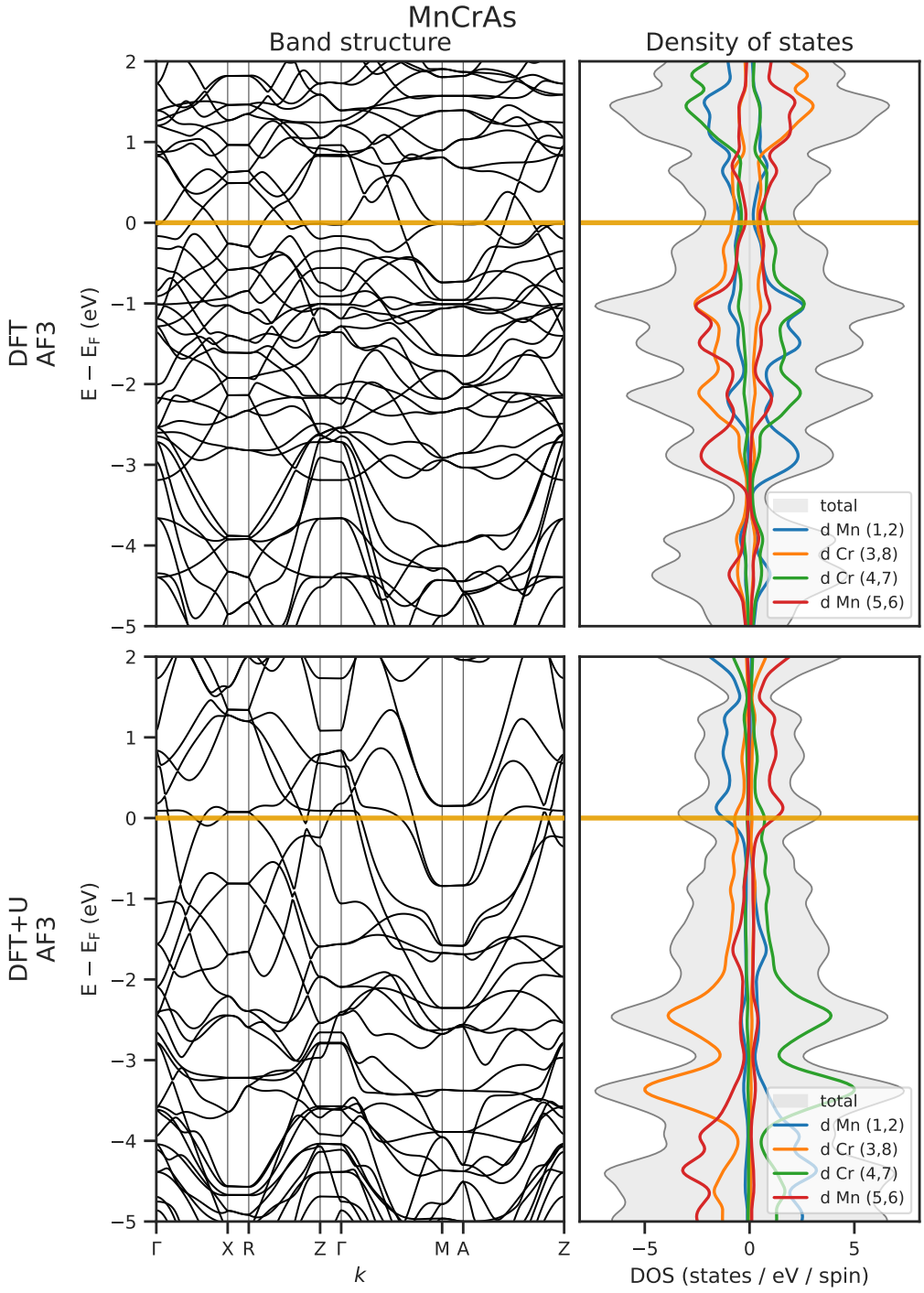


Figure 126: Band structure and Density of states of the lowest in energy calculations.

Material: CrMnSb

Configuration: CrMnSb ■ lower-energy

Structure

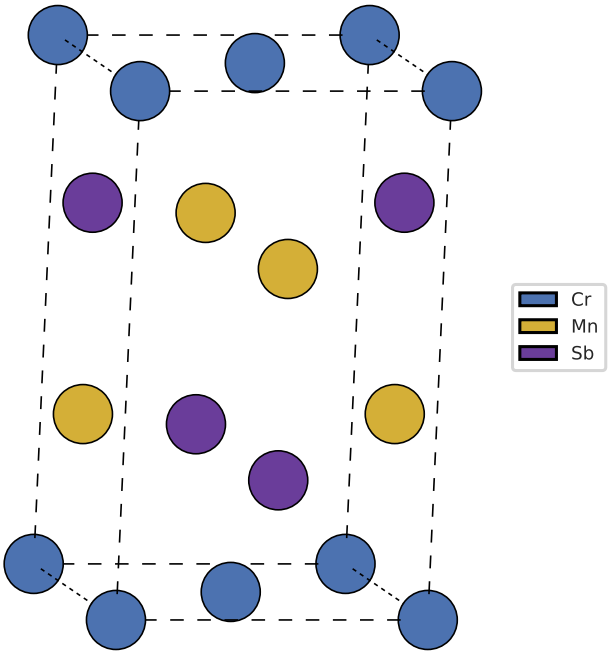


Figure 127: Structure of CrMnSb

a (Å)	c (Å)	z_1	z_2
4.0805	6.5830	0.2914	0.2846

Table 131: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

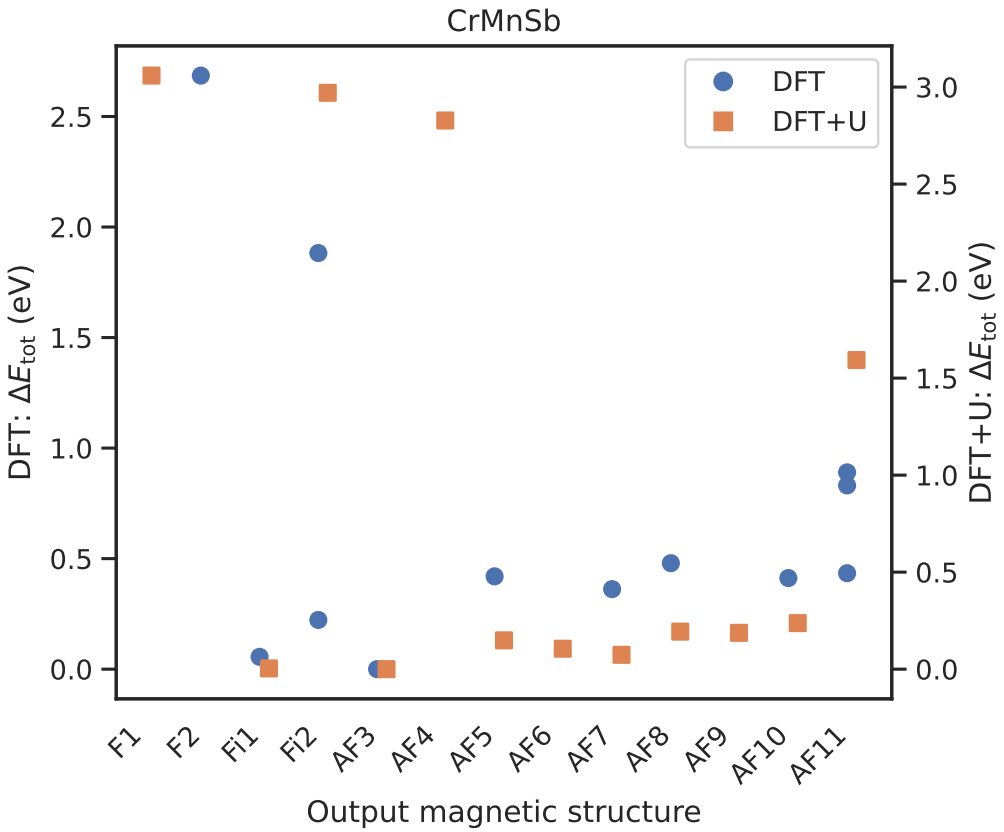


Figure 128: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF3	-30380.056049	0.000000	2.74, 2.74, -4.10, 4.10, -2.74, -2.74, 4.10, -4.10
Fi1	-30380.000218	0.055830	3.01, 3.01, -4.12, -4.12, 3.01, 3.01, -4.12, -4.12
Fi2	-30379.833412	0.222637	-2.86, -2.88, 4.10, -4.00, 3.38, -2.49, 4.11, 4.09
AF7	-30379.694010	0.362039	3.19, -3.19, 4.15, 4.15, 3.19, -3.19, -4.15, -4.15
AF10	-30379.643838	0.412211	3.09, -3.09, 4.04, 4.04, -3.09, 3.09, -4.04, -4.04
AF5	-30379.636172	0.419876	3.14, -3.14, -4.08, 4.08, 3.14, -3.14, -4.08, 4.08
AF11	-30379.621955	0.434093	3.50, -2.17, -4.01, 4.00, -3.50, 2.15, 4.00, -4.01
AF8	-30379.576705	0.479344	2.98, -2.98, -4.05, 4.05, -2.98, 2.98, -4.05, 4.05
AF11	-30379.224975	0.831073	1.91, 1.91, 3.88, 4.18, -1.91, -1.91, -3.88, -4.18
AF11	-30379.165775	0.890273	1.85, 1.85, -4.18, 4.18, -1.85, -1.85, -3.83, 3.83
Fi2	-30378.173699	1.882350	2.18, 2.18, 3.97, -3.91, -0.82, -0.82, -3.91, 3.97
F2	-30377.370916	2.685133	1.53, 1.53, 0.55, 3.89, 0.82, 0.82, 3.94, 3.89

Table 132: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-30368.543809	0.000000	4.67, 4.67, -4.84, 4.84, -4.67, -4.67, 4.84, -4.84
Fi1	-30368.539853	0.003957	4.65, 4.65, -4.88, -4.88, 4.65, 4.65, -4.88, -4.88
AF7	-30368.469904	0.073906	4.75, -4.75, 4.81, 4.81, 4.75, -4.75, -4.81, -4.81
AF6	-30368.438435	0.105375	4.76, -4.71, -4.78, 4.78, 4.71, -4.76, 4.78, -4.78
AF5	-30368.395216	0.148594	4.74, -4.74, -4.79, 4.79, 4.74, -4.74, -4.79, 4.79
AF9	-30368.356645	0.187164	4.75, -4.71, -4.79, 4.79, -4.75, 4.71, 4.79, -4.79
AF8	-30368.350317	0.193492	4.74, -4.74, -4.78, 4.78, -4.74, 4.74, -4.78, 4.78
AF10	-30368.306479	0.237330	4.74, -4.74, 4.82, 4.82, -4.74, 4.74, -4.82, -4.82
AF11	-30366.950699	1.593110	4.58, 4.58, -4.86, 4.86, -4.58, -4.58, -4.69, 4.69
AF4	-30365.715983	2.827826	4.46, 4.46, 4.64, -4.64, -4.46, -4.46, -4.64, 4.64
Fi2	-30365.573368	2.970441	1.82, -4.67, 4.83, 4.85, -2.79, -4.64, 4.84, -4.72
F1	-30365.484549	3.059260	4.42, 4.42, 4.65, 4.65, 4.42, 4.42, 4.65, 4.65

Table 133: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

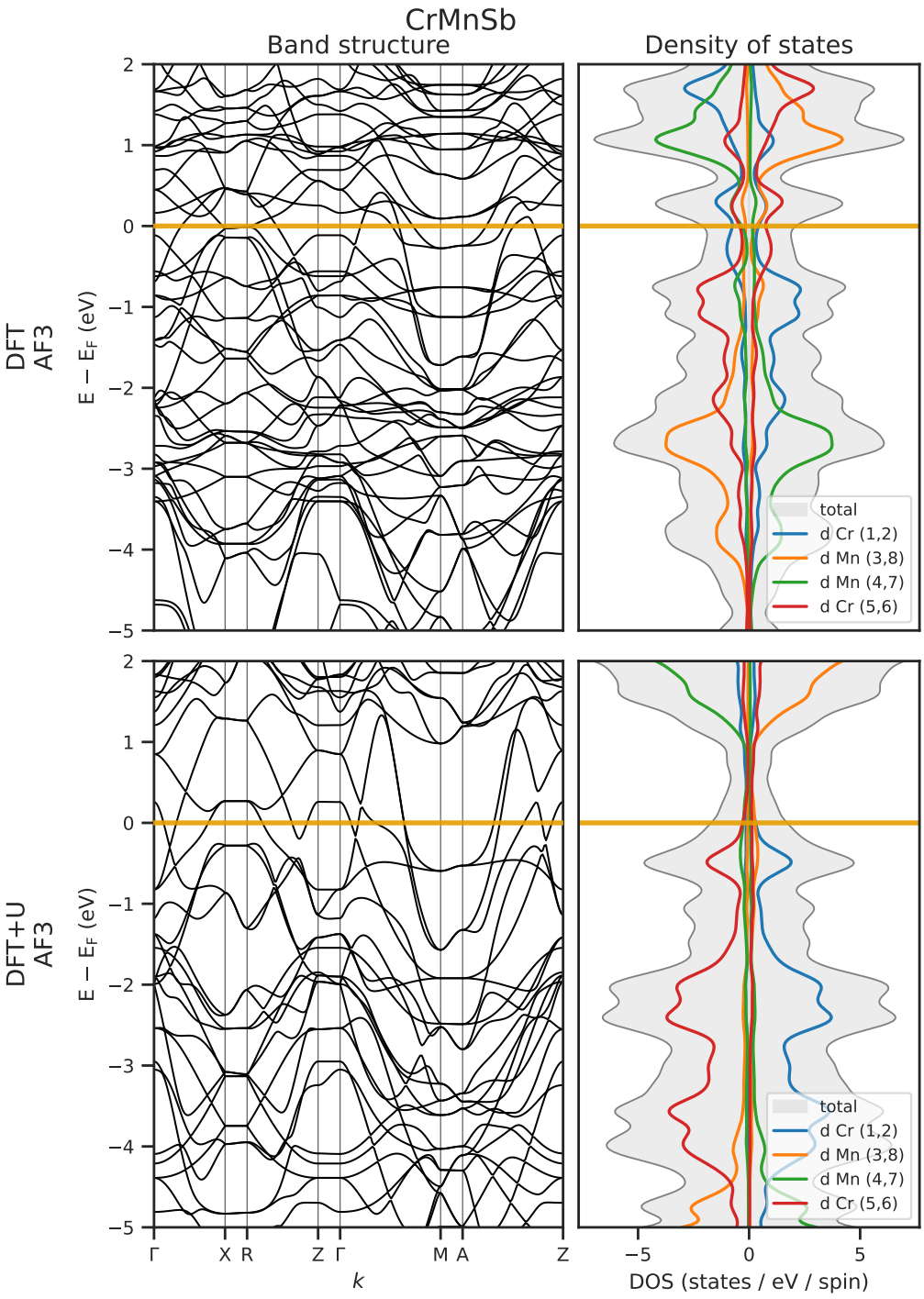


Figure 129: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnCrSb ■ higher-energy

Structure

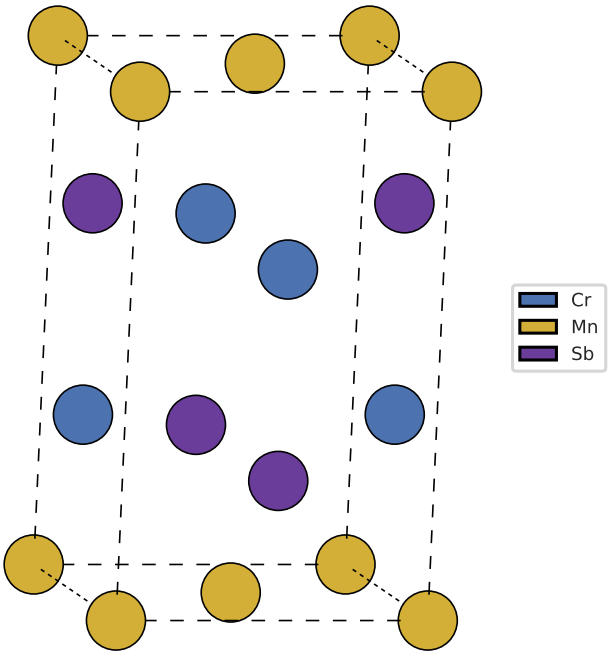


Figure 130: Structure of MnCrSb

a (Å)	c (Å)	z_1	z_2
4.1068	6.6780	0.3028	0.2812

Table 134: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

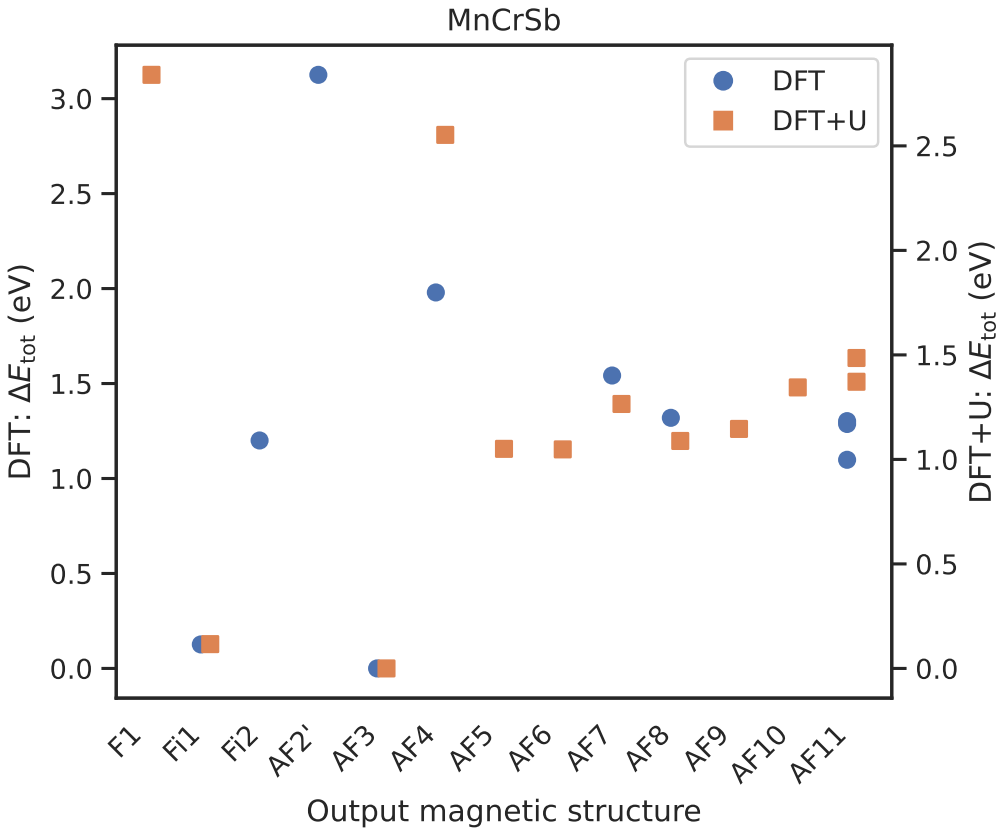


Figure 131: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF3	-30379.721245	0.000000	3.95, 3.95, -3.99, 3.99, -3.95, -3.95, 3.99, -3.99
Fi1	-30379.594936	0.126309	-3.86, -3.86, 4.07, 4.07, -3.86, -3.86, 4.07, 4.06
AF11	-30378.622749	1.098496	3.65, -3.95, -4.14, 4.14, 3.95, -3.65, 4.14, -4.14
Fi2	-30378.521098	1.200147	-3.86, -3.86, 4.00, 3.91, 3.30, 3.30, 3.91, 4.00
AF11	-30378.434182	1.287064	3.65, -3.98, -4.12, 4.12, -3.65, 3.98, 4.12, -4.12
AF11	-30378.419139	1.302106	3.62, 3.62, -4.03, 4.03, -3.62, -3.62, -3.72, 3.72
AF8	-30378.401761	1.319484	3.81, -3.81, -4.11, 4.11, -3.81, 3.81, -4.11, 4.11
AF7	-30378.179019	1.542227	3.81, -3.81, 4.11, 4.11, 3.81, -3.81, -4.11, -4.11
AF4	-30377.741742	1.979503	3.44, 3.44, 3.89, -3.89, -3.44, -3.44, -3.89, 3.89
AF2′	-30376.595946	3.125299	-0.00, -0.00, -3.92, 3.92, 0.00, 0.00, -3.92, 3.92

Table 135: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-30369.330043	0.000000	4.68, 4.68, -4.87, 4.87, -4.68, -4.68, 4.87, -4.87
Fi1	-30369.213763	0.116280	4.67, 4.67, -4.92, -4.92, 4.67, 4.67, -4.92, -4.92
AF6	-30368.282092	1.047951	4.67, -4.73, -4.85, 4.85, 4.73, -4.67, 4.85, -4.85
AF5	-30368.279523	1.050520	4.71, -4.71, -4.86, 4.86, 4.71, -4.71, -4.86, 4.86
AF8	-30368.241763	1.088280	4.71, -4.71, -4.86, 4.86, -4.71, 4.71, -4.86, 4.86
AF9	-30368.184154	1.145889	4.67, -4.74, -4.85, 4.85, -4.67, 4.74, 4.85, -4.85
AF7	-30368.064790	1.265253	4.71, -4.71, 4.87, 4.87, 4.71, -4.71, -4.87, -4.87
AF10	-30367.985553	1.344490	4.71, -4.71, 4.87, 4.87, -4.71, 4.71, -4.87, -4.87
AF11	-30367.958486	1.371557	4.61, 4.61, -4.88, 4.88, -4.61, -4.61, -4.69, 4.69
AF11	-30367.844853	1.485190	4.59, 4.59, 4.71, 4.91, -4.59, -4.59, -4.71, -4.91
AF4	-30366.777388	2.552654	4.49, 4.49, 4.63, -4.63, -4.49, -4.49, -4.63, 4.63
F1	-30366.490147	2.839896	4.45, 4.45, 4.64, 4.64, 4.45, 4.45, 4.64, 4.64

Table 136: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

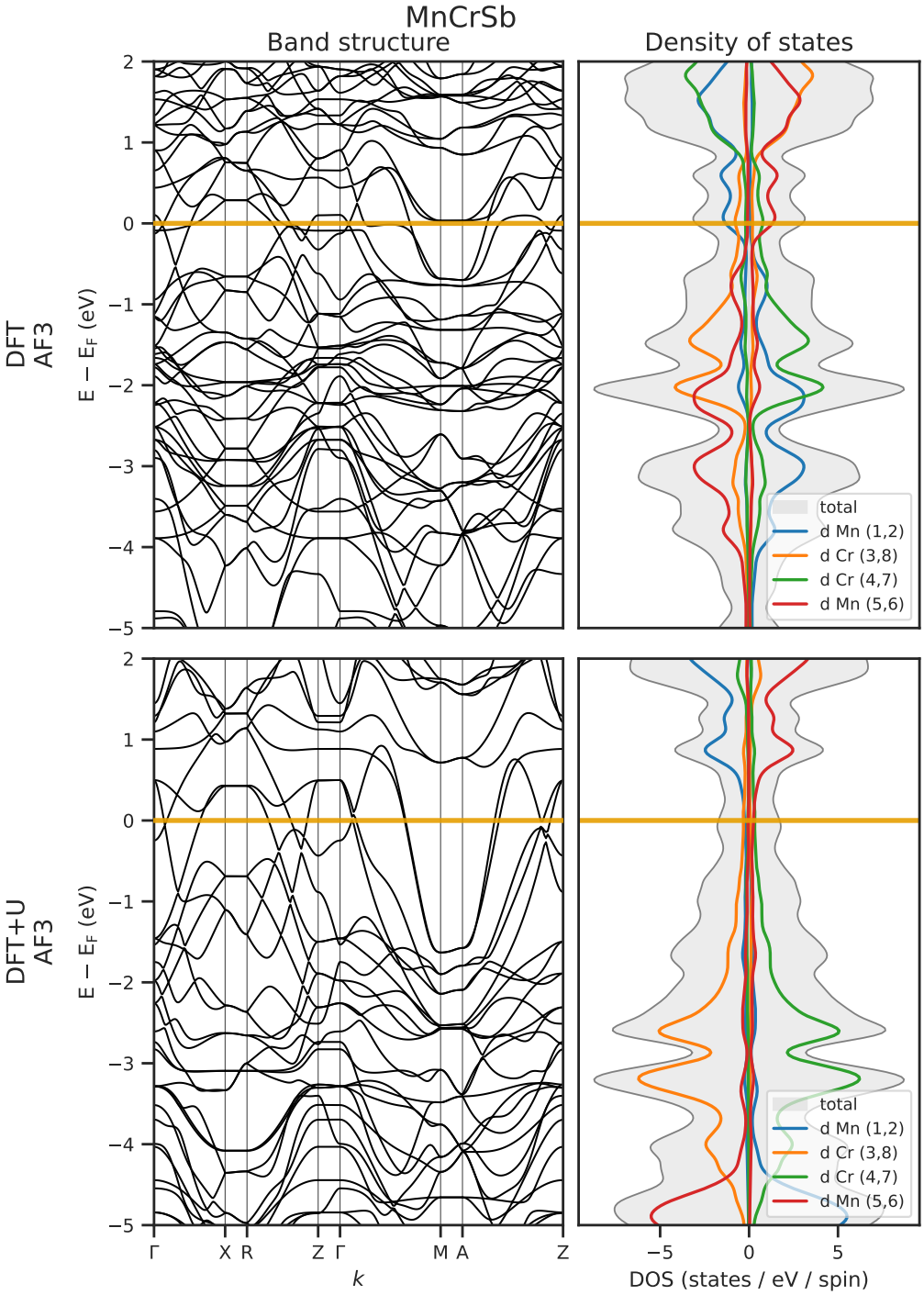


Figure 132: Band structure and Density of states of the lowest in energy calculations.

Material: NiCrAs

Configuration: NiCrAs ■ lower-energy

Structure

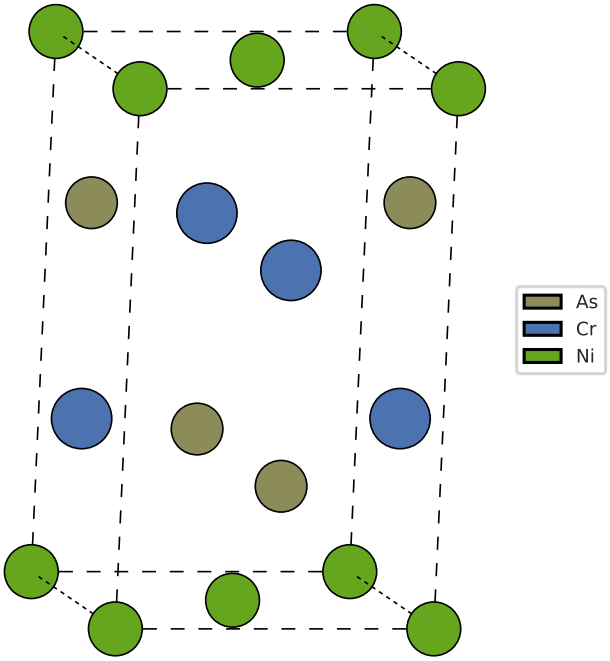


Figure 133: Structure of NiCrAs

a (Å)	c (Å)	z_1	z_2
3.6644	6.1848	0.3423	0.2600

Table 137: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1′	-39327.864214	0.000000	-0.01, -0.01, -3.33, -3.33, -0.01, -0.01, -3.33, -3.33
AF3′	-39327.674586	0.189628	-0.03, -0.03, -3.38, 3.38, 0.03, 0.03, 3.38, -3.38
AF2′	-39327.331384	0.532830	0.00, 0.00, -3.37, 3.37, 0.00, 0.00, -3.37, 3.37
AF1′	-39327.271077	0.593137	0.00, 0.00, 3.21, 3.21, 0.00, 0.00, -3.21, -3.21
AF11′	-39326.291322	1.572892	0.08, 0.08, -0.23, 0.23, -0.08, -0.08, -3.50, 3.50

Table 138: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

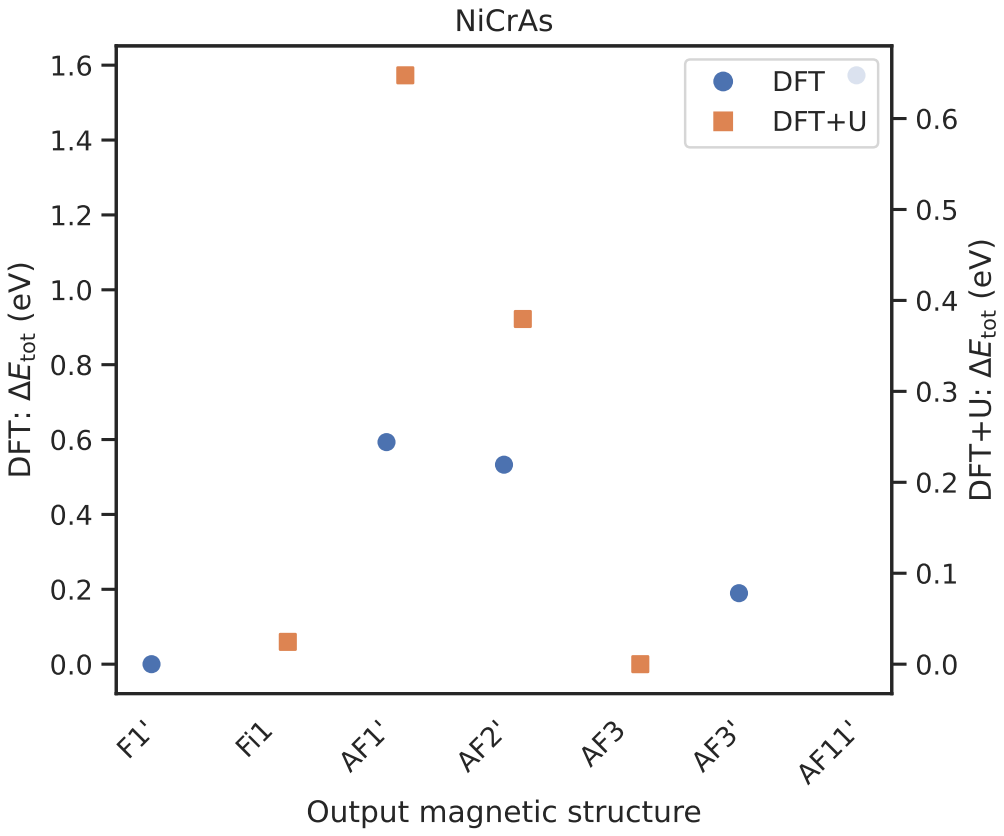


Figure 134: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF3	-39313.236898	0.000000	0.30, 0.30, -4.51, 4.51, -0.30, -0.30, 4.51, -4.51
AF3	-39313.236898	0.000000	0.30, 0.30, -4.51, 4.51, -0.30, -0.30, 4.51, -4.51
AF3	-39313.236898	0.000000	-0.30, -0.30, 4.51, -4.51, 0.30, 0.30, -4.51, 4.51
AF3	-39313.236898	0.000000	0.30, 0.30, -4.51, 4.51, -0.30, -0.30, 4.51, -4.51
Fi1	-39313.212369	0.024529	0.49, 0.49, -4.35, -4.35, 0.49, 0.49, -4.35, -4.35
Fi1	-39313.212369	0.024530	-0.49, -0.49, 4.35, 4.35, -0.49, -0.49, 4.35, 4.35
AF2′	-39312.857329	0.379569	0.00, 0.00, -4.51, 4.51, 0.00, 0.00, -4.51, 4.51
AF2′	-39312.857329	0.379570	0.00, 0.00, -4.51, 4.51, 0.00, 0.00, -4.51, 4.51
AF2′	-39312.857328	0.379570	0.00, 0.00, -4.51, 4.51, 0.00, 0.00, -4.51, 4.51
AF1′	-39312.589364	0.647534	0.00, 0.00, 4.38, 4.38, 0.00, 0.00, -4.38, -4.38
AF1′	-39312.589364	0.647534	0.00, 0.00, 4.38, 4.38, 0.00, 0.00, -4.38, -4.38
AF1′	-39312.589364	0.647535	0.00, 0.00, 4.38, 4.38, 0.00, 0.00, -4.38, -4.38

Table 139: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

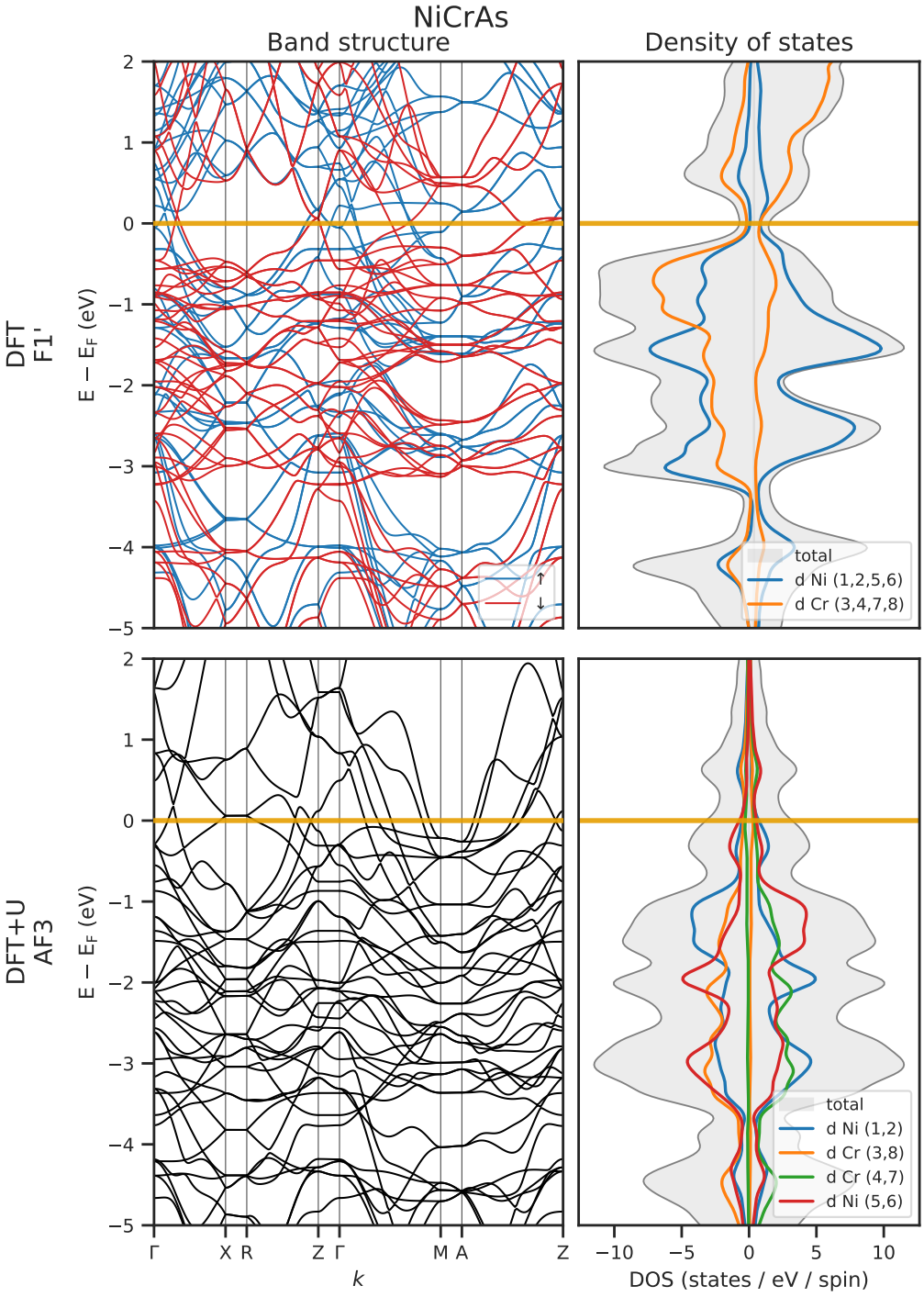


Figure 135: Band structure and Density of states of the lowest in energy calculations.

Configuration: CrNiAs ■ higher-energy

Structure

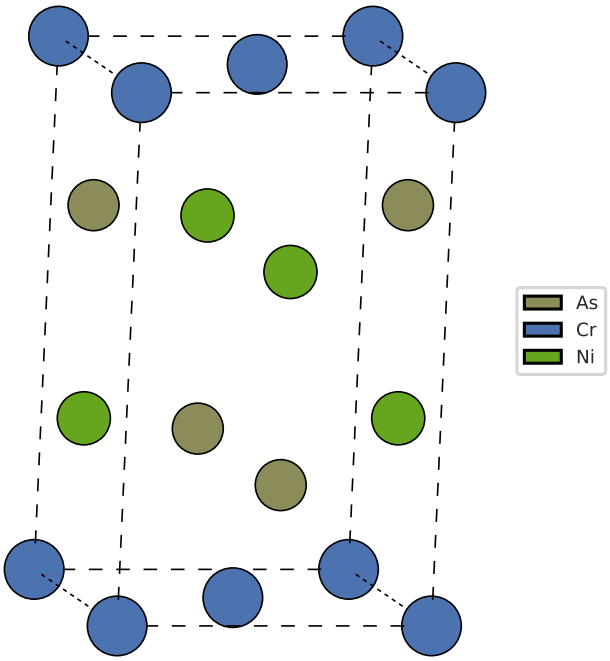


Figure 136: Structure of CrNiAs

a (Å)	c (Å)	z_1	z_2
3.6607	6.1047	0.3017	0.2966

Table 140: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-39327.258972	0.000000	2.57, -2.57, 0.00, 0.00, -2.57, 2.57, 0.00, 0.00
AF5″	-39327.099763	0.159209	2.29, -2.29, 0.00, 0.00, 2.29, -2.29, 0.00, 0.00
NM	-39326.800462	0.458510	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-39326.800356	0.458615	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 141: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

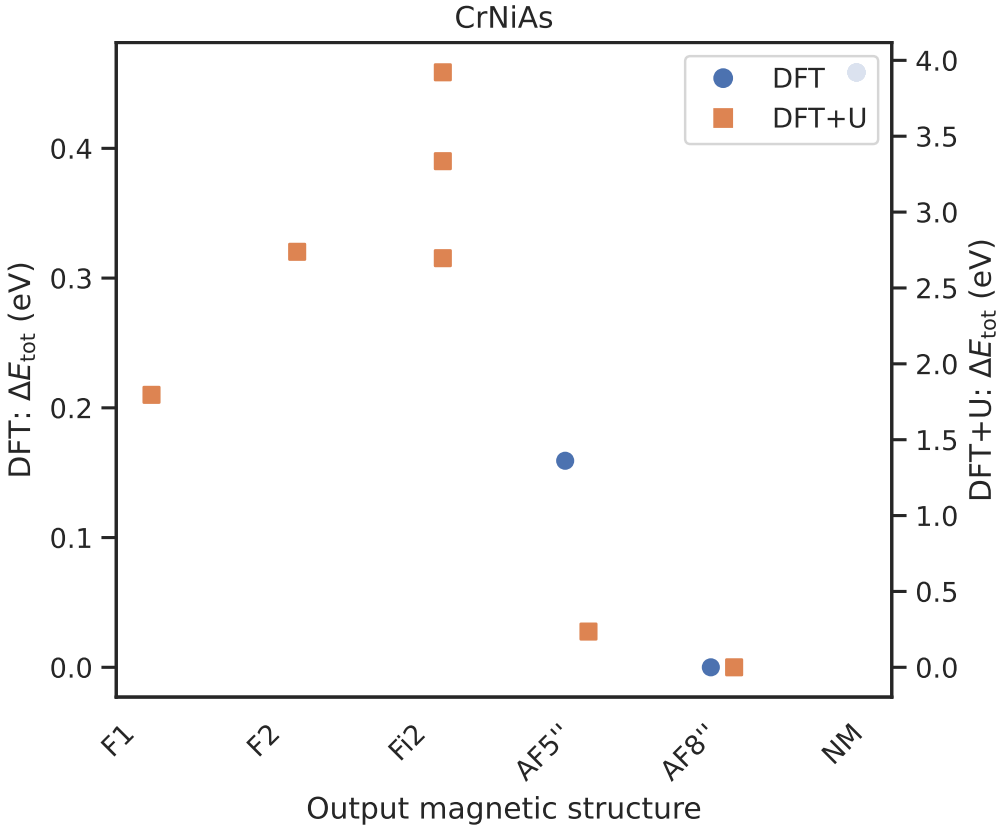


Figure 137: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF8″	-39311.025181	0.000000	4.40, -4.40, 0.00, 0.00, -4.40, 4.40, 0.00, 0.00
AF8″	-39311.025181	0.000000	4.40, -4.40, 0.00, 0.00, -4.40, 4.40, 0.00, 0.00
AF8″	-39311.025181	0.000000	4.40, -4.40, 0.00, 0.00, -4.40, 4.40, 0.00, 0.00
AF5″	-39310.789602	0.235579	4.40, -4.40, 0.00, 0.00, 4.40, -4.40, 0.00, 0.00
AF5″	-39310.789602	0.235579	4.40, -4.40, 0.00, 0.00, 4.40, -4.40, 0.00, 0.00
AF5″	-39310.789602	0.235579	4.40, -4.40, 0.00, 0.00, 4.40, -4.40, 0.00, 0.00
F1	-39309.229602	1.795579	4.04, 4.04, 0.24, 0.24, 4.04, 4.04, 0.24, 0.24
Fi2	-39308.328941	2.696240	1.95, 4.03, 0.27, -0.22, -4.08, -4.09, -0.22, 0.27
F2	-39308.286911	2.738270	4.01, 1.82, 0.26, 0.25, 4.05, 4.05, 0.25, 0.26
Fi2	-39307.689699	3.335482	4.09, 2.29, 0.14, -0.26, -4.08, -2.69, -0.66, 0.15
Fi2	-39307.103970	3.921211	-1.17, 4.26, 0.31, -0.28, -1.82, -4.02, -0.28, 0.31

Table 142: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

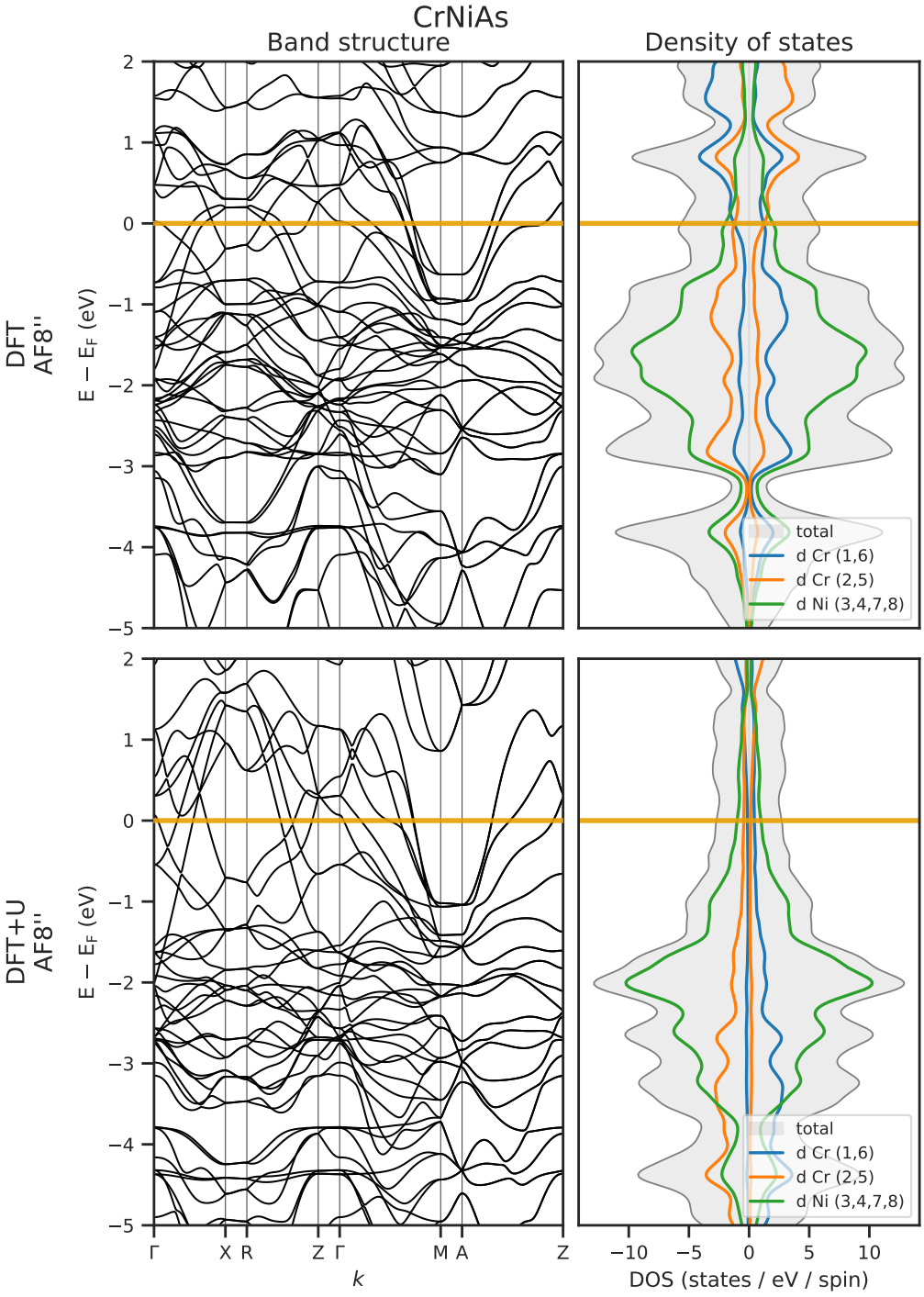


Figure 138: Band structure and Density of states of the lowest in energy calculations.

Material: CrNiSb

Configuration: CrNiSb ■ lower-energy

Structure

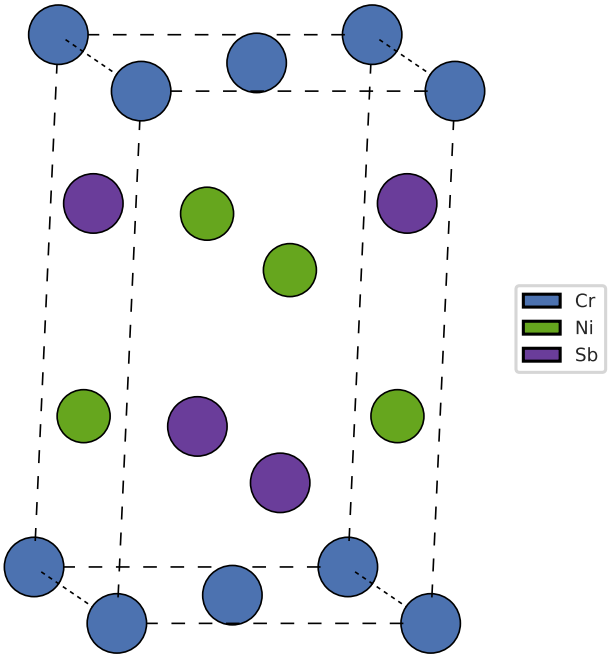


Figure 139: Structure of CrNiSb

a (Å)	c (Å)	z_1	z_2
3.8213	6.6181	0.2712	0.3214

Table 143: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cr atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF8″	-37213.268577	0.000000	3.36, -3.36, 0.00, 0.00, -3.36, 3.36, 0.00, 0.00
AF5″	-37213.157970	0.110607	3.33, -3.33, 0.00, 0.00, 3.33, -3.33, 0.00, 0.00
AF11″	-37212.533668	0.734909	-3.32, 3.32, 0.00, 0.00, 0.08, -0.08, 0.00, 0.00
NM	-37211.871363	1.397214	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-37211.870912	1.397665	-0.00, 0.00, -0.00, 0.00, -0.00, -0.00, 0.00, -0.00

Table 144: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

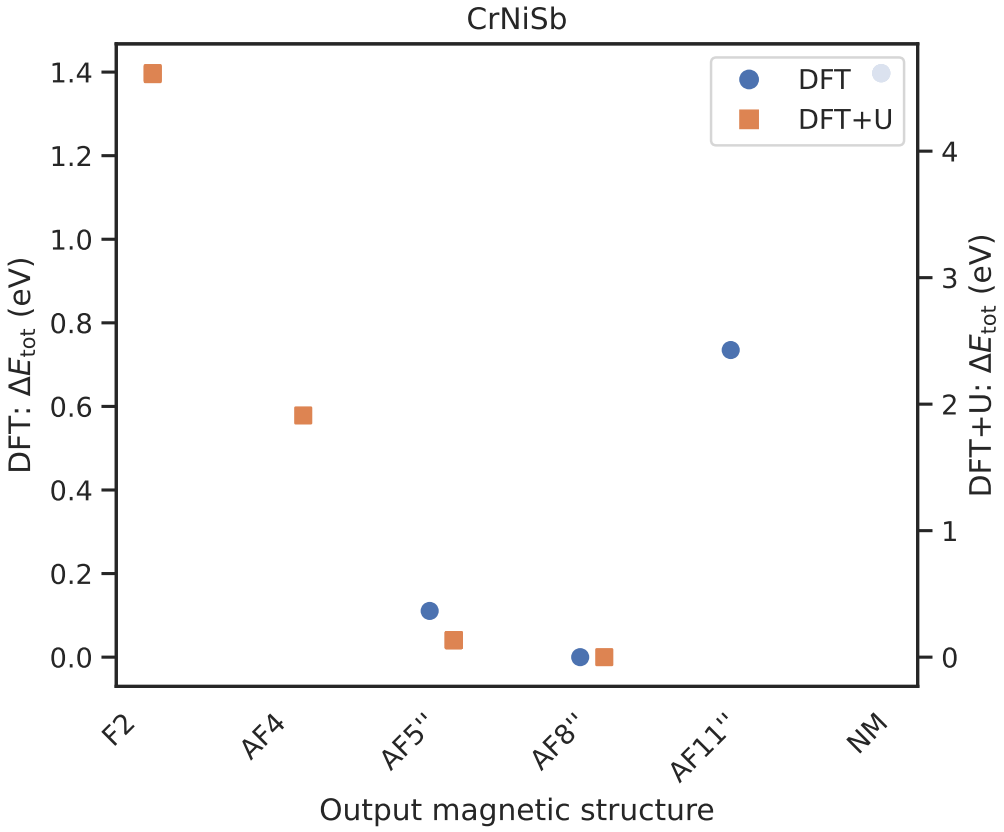


Figure 140: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF8″	-37199.273594	0.000000	4.65, -4.65, 0.00, 0.00, -4.65, 4.65, 0.00, 0.00
AF8″	-37199.273581	0.000013	4.65, -4.65, 0.00, 0.00, -4.65, 4.65, 0.00, 0.00
AF8″	-37199.273578	0.000016	4.65, -4.65, 0.00, 0.00, -4.65, 4.65, 0.00, 0.00
AF5″	-37199.139516	0.134078	4.66, -4.66, 0.00, 0.00, 4.66, -4.66, 0.00, 0.00
AF5″	-37199.139459	0.134134	4.66, -4.66, 0.00, 0.00, 4.66, -4.66, 0.00, 0.00
AF5″	-37199.139332	0.134262	4.66, -4.66, 0.00, 0.00, 4.66, -4.66, 0.00, 0.00
AF4	-37197.362917	1.910677	4.37, 4.37, 0.12, -0.12, -4.37, -4.37, -0.12, 0.12
AF4	-37197.362917	1.910677	4.37, 4.37, 0.12, -0.12, -4.37, -4.37, -0.12, 0.12
AF4	-37197.362917	1.910677	4.37, 4.37, 0.12, -0.12, -4.37, -4.37, -0.12, 0.12
AF4	-37197.362917	1.910677	4.37, 4.37, 0.12, -0.12, -4.37, -4.37, -0.12, 0.12
F2	-37194.664713	4.608881	2.09, 4.28, 0.15, 0.15, 4.28, 2.09, 0.15, 0.15
F2	-37194.656242	4.617352	2.07, 4.28, 0.14, 0.14, 2.07, 4.28, 0.14, 0.14

Table 145: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

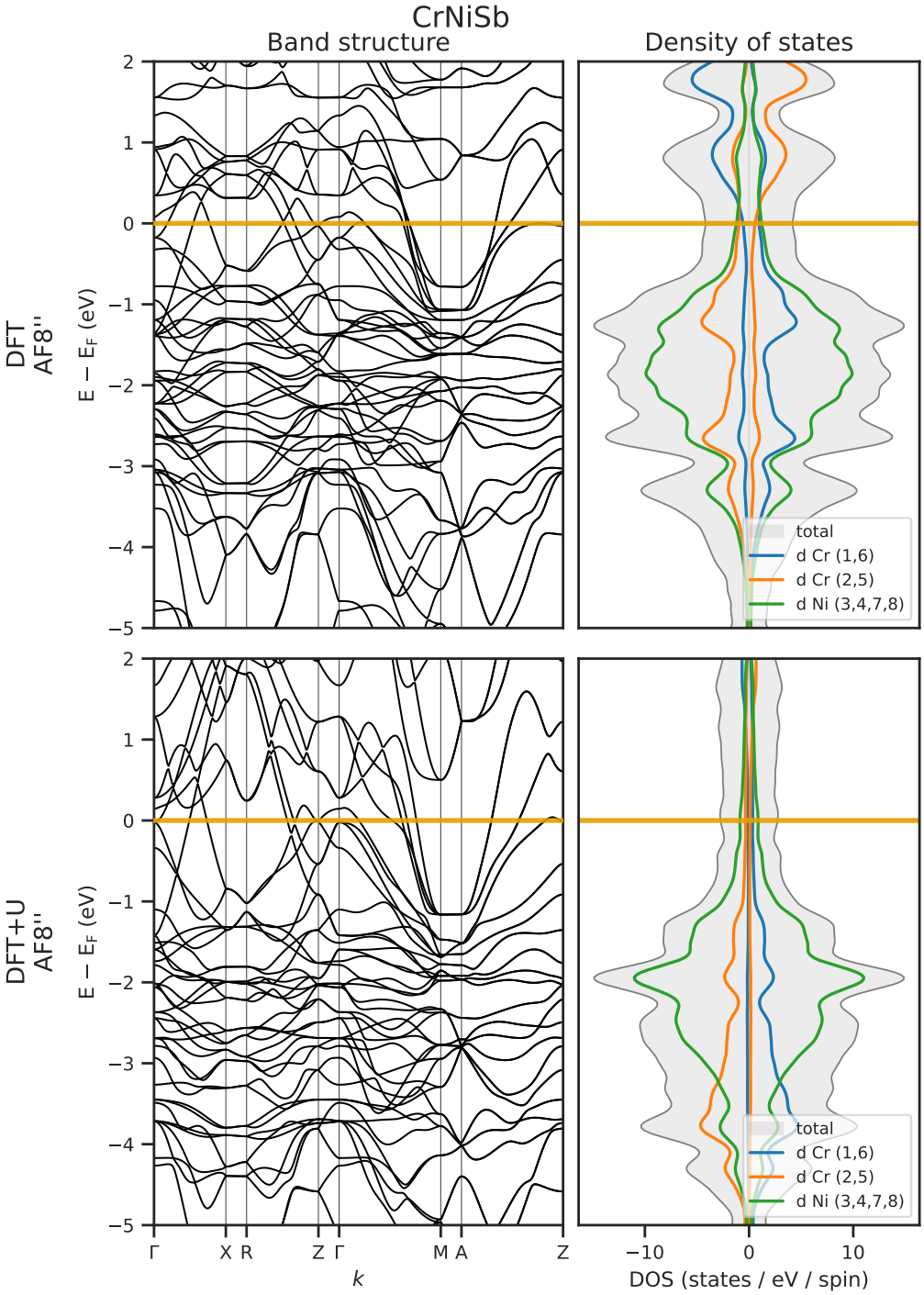


Figure 141: Band structure and Density of states of the lowest in energy calculations.

Configuration: NiCrSb ■ higher-energy

Structure

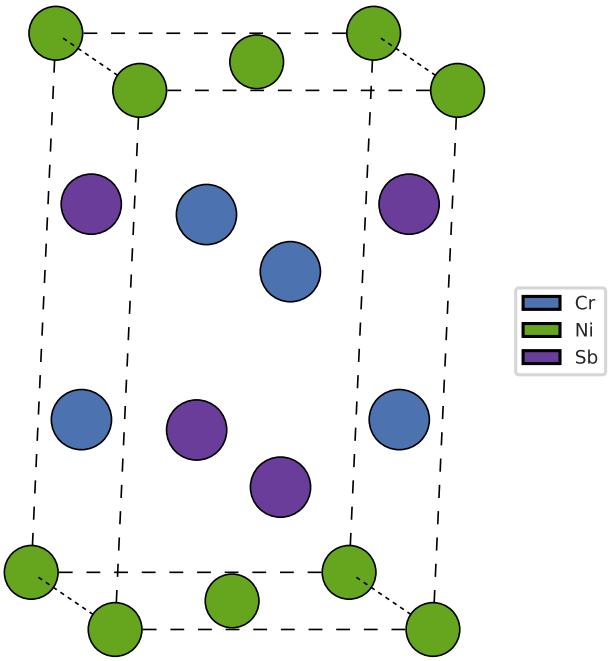


Figure 142: Structure of NiCrSb

a (Å)	c (Å)	z_1	z_2
4.0807	6.2054	0.2886	0.2668

Table 146: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Cr atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-37212.266508	0.000000	0.12, 0.12, -3.88, -3.88, 0.12, 0.12, -3.88, -3.88
AF3′	-37212.263310	0.003198	0.02, 0.02, -3.93, 3.93, -0.02, -0.02, 3.93, -3.93
AF3′	-37212.263110	0.003397	0.02, 0.02, -3.93, 3.93, -0.02, -0.02, 3.93, -3.93
AF2′	-37212.030257	0.236250	0.00, 0.00, -3.95, 3.95, 0.00, 0.00, -3.95, 3.95
AF1′	-37211.951084	0.315424	0.00, 0.00, 3.97, 3.97, 0.00, 0.00, -3.97, -3.97

Table 147: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

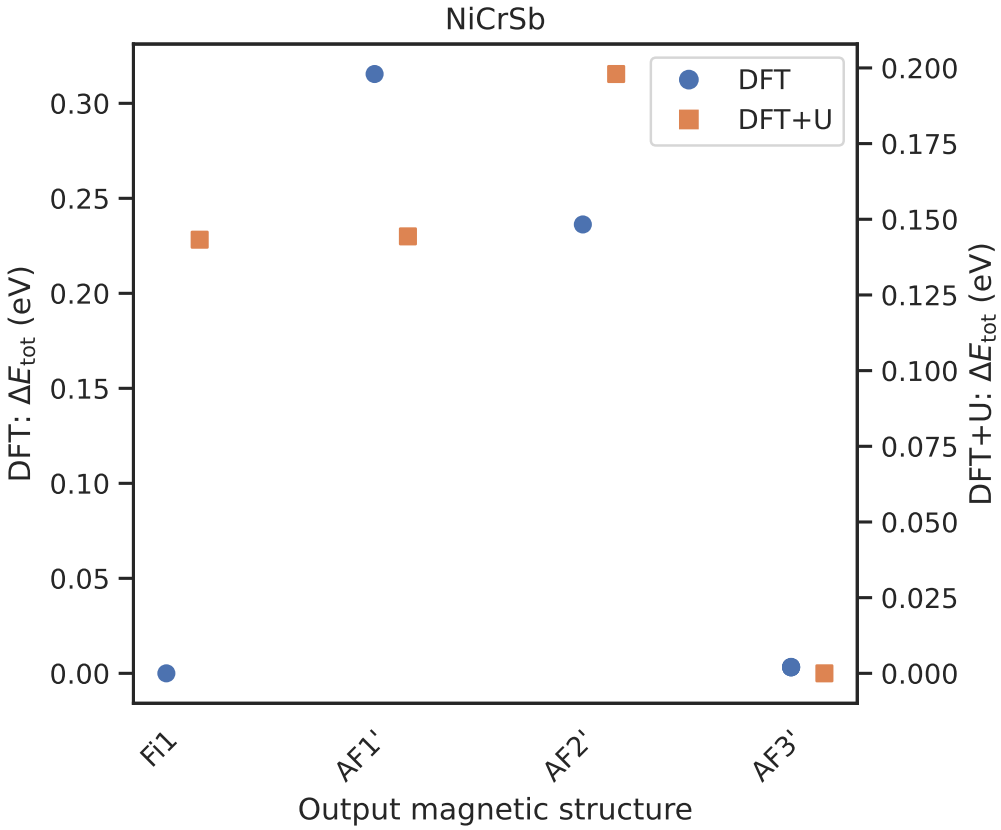


Figure 143: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-37199.991764	0.000000	0.08, 0.08, -4.72, 4.72, -0.08, -0.08, 4.72, -4.72
AF3′	-37199.991764	0.000000	0.08, 0.08, -4.72, 4.72, -0.08, -0.08, 4.72, -4.72
AF3′	-37199.991764	0.000000	-0.08, -0.08, 4.72, -4.72, 0.08, 0.08, -4.72, 4.72
AF3′	-37199.991763	0.000001	0.08, 0.08, -4.72, 4.72, -0.08, -0.08, 4.72, -4.72
Fi1	-37199.848508	0.143257	0.17, 0.17, -4.71, -4.71, 0.17, 0.17, -4.71, -4.71
Fi1	-37199.848505	0.143259	-0.17, -0.17, 4.71, 4.71, -0.17, -0.17, 4.71, 4.71
AF1′	-37199.847413	0.144351	0.00, 0.00, 4.75, 4.75, 0.00, 0.00, -4.75, -4.75
AF1′	-37199.847413	0.144351	0.00, 0.00, 4.75, 4.75, 0.00, 0.00, -4.75, -4.75
AF1′	-37199.847413	0.144351	0.00, 0.00, 4.75, 4.75, 0.00, 0.00, -4.75, -4.75
AF2′	-37199.793778	0.197986	0.00, 0.00, -4.72, 4.72, 0.00, 0.00, -4.72, 4.72
AF2′	-37199.793778	0.197986	0.00, 0.00, -4.72, 4.72, 0.00, 0.00, -4.72, 4.72
AF2′	-37199.793773	0.197991	0.00, 0.00, -4.72, 4.72, 0.00, 0.00, -4.72, 4.72

Table 148: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

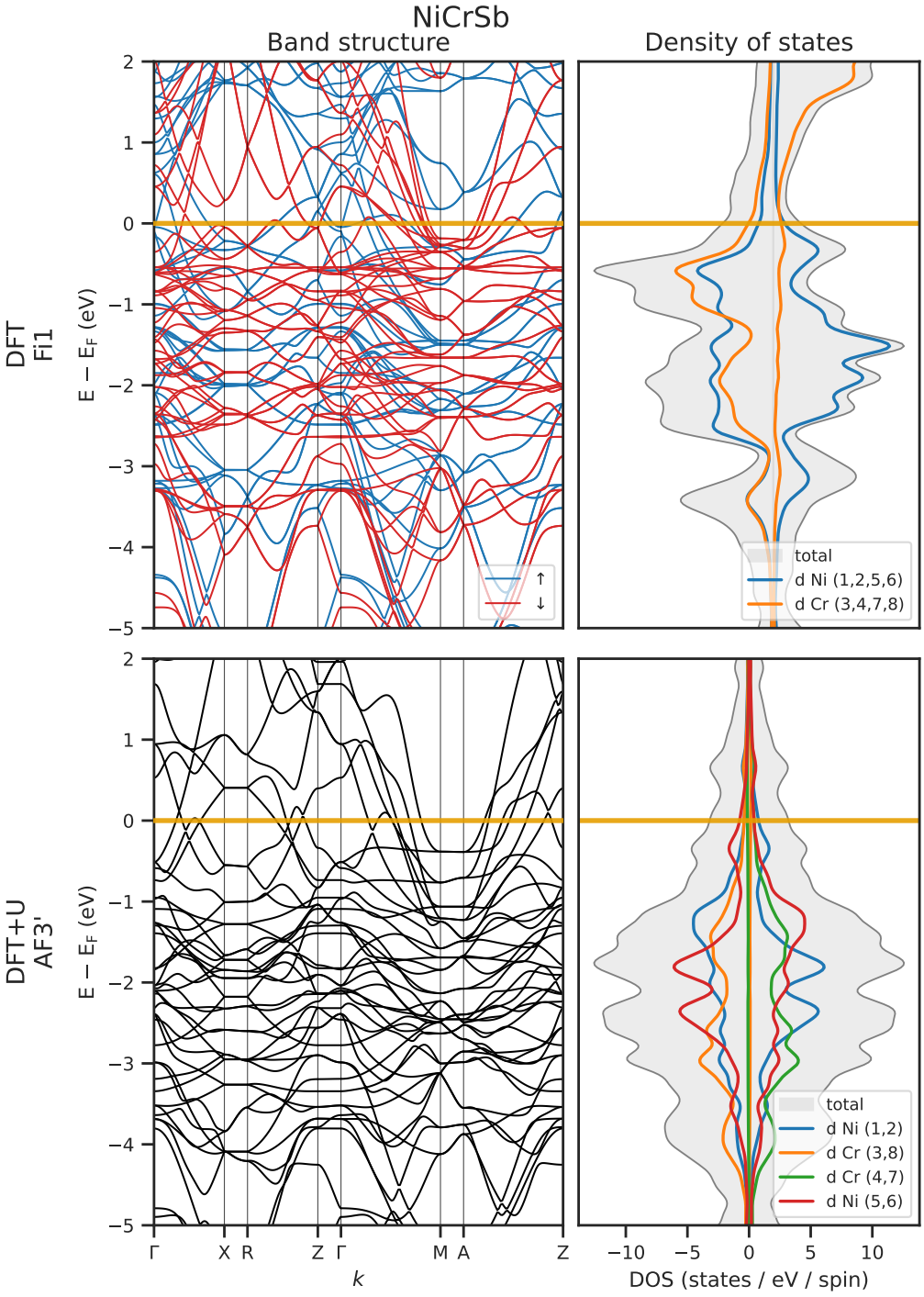


Figure 144: Band structure and Density of states of the lowest in energy calculations.

Material: Cu_2As

Configuration: Cu_2As

Structure

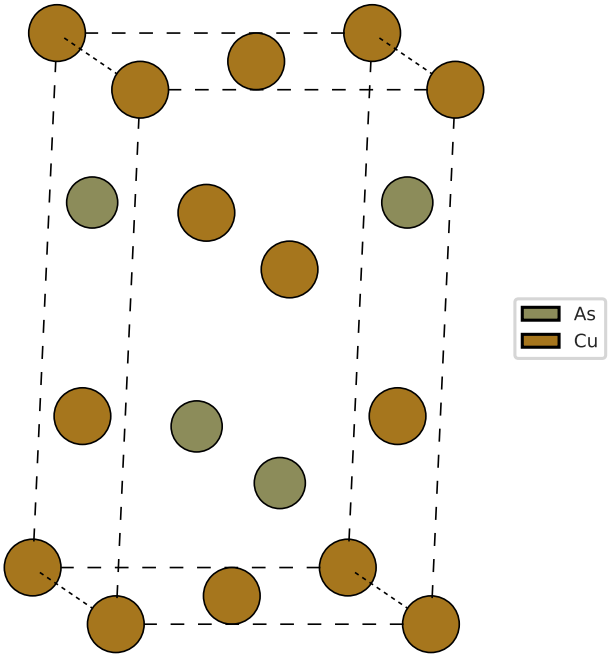


Figure 145: Structure of Cu_2As

a (Å)	c (Å)	z_1	z_2
3.8264	6.0177	0.2998	0.2884

Table 149: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-54584.603510	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 150: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

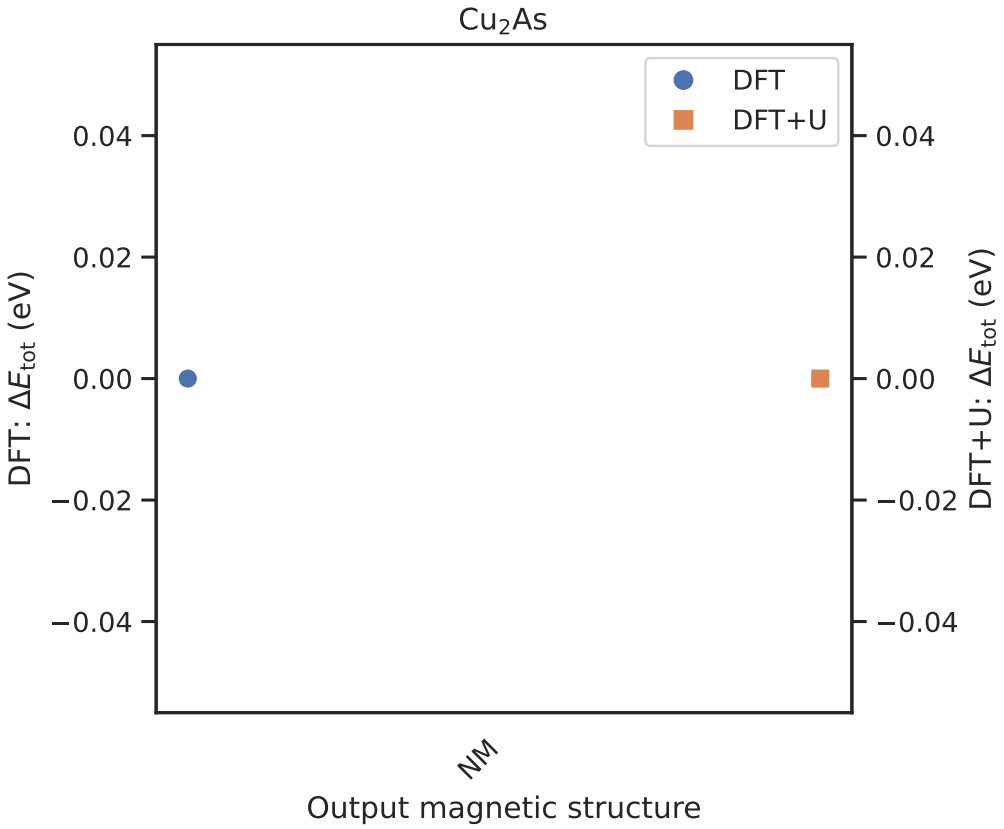


Figure 146: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-54584.603459	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 151: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

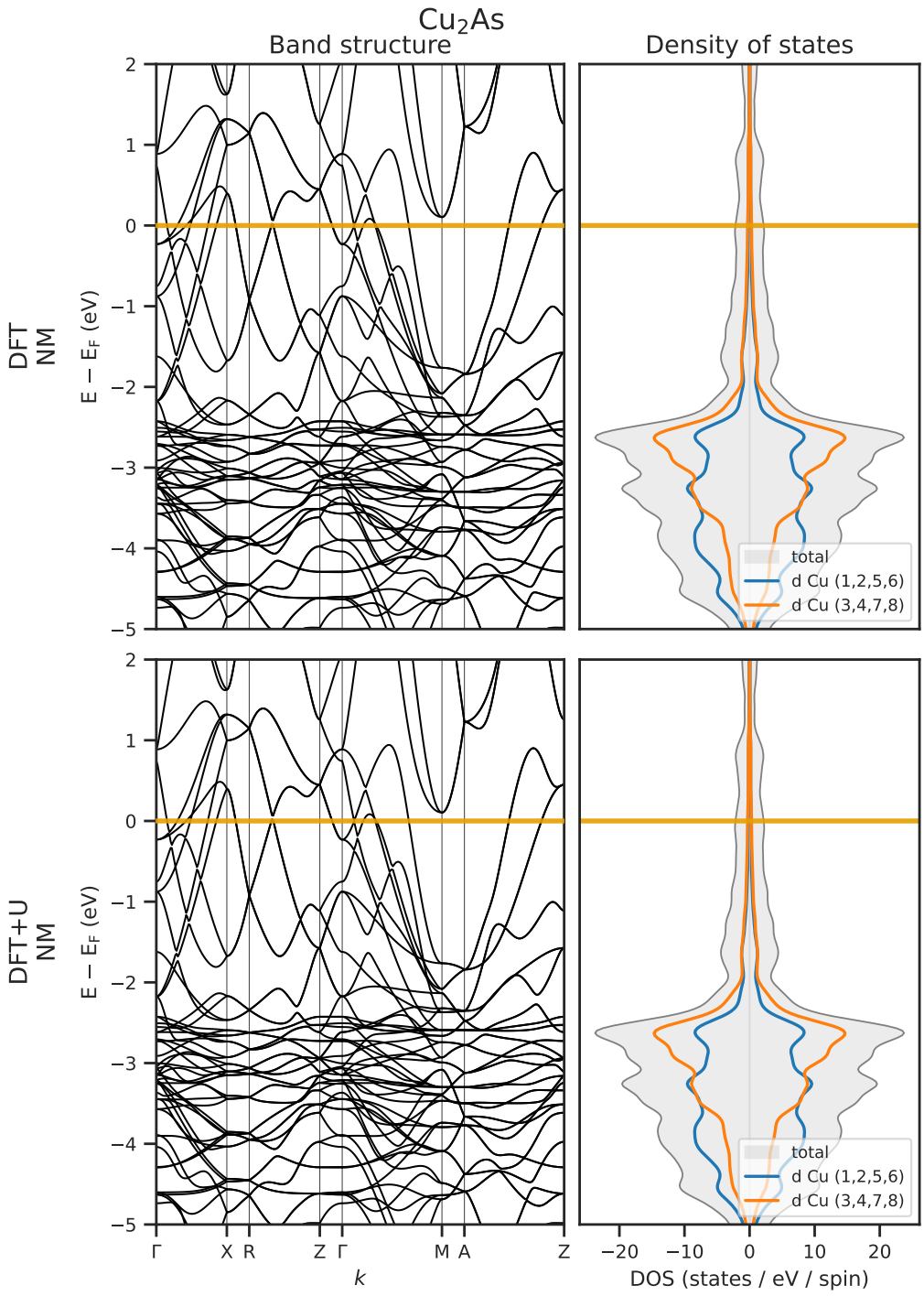


Figure 147: Band structure and Density of states of the lowest in energy calculations.

Material: FeCuAs

Configuration: FeCuAs ■ lower-energy

Structure

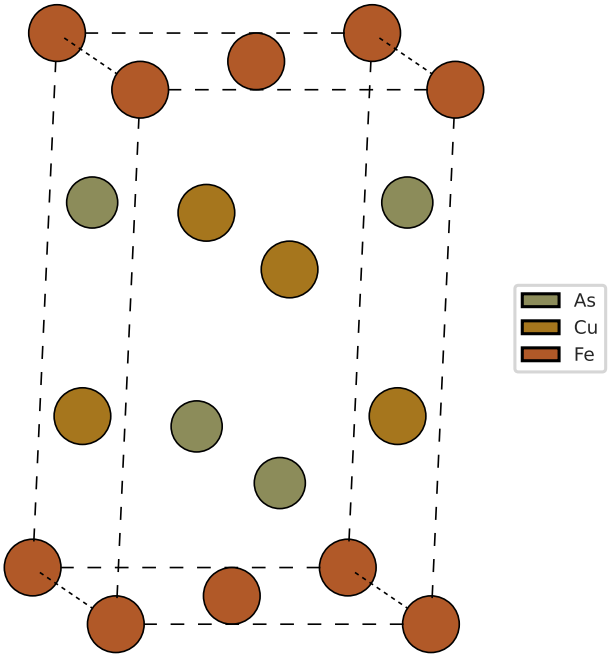


Figure 148: Structure of FeCuAs

a (Å)	c (Å)	z_1	z_2
3.7822	5.8142	0.3258	0.2550

Table 152: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-46619.768735	0.000000	1.35, -1.35, 0.00, 0.00, 1.35, -1.35, 0.00, 0.00
AF1″	-46619.766898	0.001837	0.60, 0.60, -0.01, 0.01, -0.60, -0.60, 0.01, -0.01
AF8″	-46619.749050	0.019685	1.25, -1.25, 0.00, 0.00, -1.25, 1.25, 0.00, 0.00
F1″	-46619.742197	0.026537	0.49, 0.49, -0.03, -0.03, 0.49, 0.49, -0.03, -0.03

Table 153: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

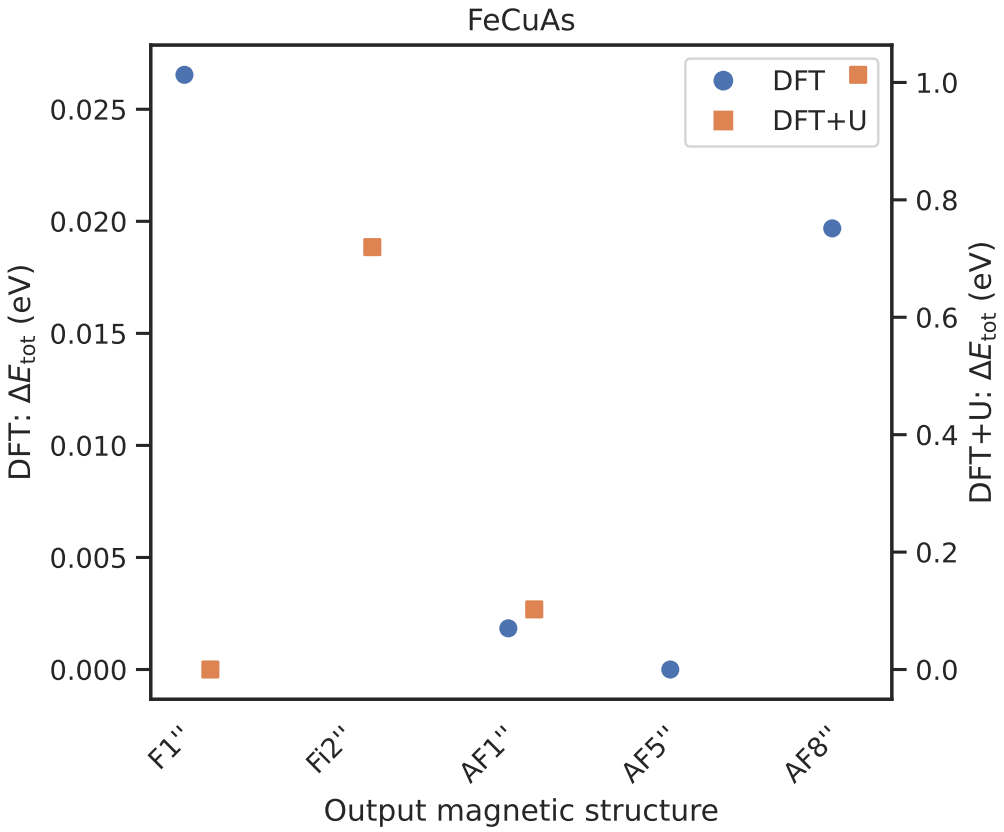


Figure 149: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-46610.862751	0.000000	2.79, 2.79, -0.08, -0.08, 2.79, 2.79, -0.08, -0.08
AF1″	-46610.760353	0.102398	2.81, 2.81, -0.08, 0.08, -2.81, -2.81, 0.08, -0.08
Fi2″	-46610.143270	0.719481	2.86, -3.04, -0.01, -0.00, 2.86, -2.90, -0.02, -0.03
AF8″	-46609.849763	1.012988	2.87, -2.87, -0.00, -0.00, -2.87, 2.87, 0.00, 0.00

Table 154: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

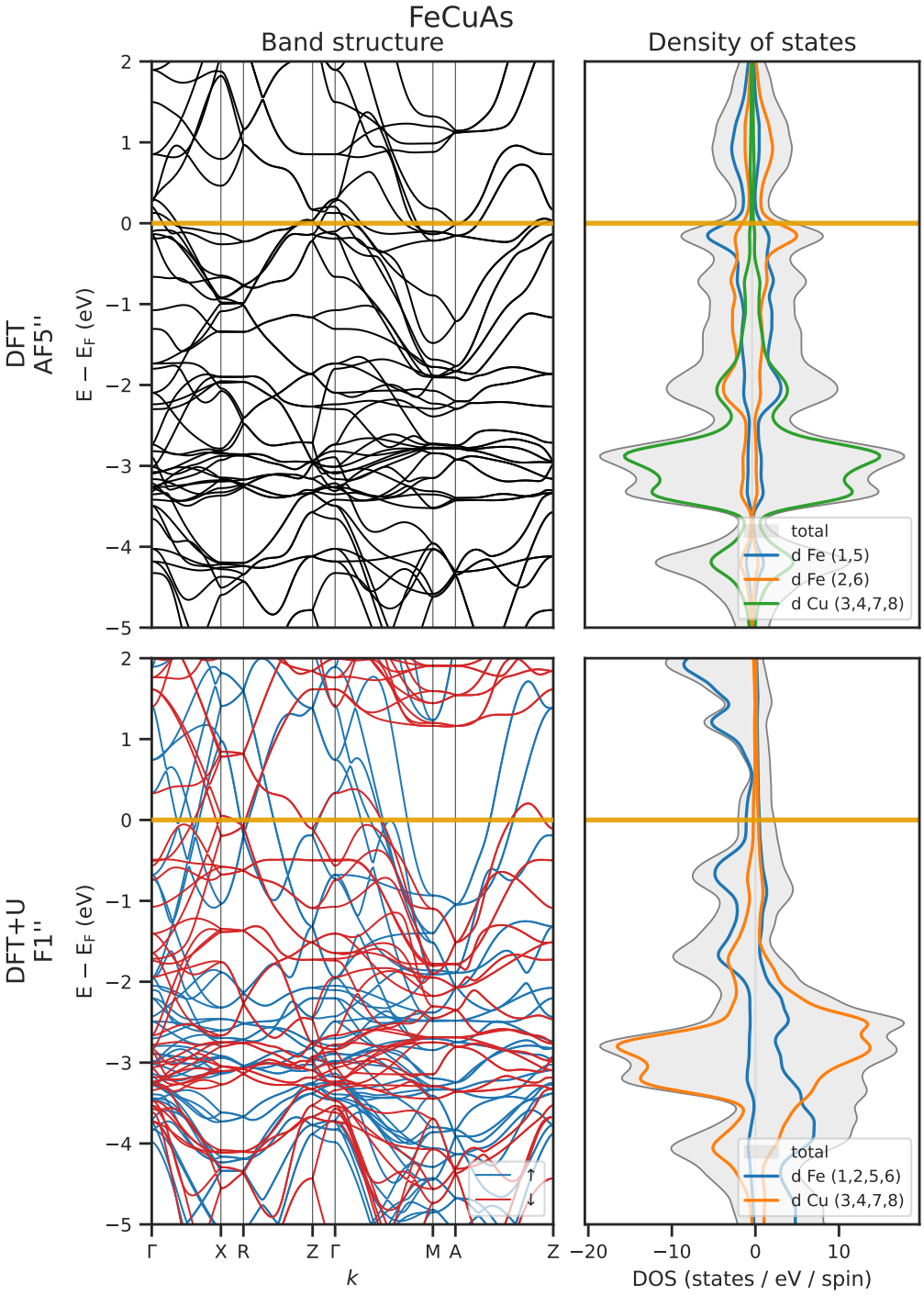


Figure 150: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuFeAs ■ higher-energy

Structure

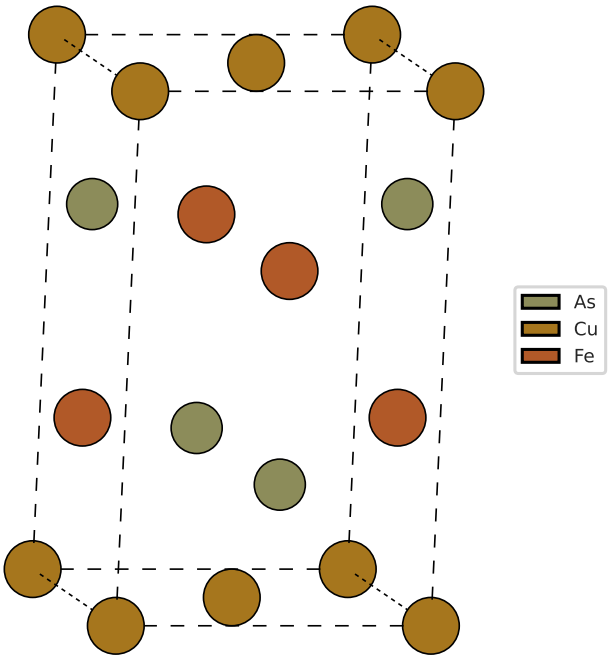


Figure 151: Structure of CuFeAs

a (Å)	c (Å)	z_1	z_2
3.5648	6.4537	0.3526	0.2826

Table 155: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-46618.159022	0.000000	0.06, 0.06, -2.35, 2.35, -0.06, -0.06, 2.35, -2.35
AF1′	-46618.067518	0.091504	0.00, 0.00, 2.51, 2.51, 0.00, 0.00, -2.51, -2.51
AF2′	-46618.047753	0.111269	0.00, 0.00, -2.29, 2.29, 0.00, 0.00, -2.29, 2.29
F1′	-46617.946087	0.212936	-0.03, -0.03, 2.46, 2.46, -0.03, -0.03, 2.46, 2.46

Table 156: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

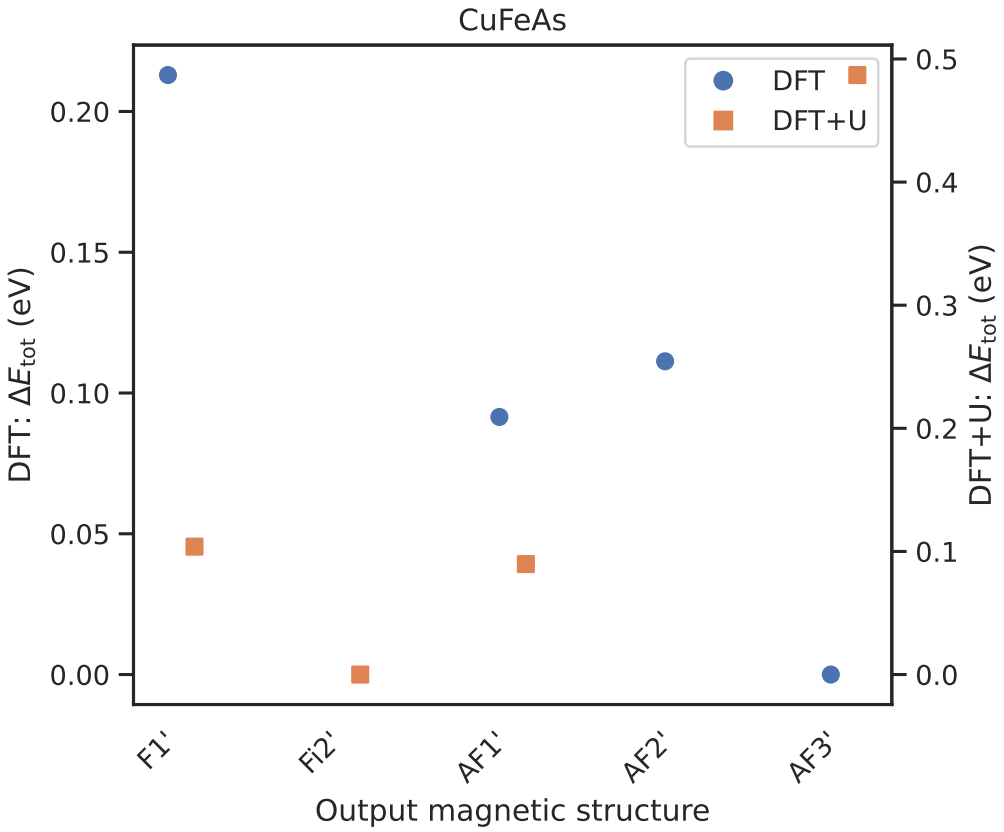


Figure 152: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi2′	-46610.507346	0.000000	-0.01, -0.00, -2.94, 3.21, 0.01, 0.01, -3.05, 3.16
AF1′	-46610.417627	0.089718	0.00, 0.00, 3.22, 3.22, 0.00, 0.00, -3.22, -3.22
F1′	-46610.403446	0.103899	-0.04, -0.04, 3.23, 3.23, -0.04, -0.04, 3.23, 3.23
AF3′	-46610.020410	0.486936	0.03, 0.03, -3.08, 3.08, -0.03, -0.03, 3.08, -3.08

Table 157: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

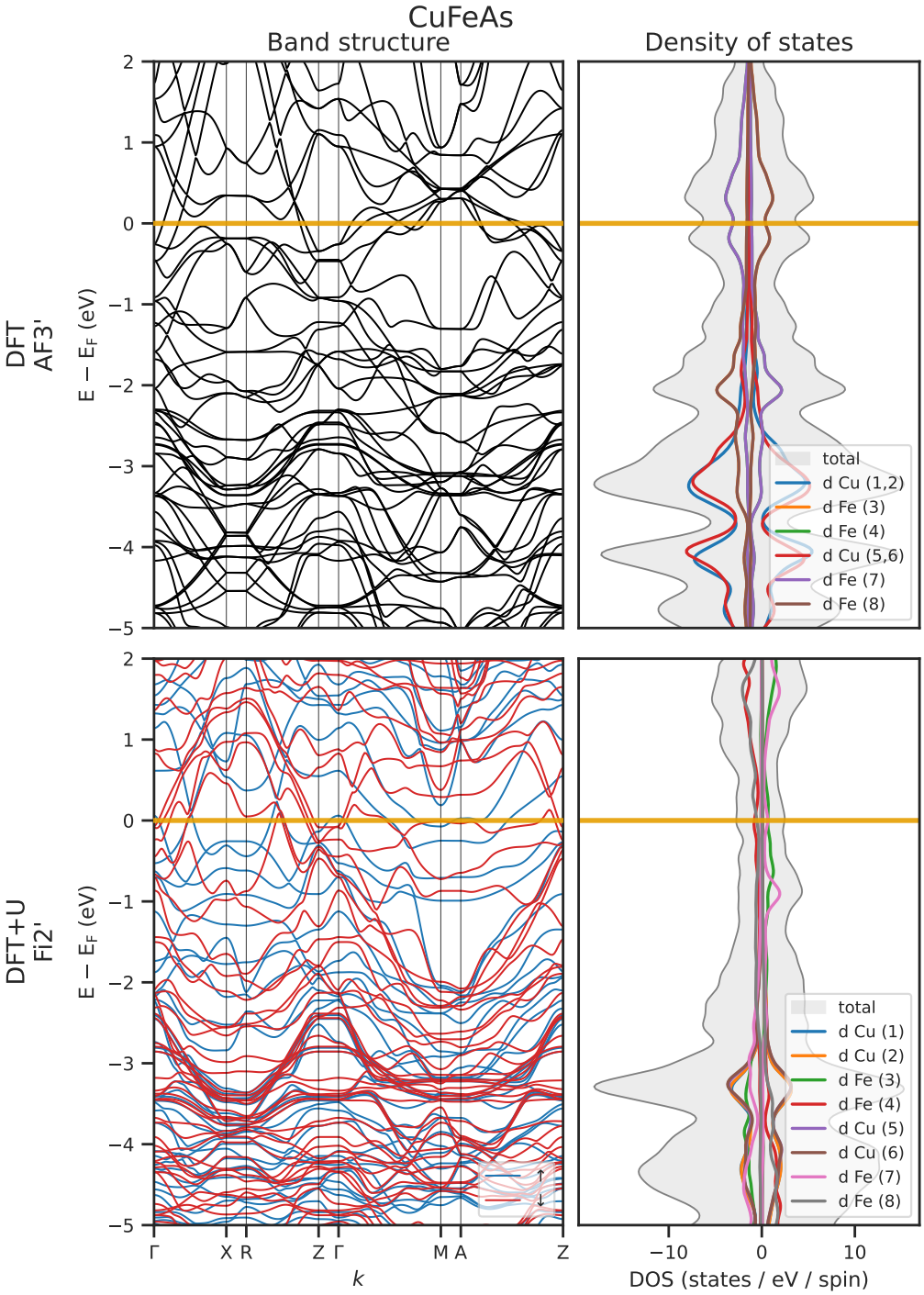


Figure 153: Band structure and Density of states of the lowest in energy calculations.

Material: FeCuSb

Configuration: FeCuSb ■ lower-energy

Structure

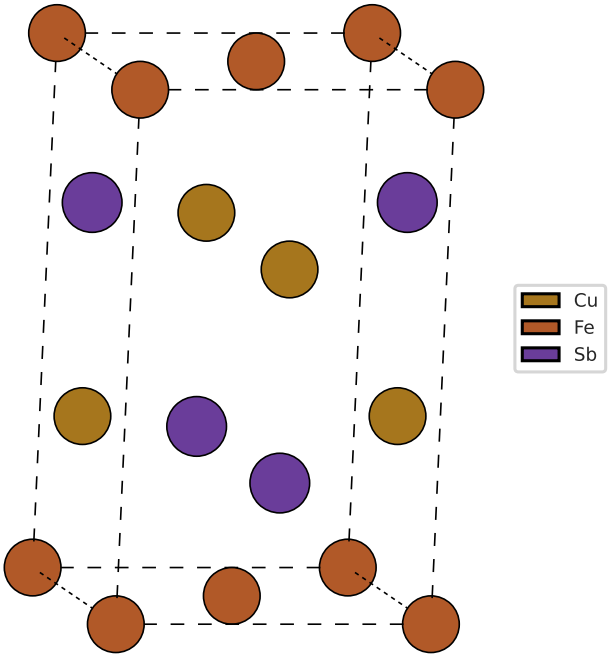


Figure 154: Structure of FeCuSb

a (Å)	c (Å)	z_1	z_2
3.9972	6.2688	0.2751	0.2866

Table 158: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-44506.203791	0.000000	2.56, 2.56, -0.04, -0.04, 2.56, 2.56, -0.04, -0.04
AF1″	-44506.072734	0.131057	2.60, 2.60, -0.03, 0.03, -2.60, -2.60, 0.03, -0.03
AF5″	-44505.704154	0.499637	2.48, -2.48, 0.00, 0.00, 2.48, -2.48, 0.00, 0.00
AF8″	-44505.578902	0.624889	2.45, -2.45, 0.00, 0.00, -2.44, 2.44, 0.00, 0.00

Table 159: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

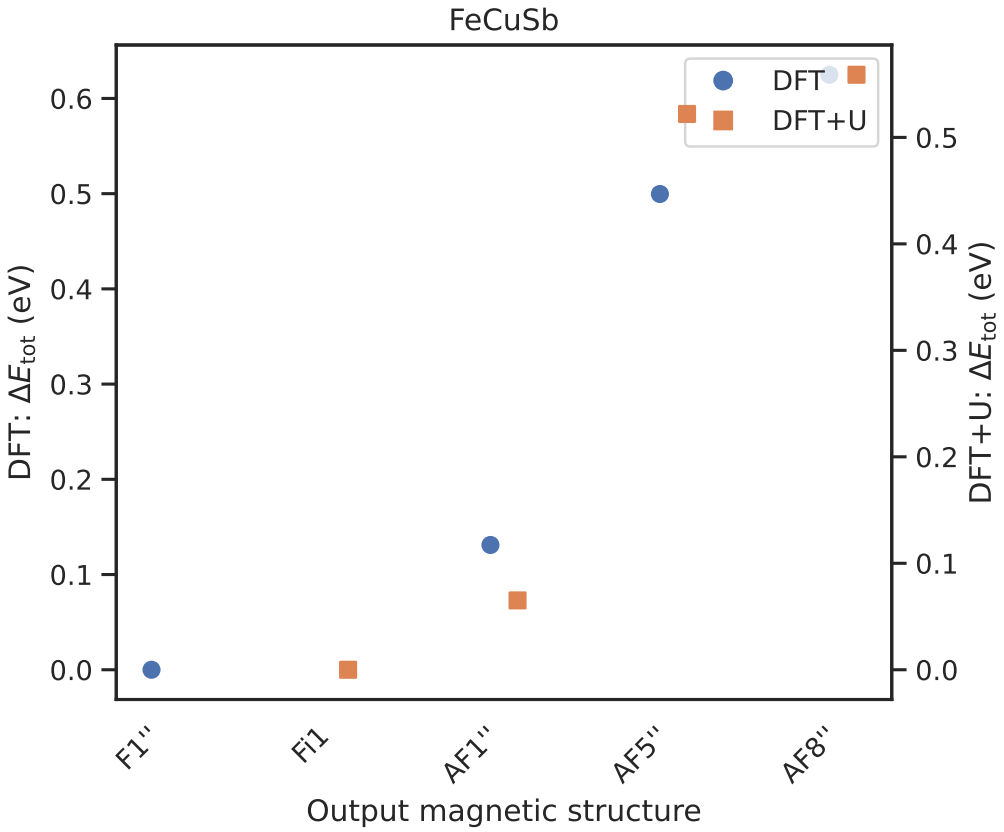


Figure 155: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-44498.654488	0.000000	3.04, 3.04, -0.11, -0.11, 3.04, 3.04, -0.11, -0.11
AF1″	-44498.589351	0.065137	3.07, 3.07, -0.09, 0.09, -3.07, -3.07, 0.09, -0.09
AF5″	-44498.132479	0.522008	3.19, -3.19, 0.00, 0.00, 3.19, -3.19, 0.00, 0.00
AF8″	-44498.095631	0.558857	3.19, -3.19, 0.00, 0.00, -3.19, 3.19, 0.00, 0.00

Table 160: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

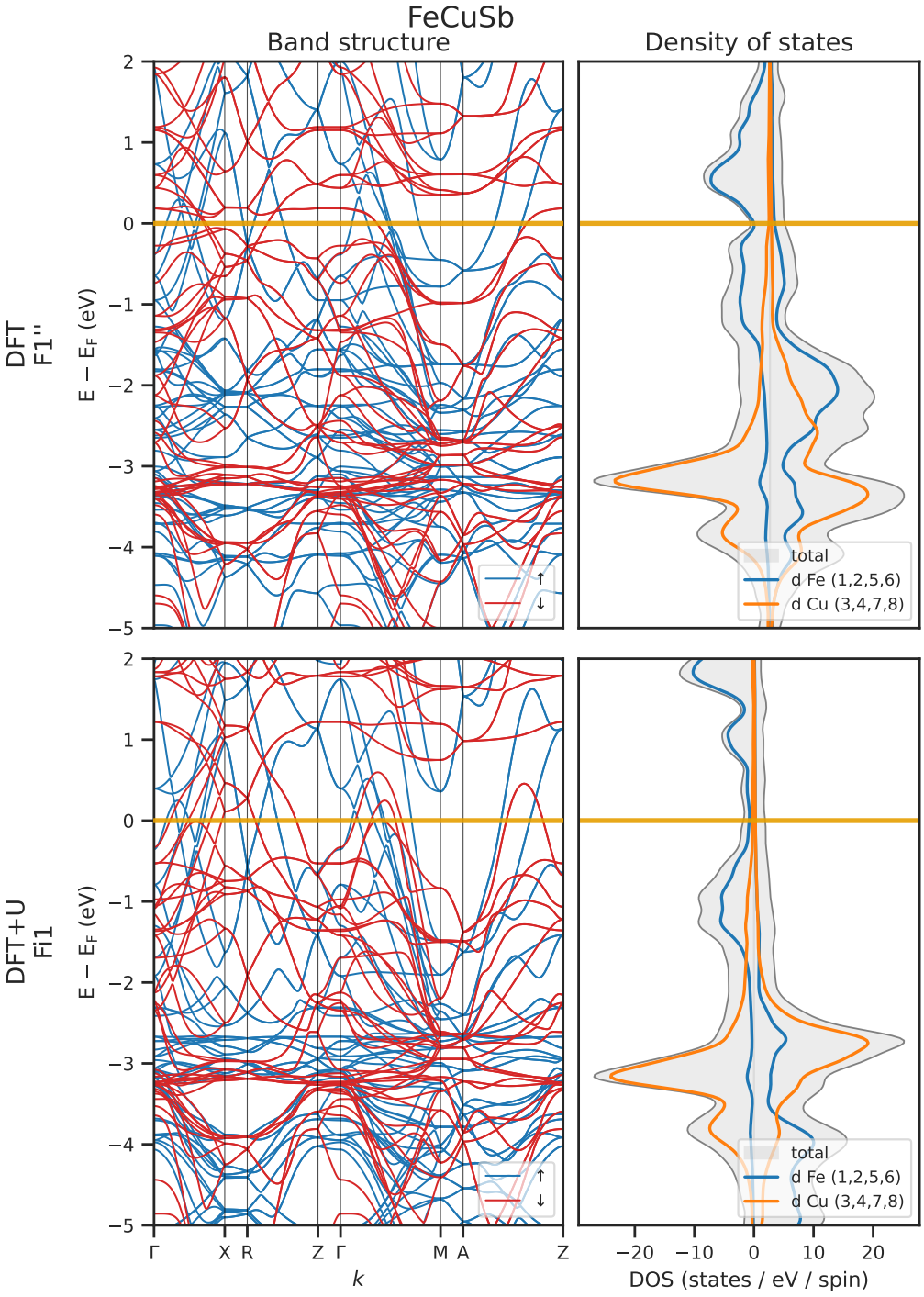


Figure 156: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuFeSb ■ higher-energy

Structure

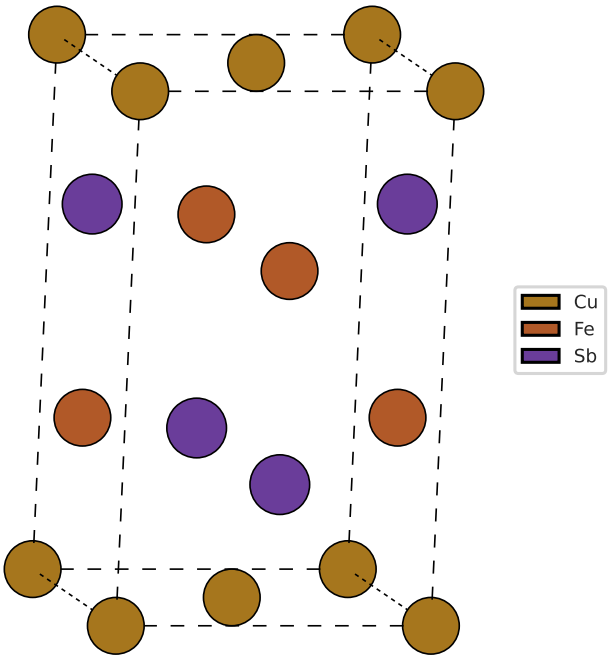


Figure 157: Structure of CuFeSb

a (Å)	c (Å)	z_1	z_2
3.9261	6.4845	0.2571	0.3158

Table 161: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-44503.977561	0.000000	0.00, 0.00, -2.78, 2.78, 0.00, 0.00, -2.78, 2.78
AF3′	-44503.966812	0.010749	0.03, 0.03, -2.74, 2.74, -0.03, -0.03, 2.74, -2.74
AF1′	-44503.754123	0.223438	0.00, 0.00, 2.76, 2.76, 0.00, 0.00, -2.76, -2.76
F1′	-44503.592733	0.384828	-0.00, -0.00, 2.74, 2.74, -0.00, -0.00, 2.74, 2.74

Table 162: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

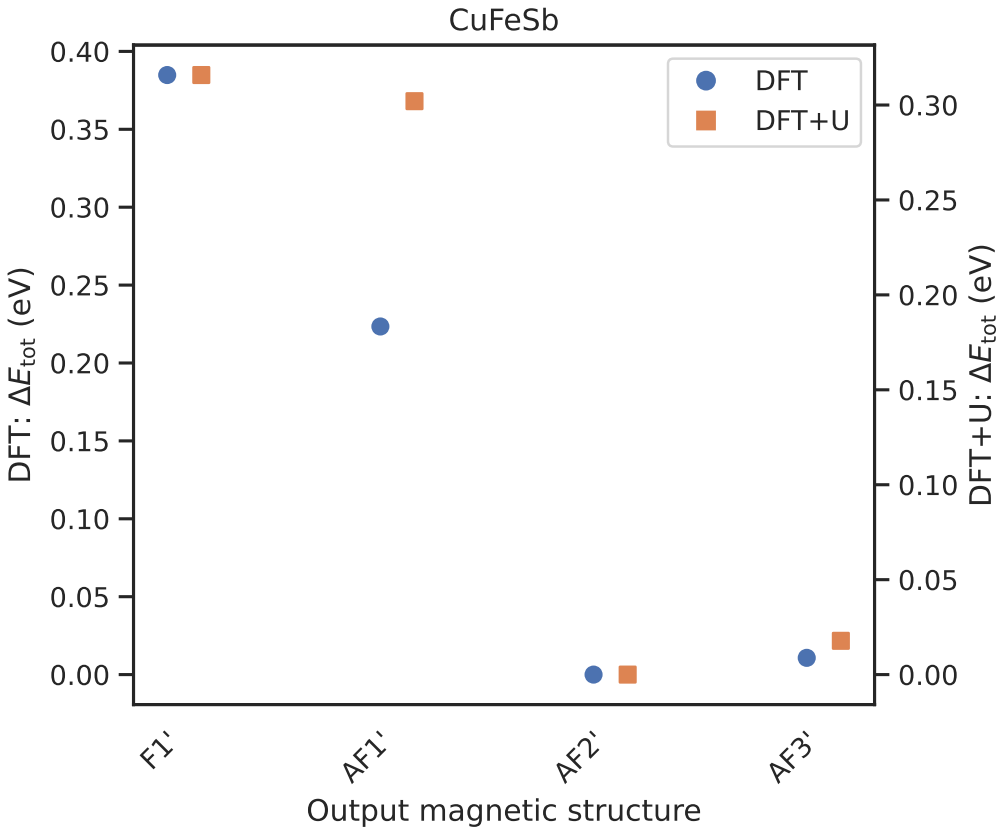


Figure 158: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-44497.600696	0.000000	0.00, 0.00, -3.12, 3.12, 0.00, 0.00, -3.12, 3.12
AF3′	-44497.582902	0.017794	0.05, 0.05, -3.08, 3.08, -0.05, -0.05, 3.08, -3.08
AF1′	-44497.298671	0.302025	0.00, 0.00, 3.07, 3.07, 0.00, 0.00, -3.07, -3.07
F1′	-44497.284904	0.315792	-0.04, -0.04, 3.02, 3.02, -0.04, -0.04, 3.02, 3.02

Table 163: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

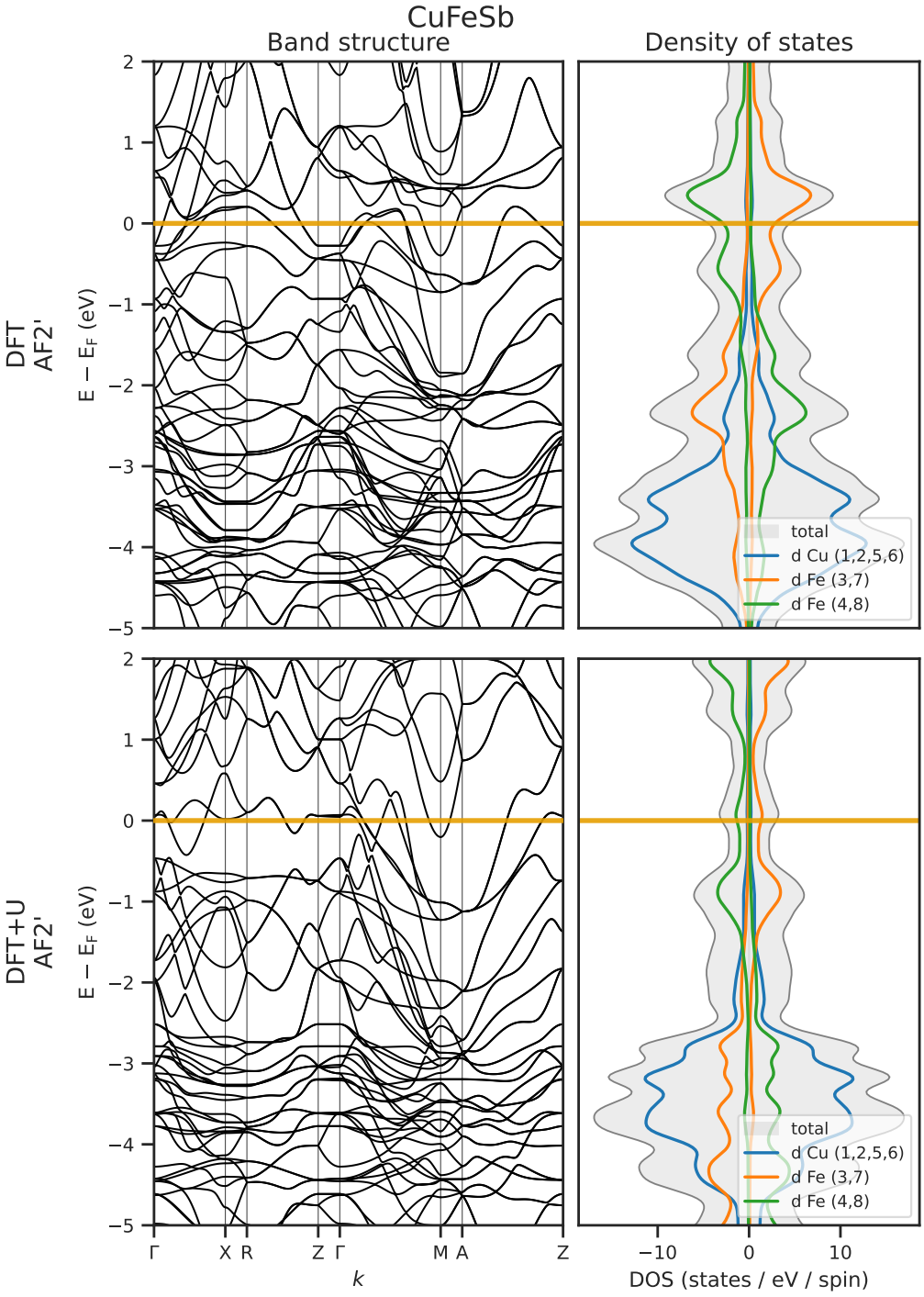


Figure 159: Band structure and Density of states of the lowest in energy calculations.

Material: CuGaAs

Configuration: CuGaAs ■ lower-energy

Structure

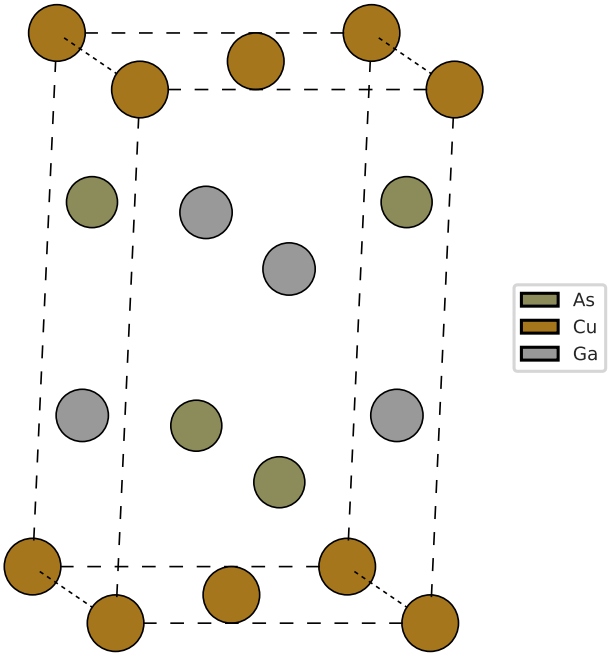


Figure 160: Structure of CuGaAs

a (Å)	c (Å)	z_1	z_2
3.9457	6.7981	0.3276	0.2537

Table 164: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-41426.648890	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 165: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

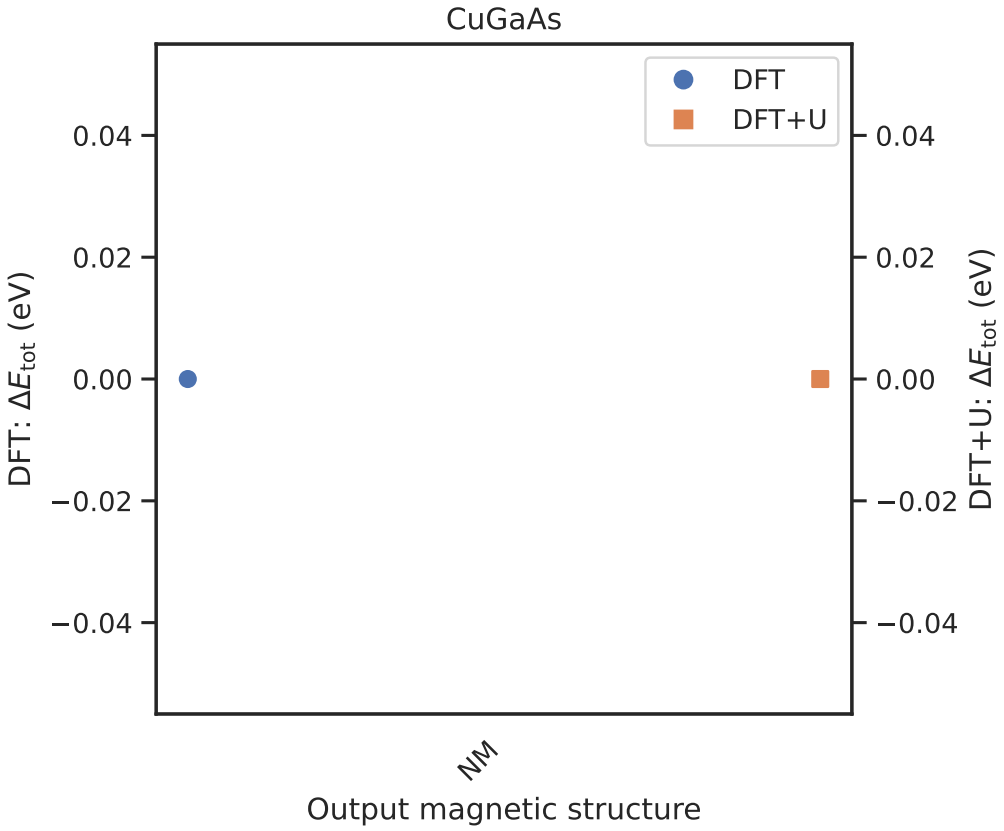


Figure 161: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-41426.648887	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 166: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

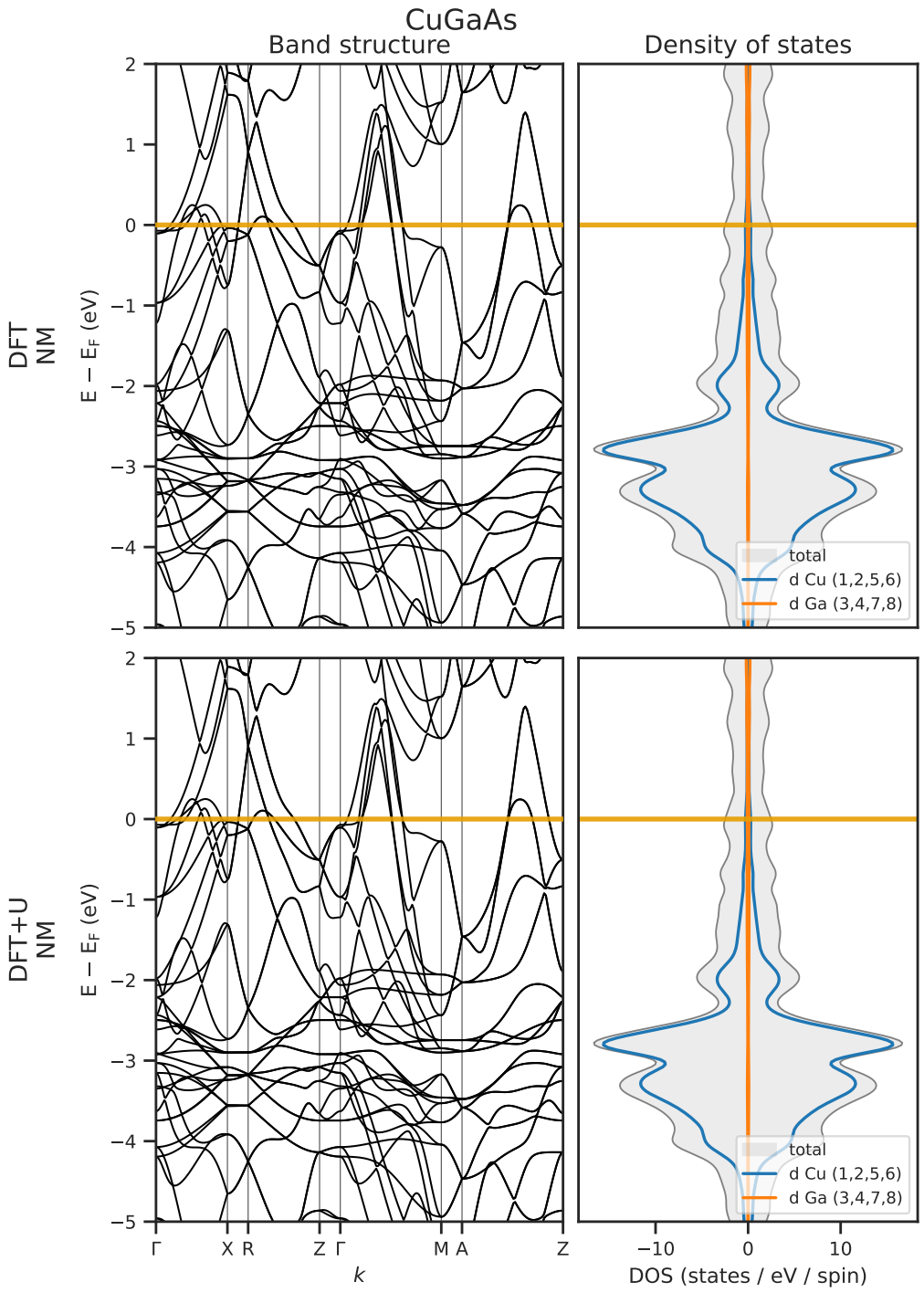


Figure 162: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaCuAs ■ higher-energy

Structure

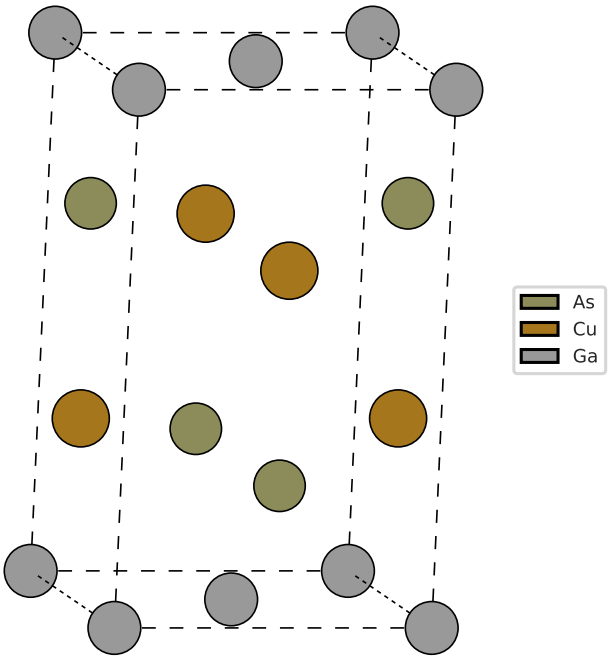


Figure 163: Structure of GaCuAs

a (Å)	c (Å)	z_1	z_2
3.8300	6.8895	0.2639	0.3790

Table 167: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-41425.442512	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 168: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

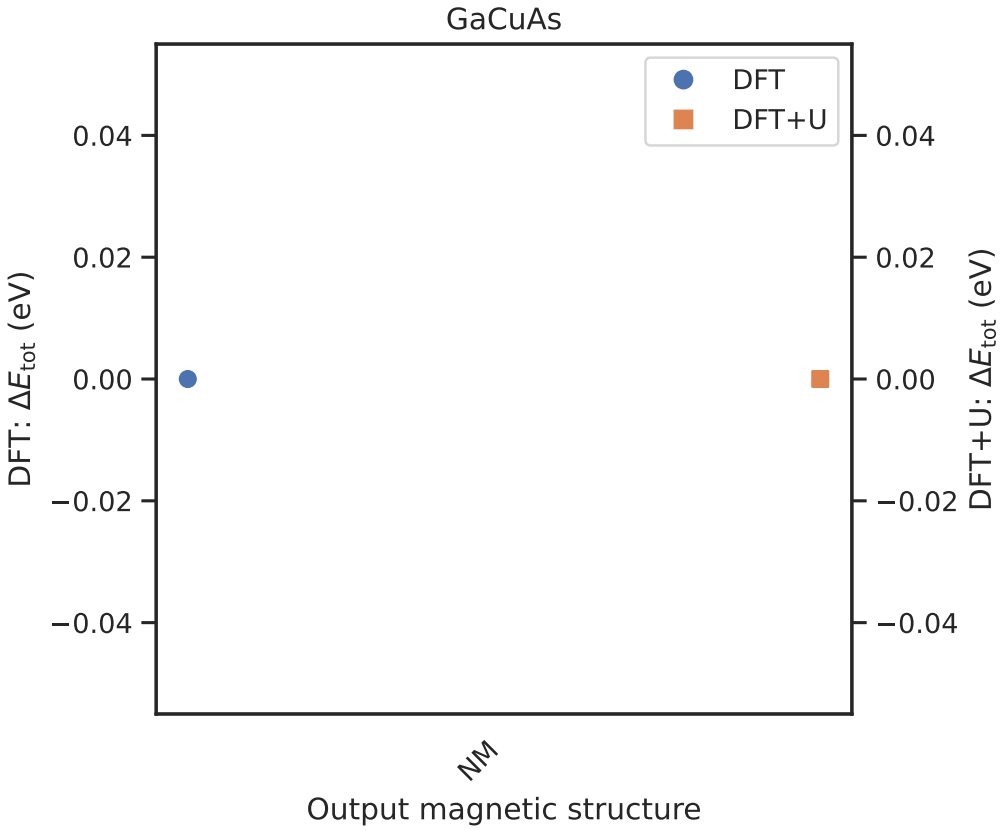


Figure 164: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-41425.442505	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 169: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

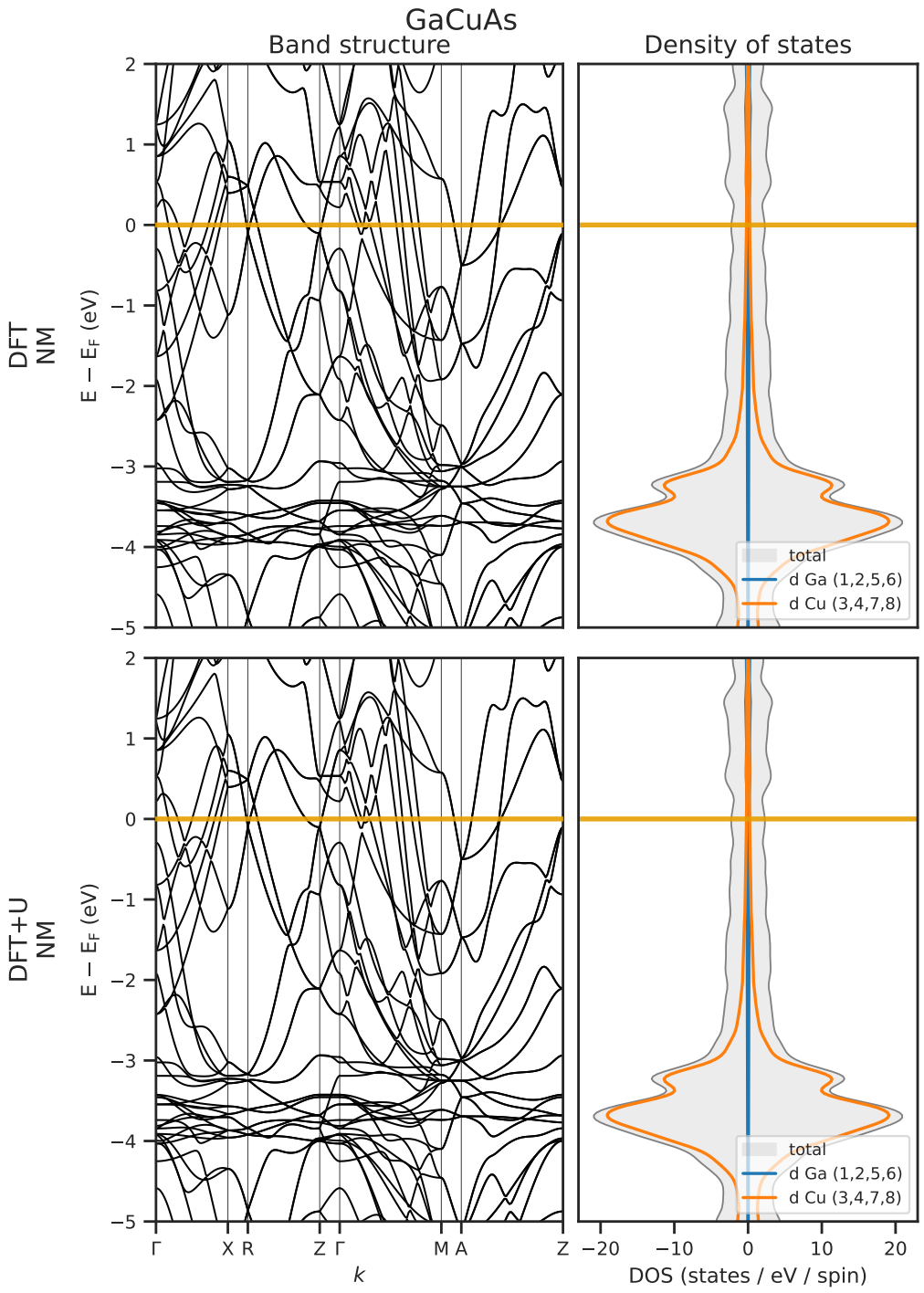


Figure 165: Band structure and Density of states of the lowest in energy calculations.

Material: GaCuSb

Configuration: GaCuSb ■ lower-energy

Structure

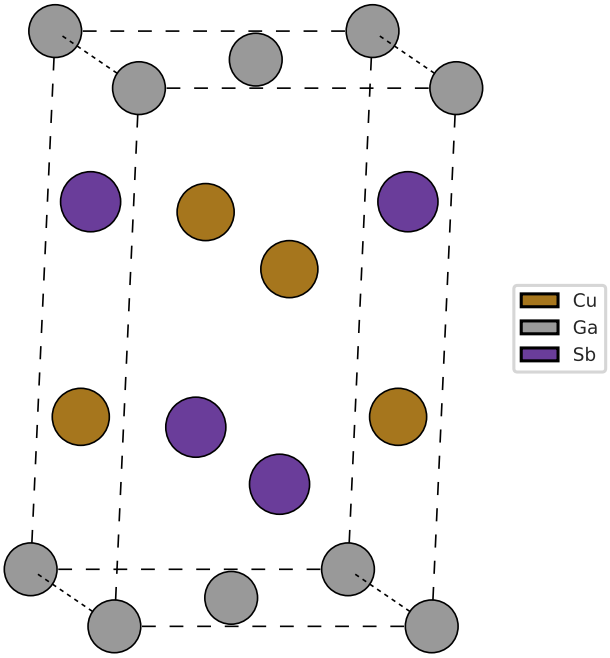


Figure 166: Structure of GaCuSb

a (Å)	c (Å)	z_1	z_2
4.0166	7.2177	0.2422	0.3760

Table 170: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-39313.287925	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 171: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

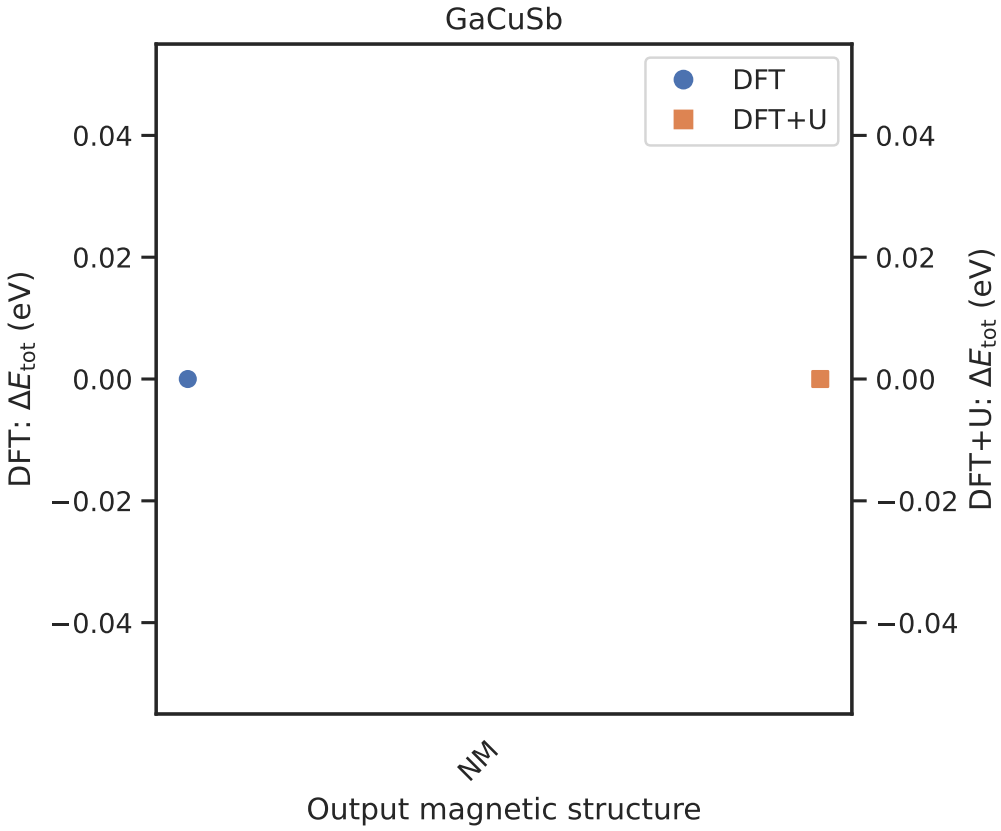


Figure 167: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-39313.287859	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 172: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

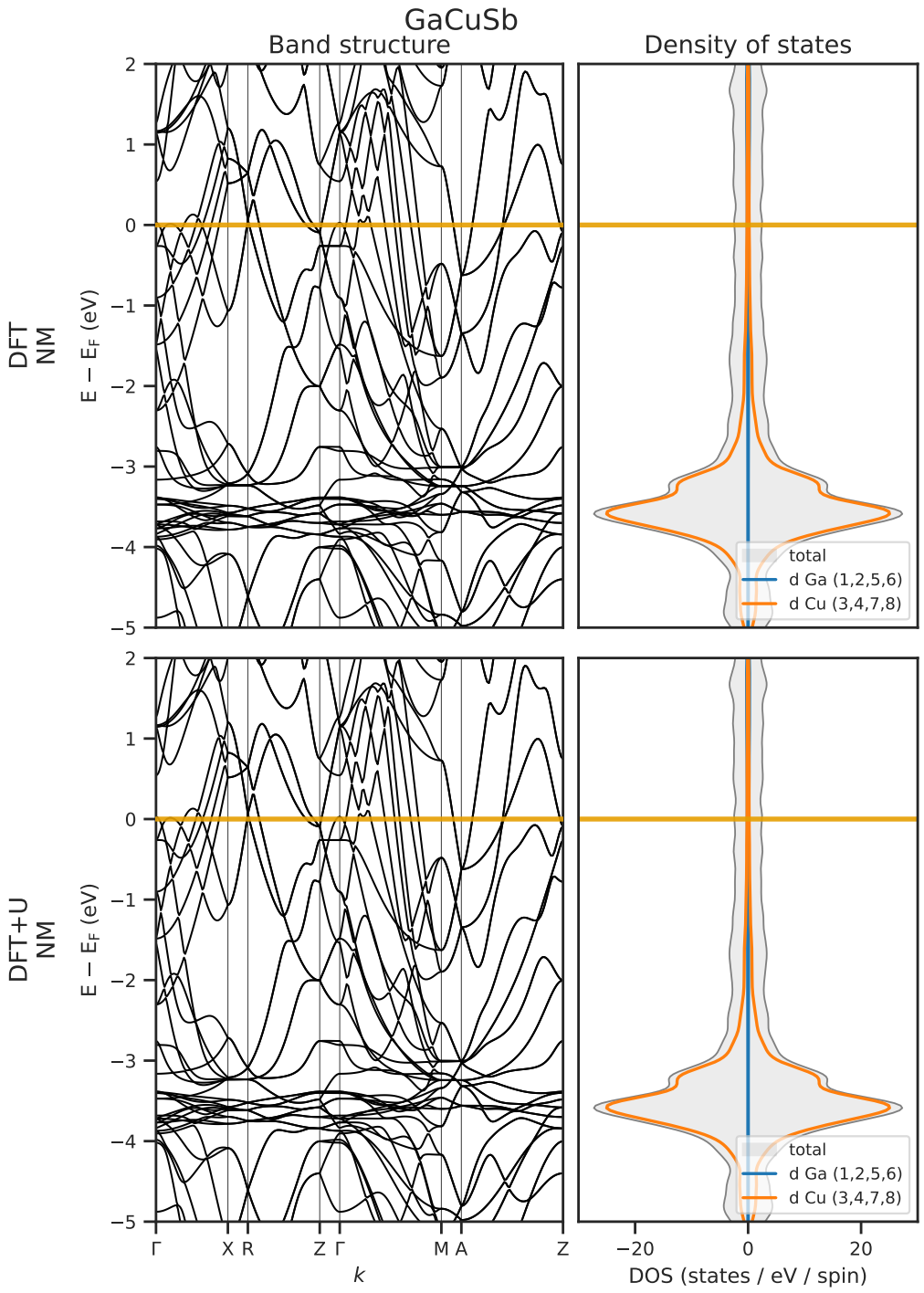


Figure 168: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuGaSb ■ higher-energy

Structure

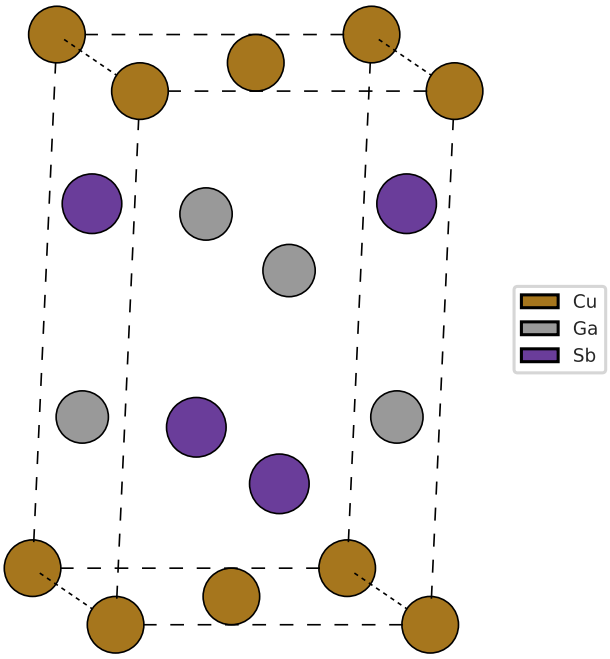


Figure 169: Structure of CuGaSb

a (Å)	c (Å)	z_1	z_2
4.3024	6.7588	0.2721	0.2689

Table 173: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-39313.074714	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 174: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

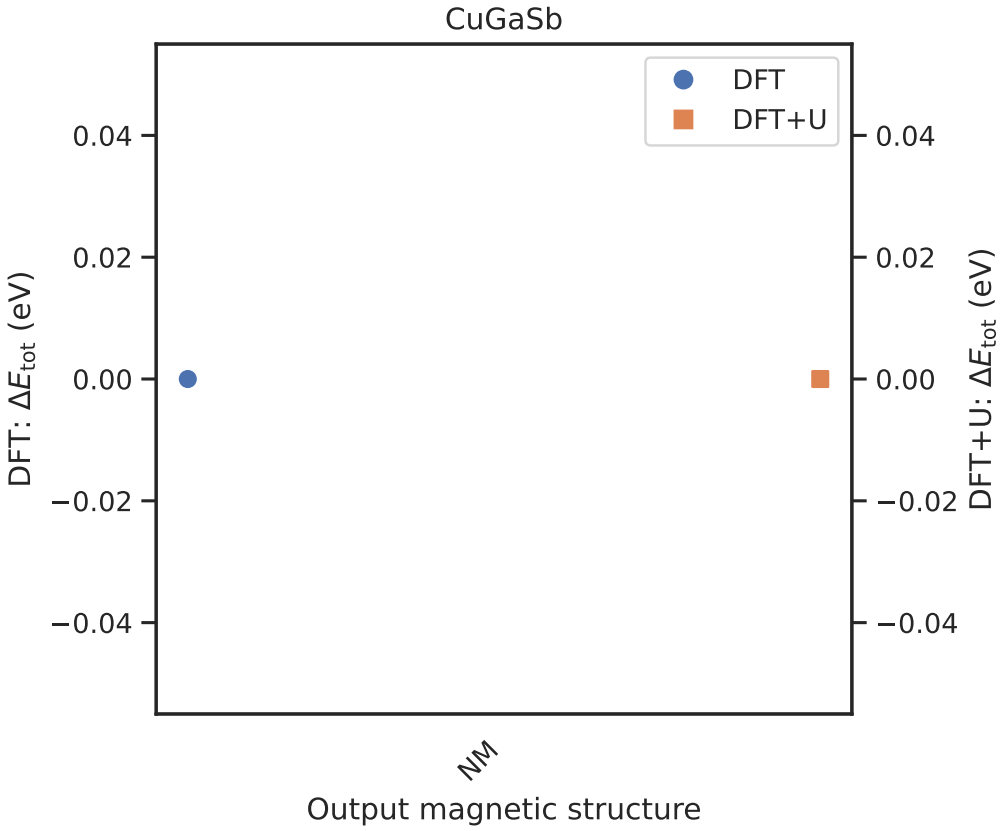


Figure 170: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-39313.074714	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 175: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

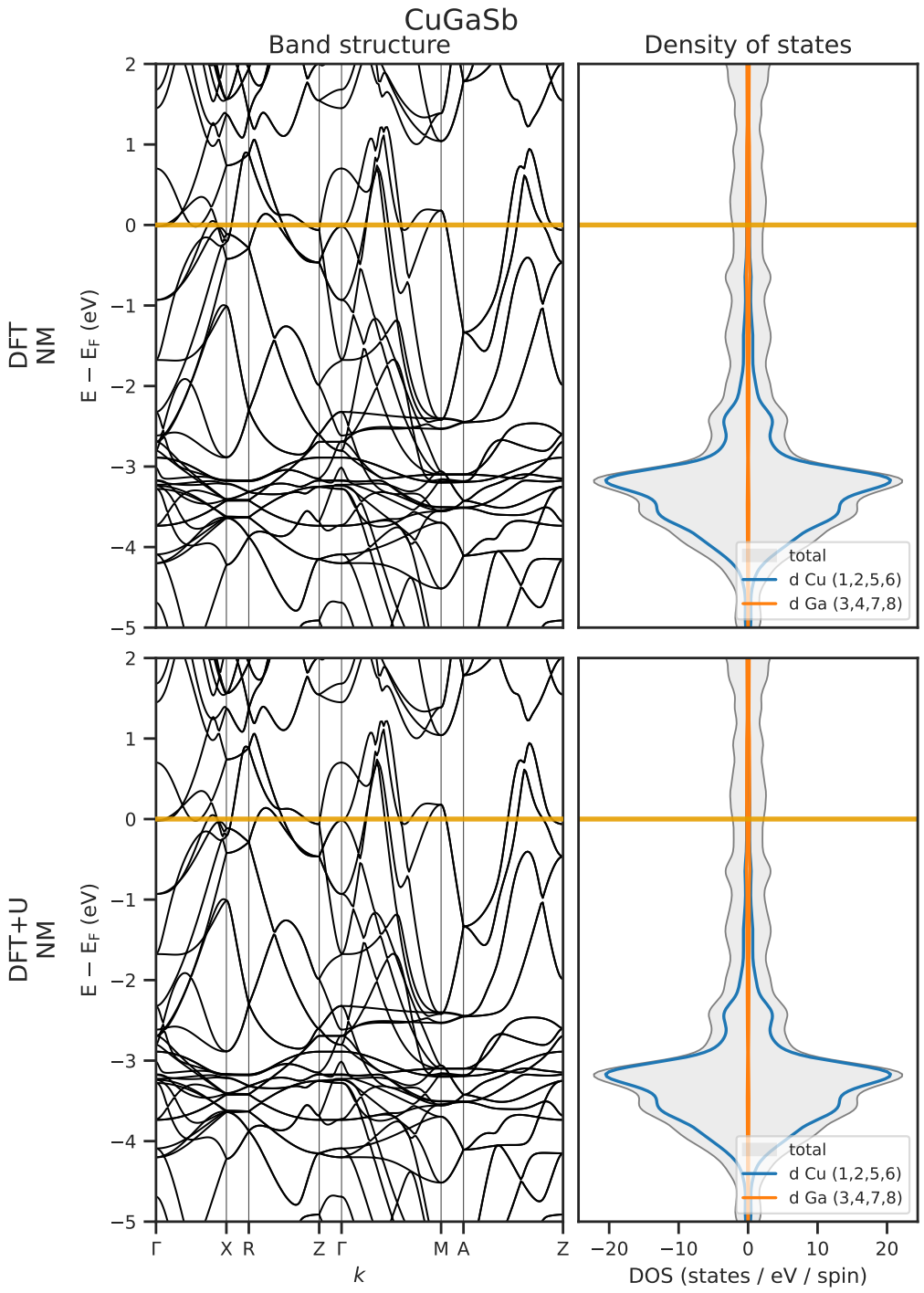


Figure 171: Band structure and Density of states of the lowest in energy calculations.

Material: CuMnAs

Configuration: CuMnAs ■ lower-energy

Structure

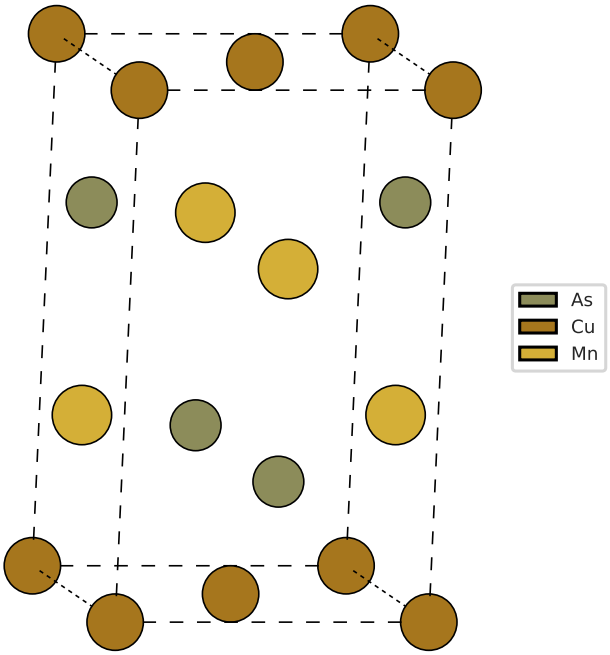


Figure 172: Structure of CuMnAs

a (Å)	c (Å)	z_1	z_2
3.7126	6.4662	0.3497	0.2712

Table 176: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-44491.684658	0.000000	0.00, 0.00, -3.95, 3.95, 0.00, 0.00, -3.95, 3.95
AF3′	-44491.565870	0.118788	0.04, 0.04, -3.98, 3.98, -0.04, -0.04, 3.98, -3.98
F1′	-44490.889306	0.795352	-0.03, -0.03, 3.95, 3.95, -0.03, -0.03, 3.95, 3.95
Fi2′	-44490.257873	1.426785	0.03, 0.03, -0.21, -3.77, 0.01, 0.01, 3.97, -3.92

Table 177: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

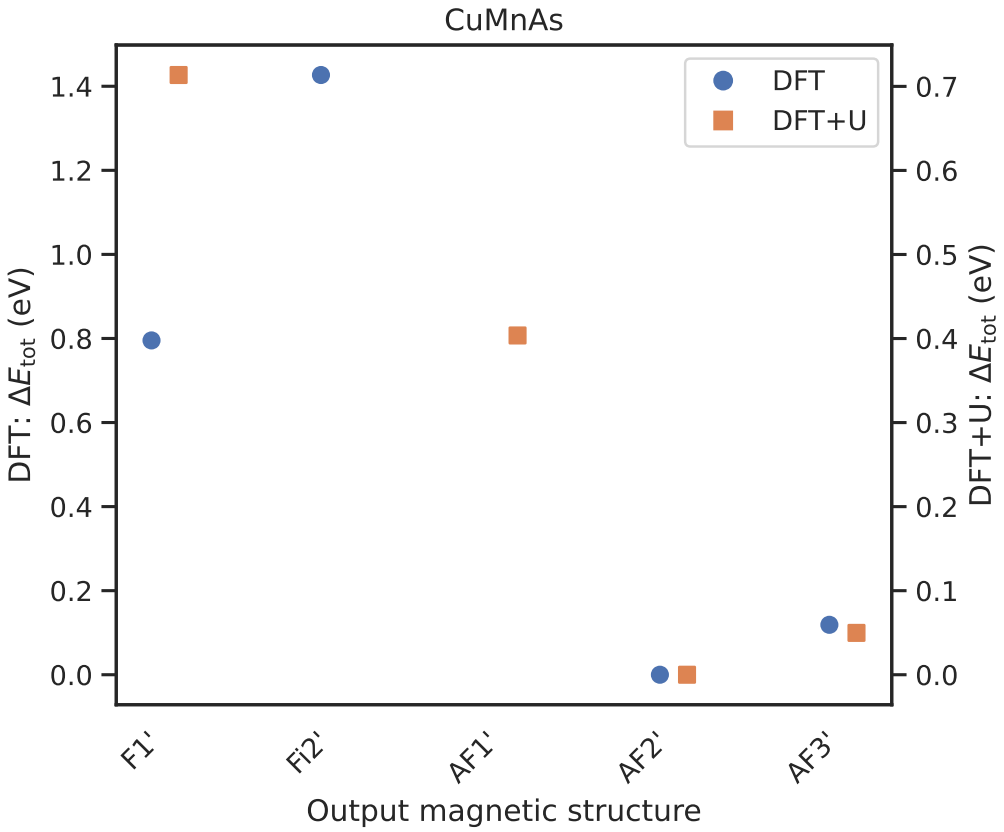


Figure 173: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF2′	-44486.500244	0.000000	0.00, 0.00, -4.71, 4.71, 0.00, 0.00, -4.71, 4.71
AF3′	-44486.450457	0.049787	0.06, 0.06, -4.69, 4.69, -0.06, -0.06, 4.69, -4.69
AF1′	-44486.096596	0.403647	0.00, 0.00, 4.66, 4.66, 0.00, 0.00, -4.66, -4.66
F1′	-44485.786714	0.713529	-0.01, -0.01, 4.69, 4.69, -0.01, -0.01, 4.69, 4.69

Table 178: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

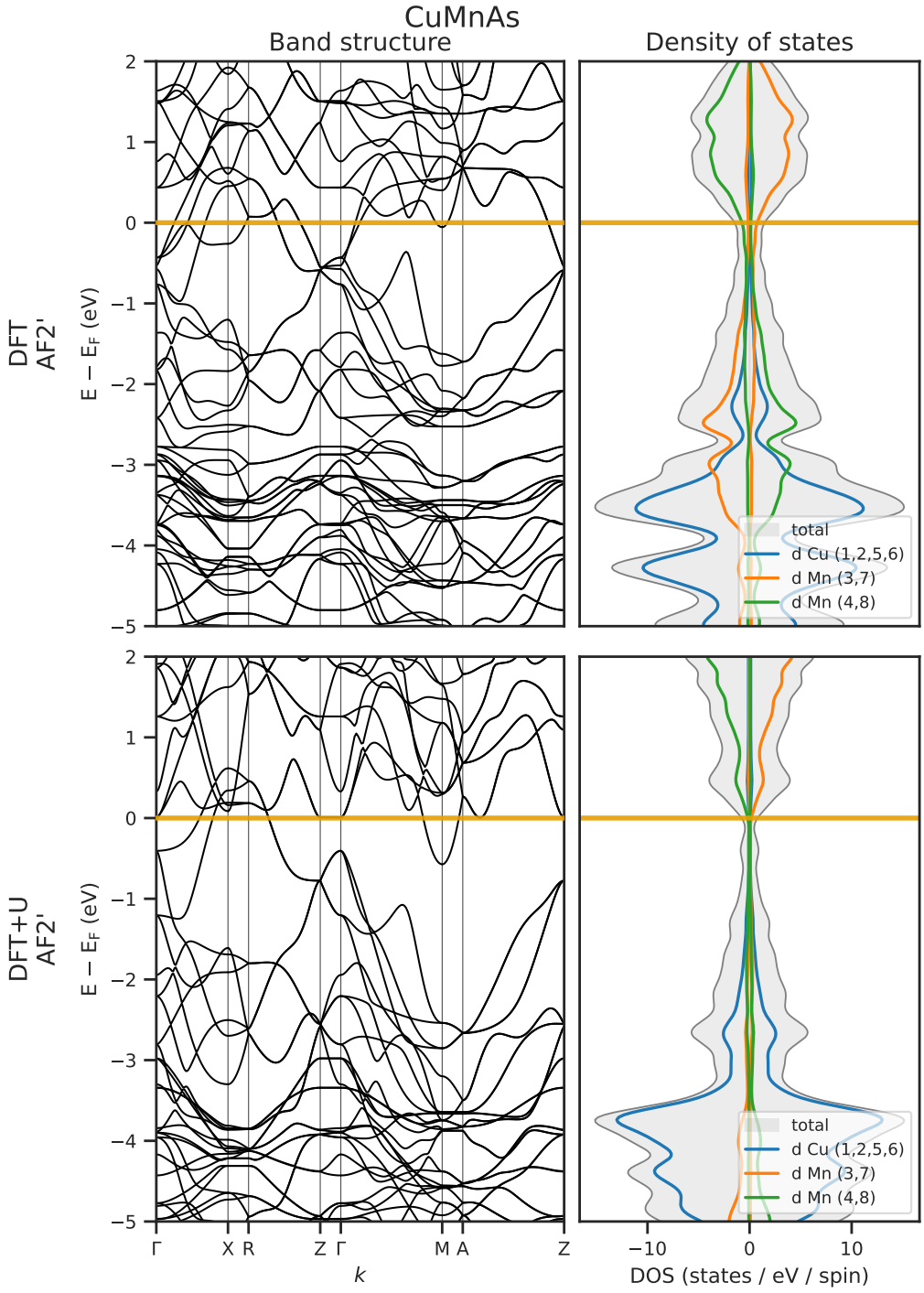


Figure 174: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnCuAs ■ higher-energy

Structure

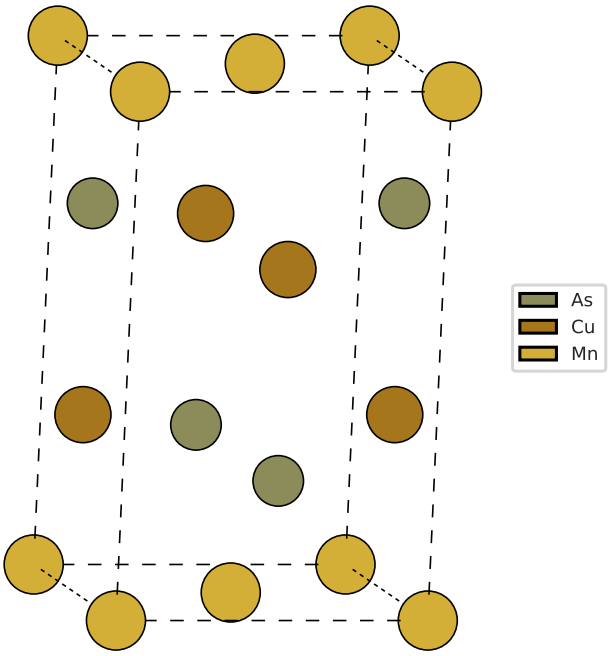


Figure 175: Structure of MnCuAs

a (Å)	c (Å)	z_1	z_2
3.8758	6.0060	0.3147	0.2717

Table 179: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-44491.345468	0.000000	3.38, -3.38, 0.00, 0.00, 3.38, -3.38, 0.00, 0.00
AF8″	-44491.260768	0.084700	3.39, -3.39, 0.00, 0.00, -3.39, 3.39, 0.00, 0.00
F1″	-44491.021515	0.323952	2.56, 2.56, -0.06, -0.06, 2.56, 2.56, -0.06, -0.06
AF1″	-44491.003731	0.341737	2.37, 2.37, -0.05, 0.05, -2.37, -2.37, 0.05, -0.05

Table 180: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

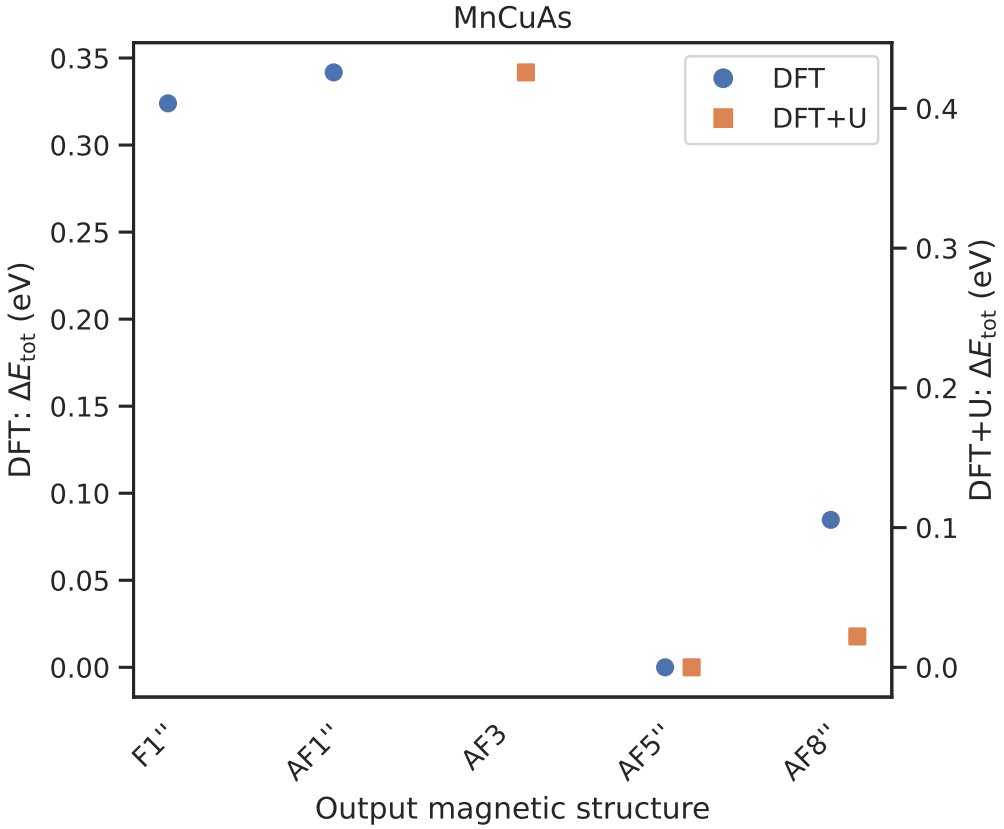


Figure 176: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-44484.043231	0.000000	4.49, -4.49, 0.00, 0.00, 4.49, -4.49, 0.00, 0.00
AF8″	-44484.021140	0.022091	4.49, -4.49, 0.00, 0.00, -4.49, 4.49, 0.00, 0.00
AF3	-44483.617453	0.425778	4.43, 4.43, -0.12, 0.12, -4.43, -4.43, 0.12, -0.12

Table 181: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

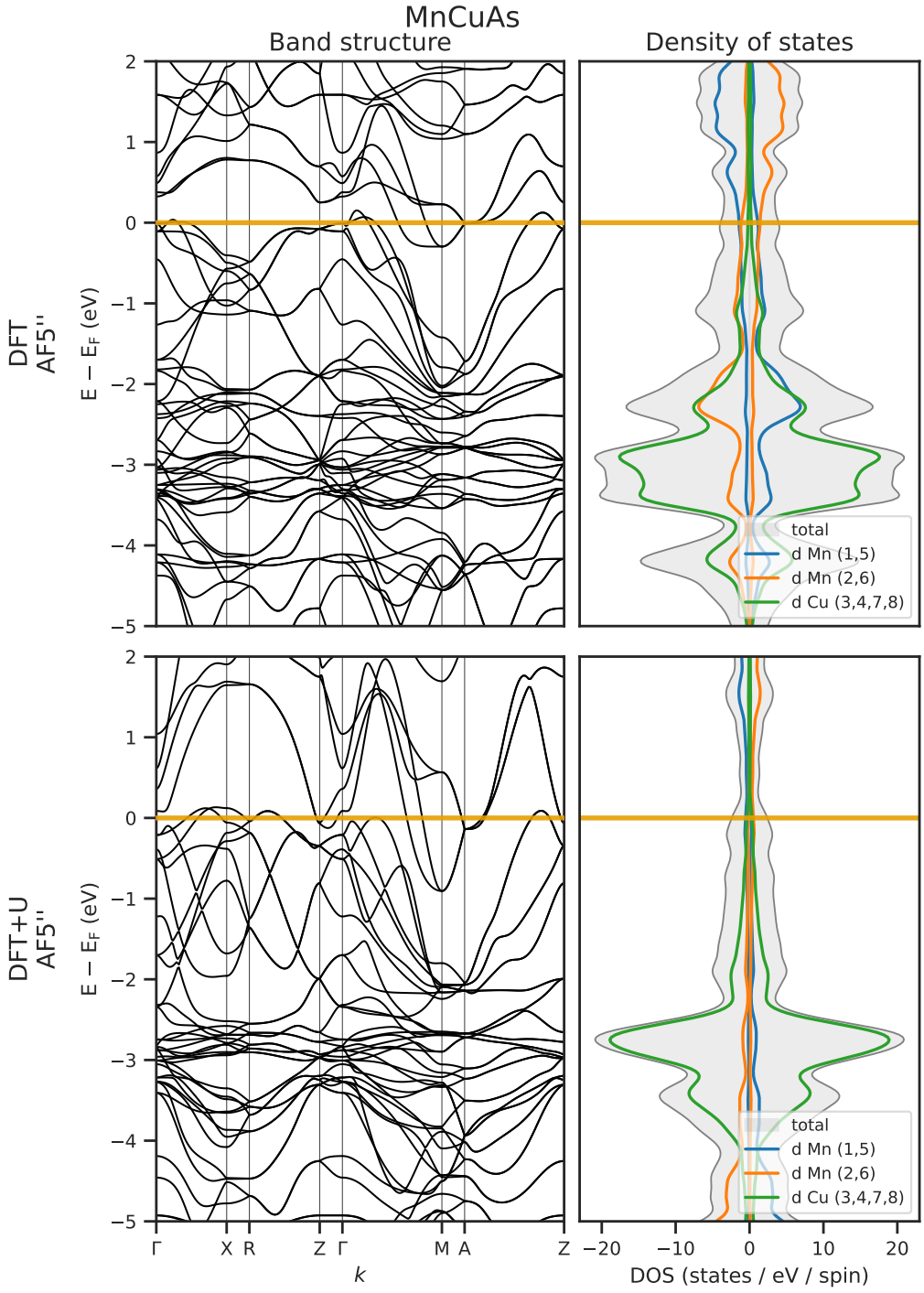


Figure 177: Band structure and Density of states of the lowest in energy calculations.

Material: MnCuSb

Configuration: MnCuSb ■ lower-energy

Structure

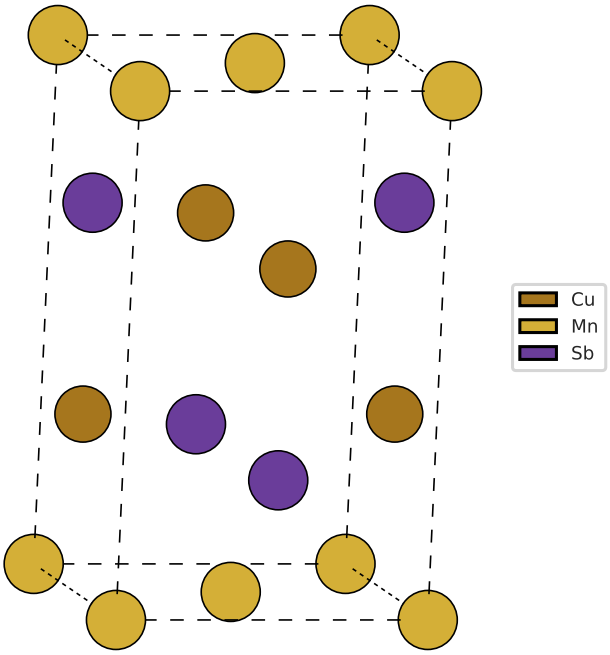


Figure 178: Structure of MnCuSb

a (Å)	c (Å)	z_1	z_2
4.0663	6.4115	0.2751	0.2953

Table 182: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-42376.930633	0.000000	3.64, 3.64, -0.09, -0.09, 3.65, 3.65, -0.09, -0.09
AF8″	-42376.920803	0.009830	3.71, -3.71, 0.00, 0.00, -3.72, 3.72, 0.00, 0.00
AF1″	-42376.875969	0.054664	3.67, 3.67, -0.08, 0.08, -3.67, -3.67, 0.08, -0.08
F2″	-42375.378878	1.551756	-3.70, -3.70, 0.08, -0.00, 0.01, 0.01, -0.00, 0.08

Table 183: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

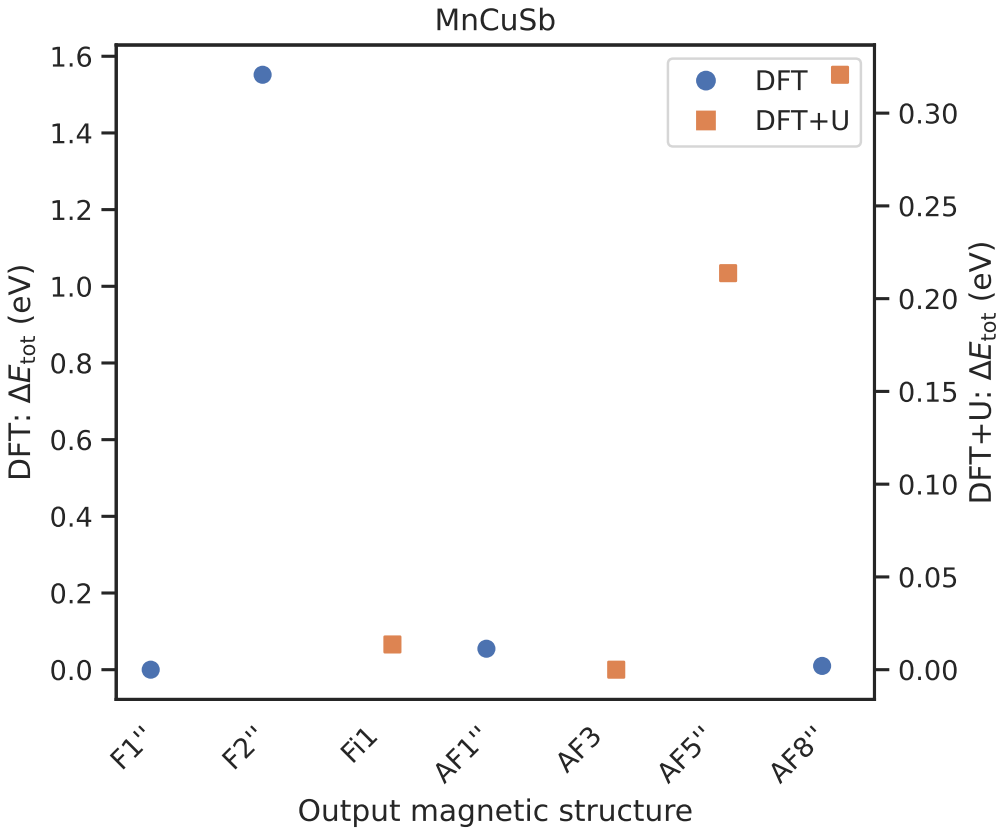


Figure 179: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-42371.200182	0.000000	4.55, 4.55, -0.13, 0.13, -4.55, -4.55, 0.13, -0.13
Fi1	-42371.186587	0.013595	4.54, 4.54, -0.14, -0.14, 4.54, 4.54, -0.14, -0.14
AF5″	-42370.986442	0.213740	4.64, -4.64, 0.00, 0.00, 4.64, -4.64, 0.00, 0.00
AF8″	-42370.879500	0.320682	4.65, -4.65, 0.00, 0.00, -4.65, 4.65, 0.00, 0.00

Table 184: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

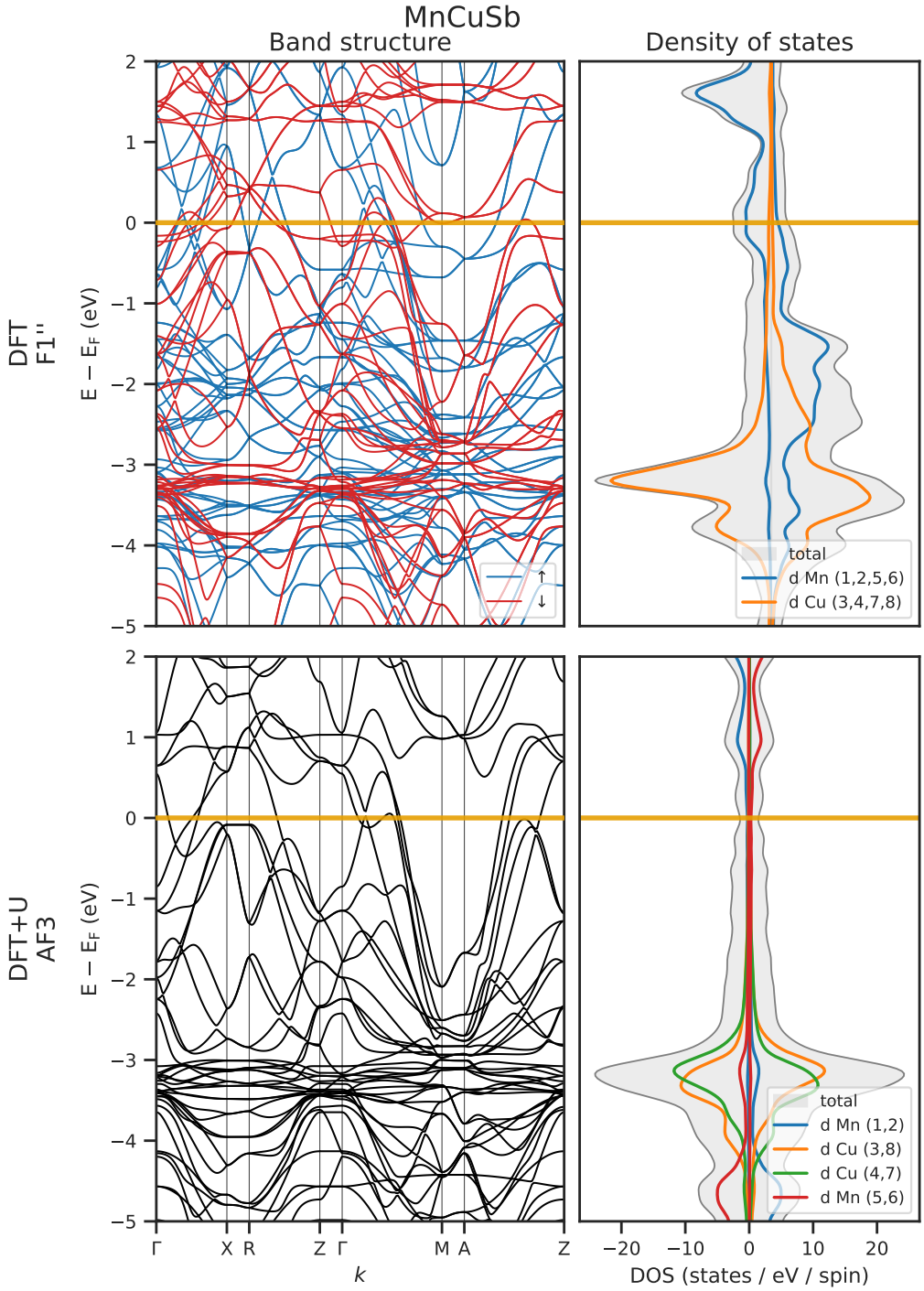


Figure 180: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuMnSb ■ higher-energy

Structure

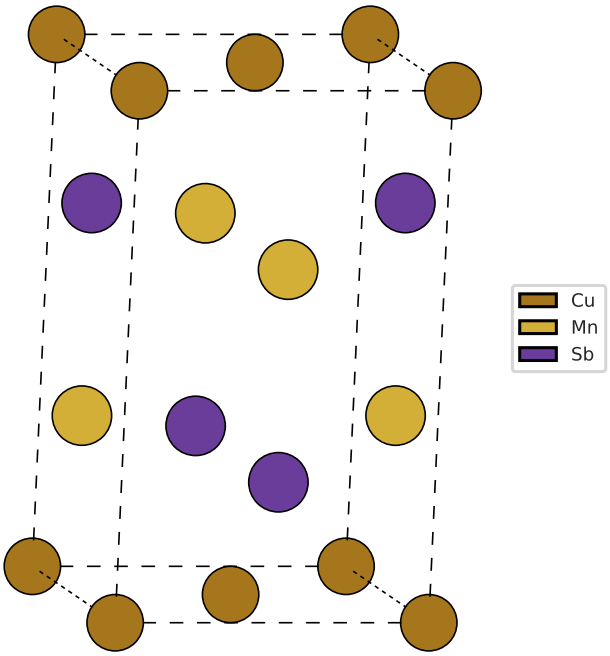


Figure 181: Structure of CuMnSb

a (Å)	c (Å)	z_1	z_2
4.1097	6.5254	0.2907	0.2806

Table 185: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1′	-42376.897185	0.000000	0.00, 0.00, 4.30, 4.30, 0.00, 0.00, -4.30, -4.30
AF2′	-42376.688839	0.208347	0.00, 0.00, -4.30, 4.30, 0.00, 0.00, -4.30, 4.30
F1′	-42376.679272	0.217914	-0.00, -0.00, 4.32, 4.32, -0.00, -0.00, 4.32, 4.32
AF3′	-42376.669268	0.227917	0.01, 0.01, -4.28, 4.28, -0.01, -0.01, 4.28, -4.28

Table 186: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

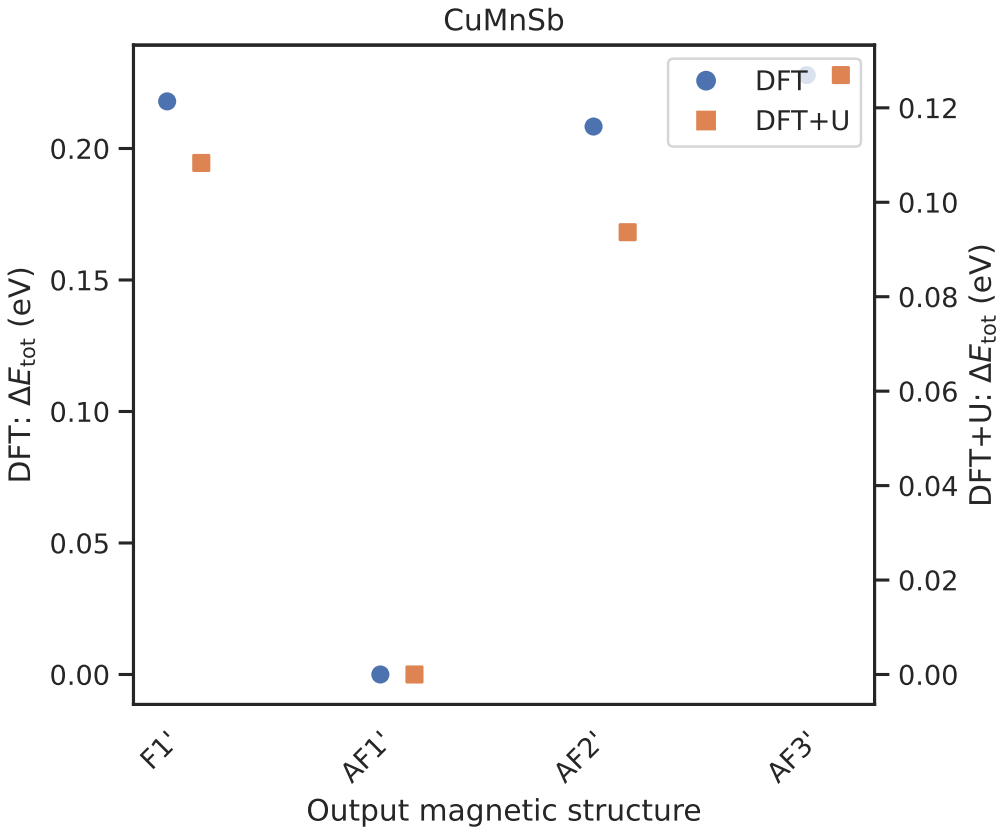


Figure 182: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1′	-42372.731297	0.000000	0.00, 0.00, 4.84, 4.84, 0.00, 0.00, -4.84, -4.84
AF2′	-42372.637635	0.093662	0.00, 0.00, -4.83, 4.83, 0.00, 0.00, -4.83, 4.83
F1′	-42372.622975	0.108322	-0.03, -0.03, 4.88, 4.88, -0.03, -0.03, 4.88, 4.88
AF3′	-42372.604360	0.126936	0.05, 0.05, -4.82, 4.82, -0.05, -0.05, 4.82, -4.82

Table 187: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

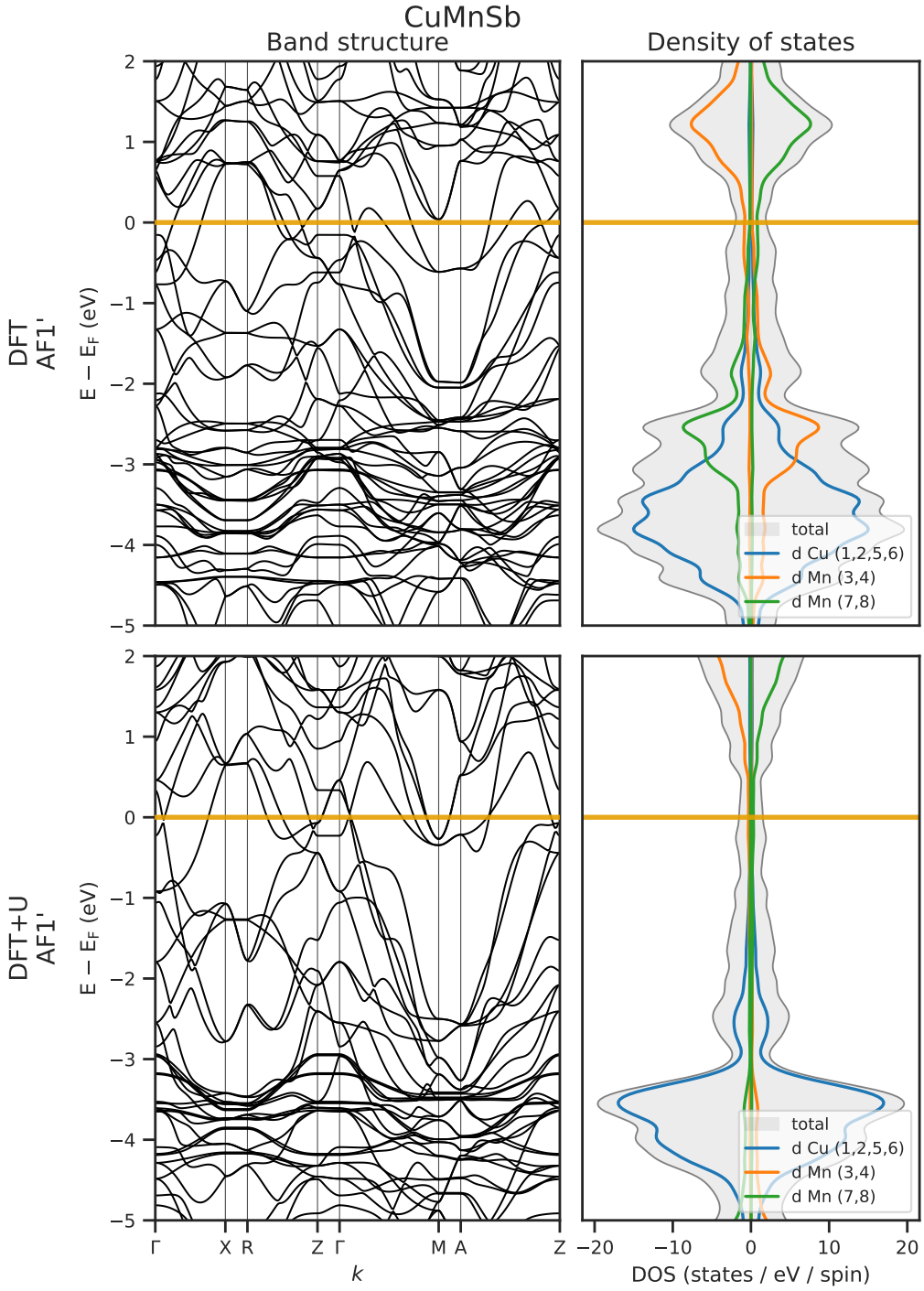


Figure 183: Band structure and Density of states of the lowest in energy calculations.

Material: NiCuAs

Configuration: NiCuAs ■ lower-energy

Structure

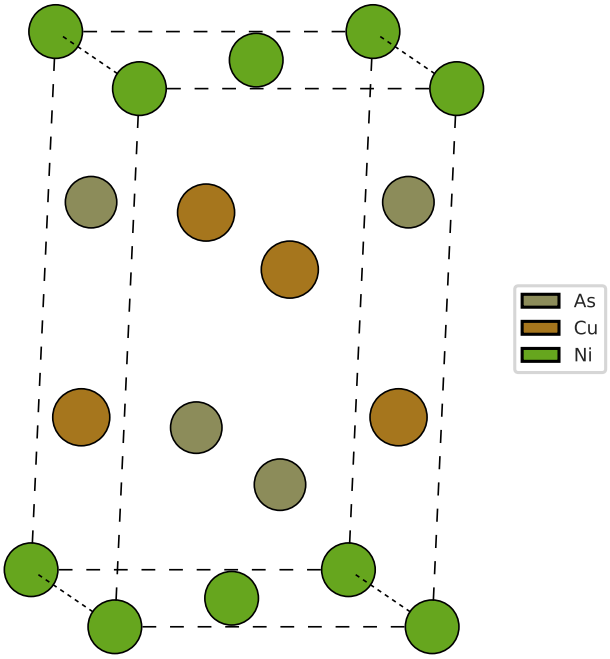


Figure 184: Structure of NiCuAs

a (Å)	c (Å)	z_1	z_2
3.7963	5.7888	0.2990	0.2733

Table 188: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-51323.262250	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 189: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

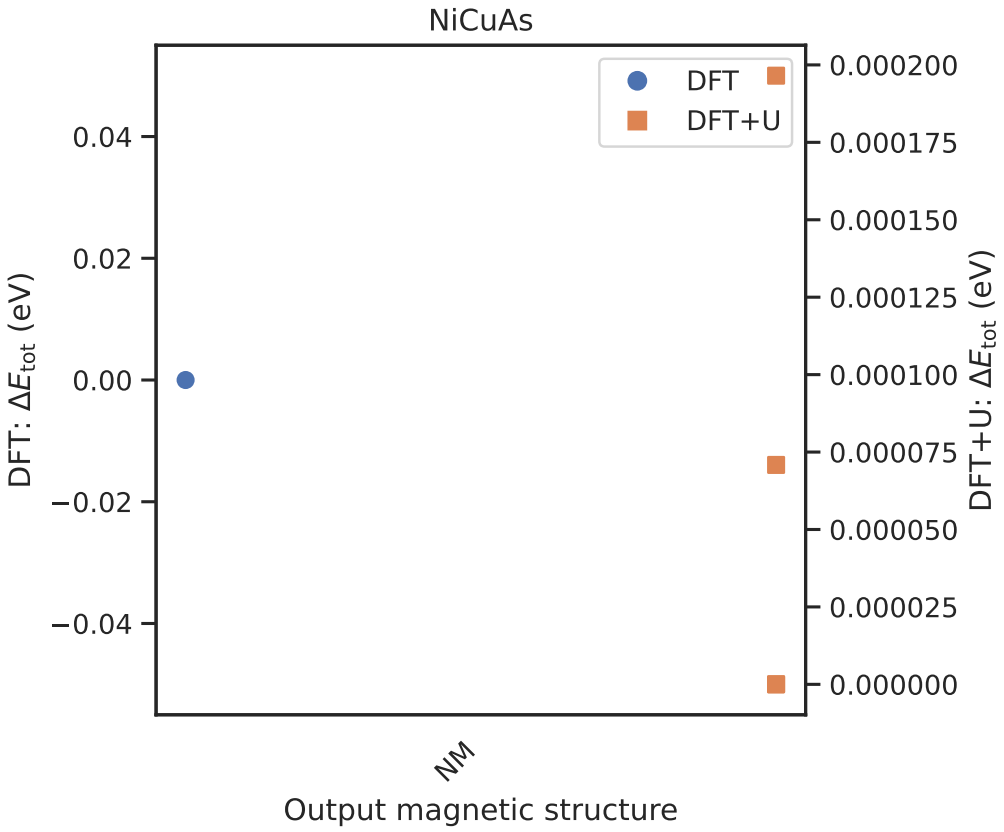


Figure 185: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-51315.840128	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-51315.840128	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-51315.840057	0.000071	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-51315.839931	0.000197	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 190: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

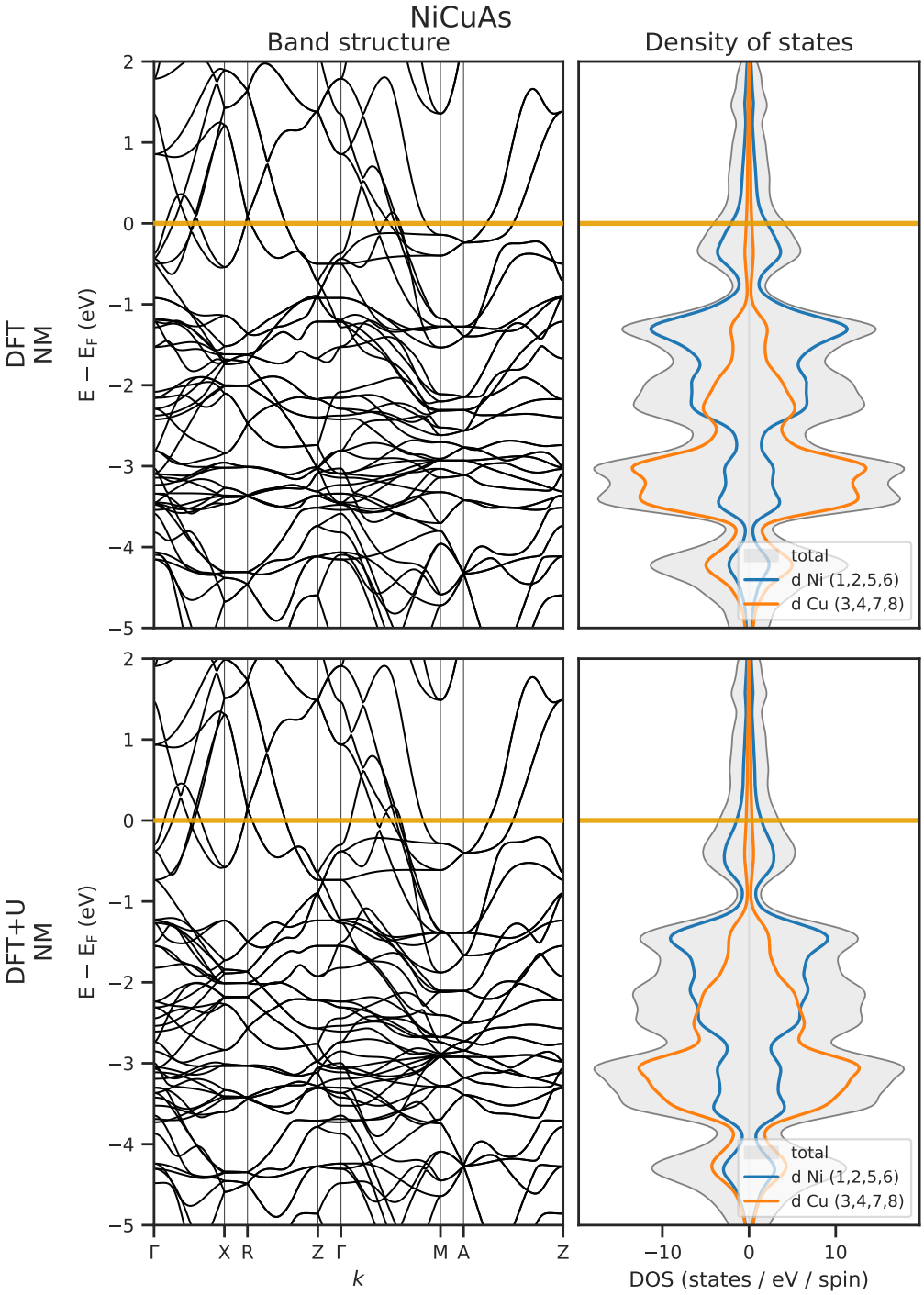


Figure 186: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuNiAs ■ higher-energy

Structure

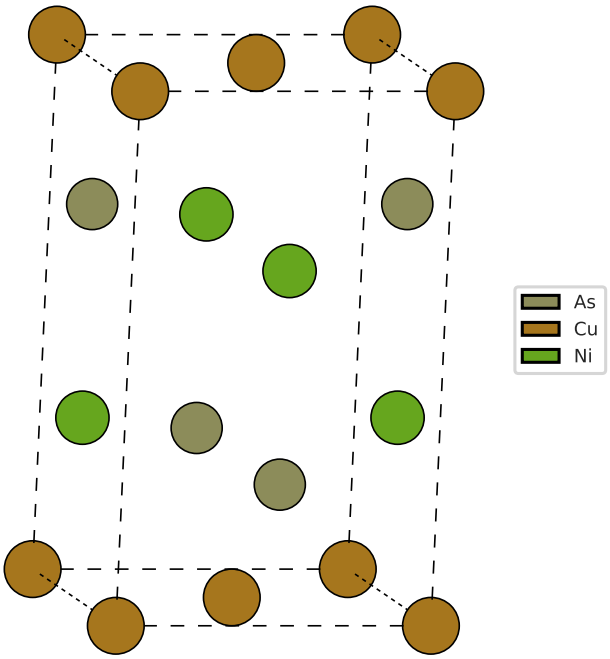


Figure 187: Structure of CuNiAs

a (Å)	c (Å)	z_1	z_2
3.6371	6.1556	0.3087	0.2999

Table 191: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-51322.532760	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 192: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

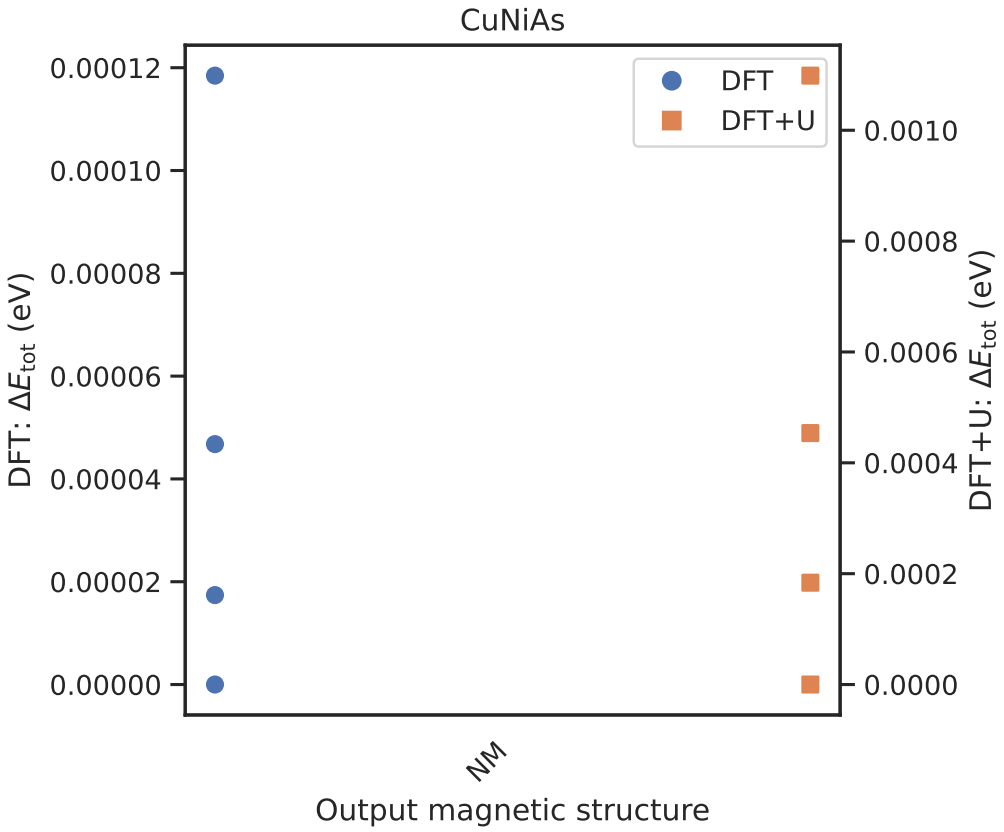


Figure 188: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-51315.494935	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-51315.494751	0.000184	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-51315.494481	0.000454	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-51315.493836	0.001099	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 193: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

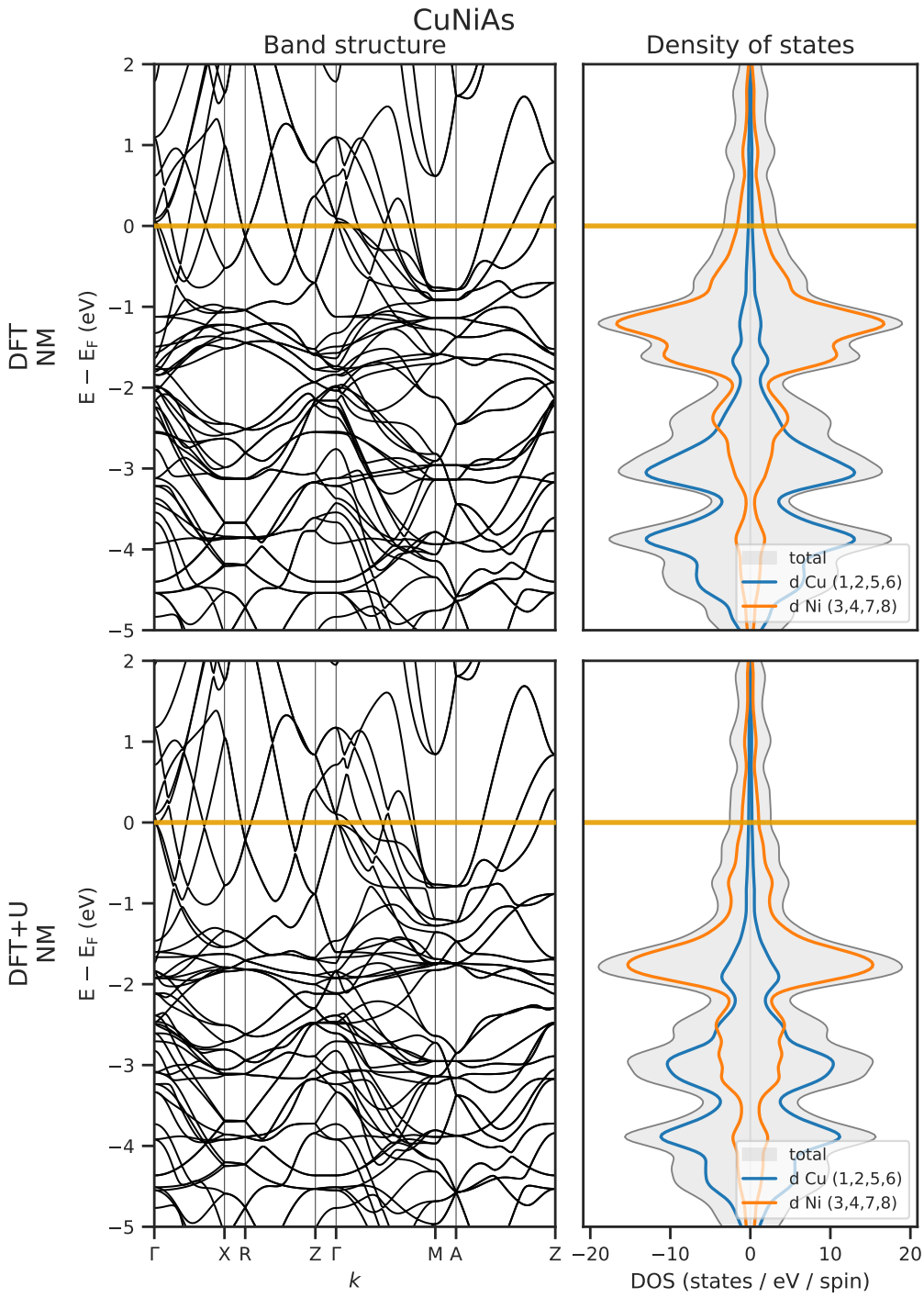


Figure 189: Band structure and Density of states of the lowest in energy calculations.

Material: NiCuSb

Configuration: NiCuSb ■ lower-energy

Structure

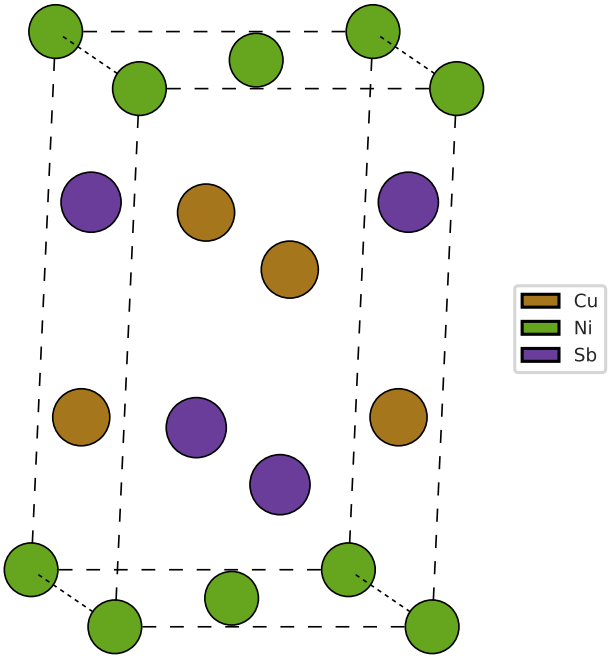


Figure 190: Structure of NiCuSb

a (Å)	c (Å)	z_1	z_2
3.9996	6.0838	0.2697	0.2850

Table 194: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Cu atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-49210.158114	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 195: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

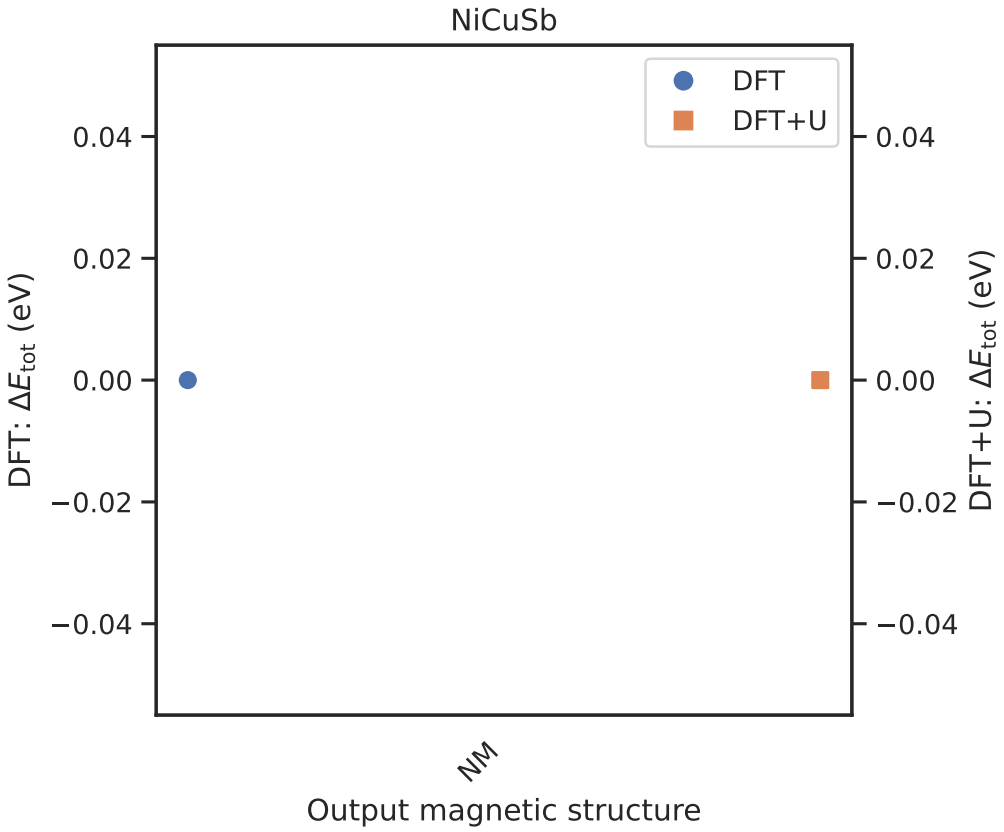


Figure 191: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-49203.023786	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-49203.023786	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-49203.023786	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-49203.023786	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 196: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

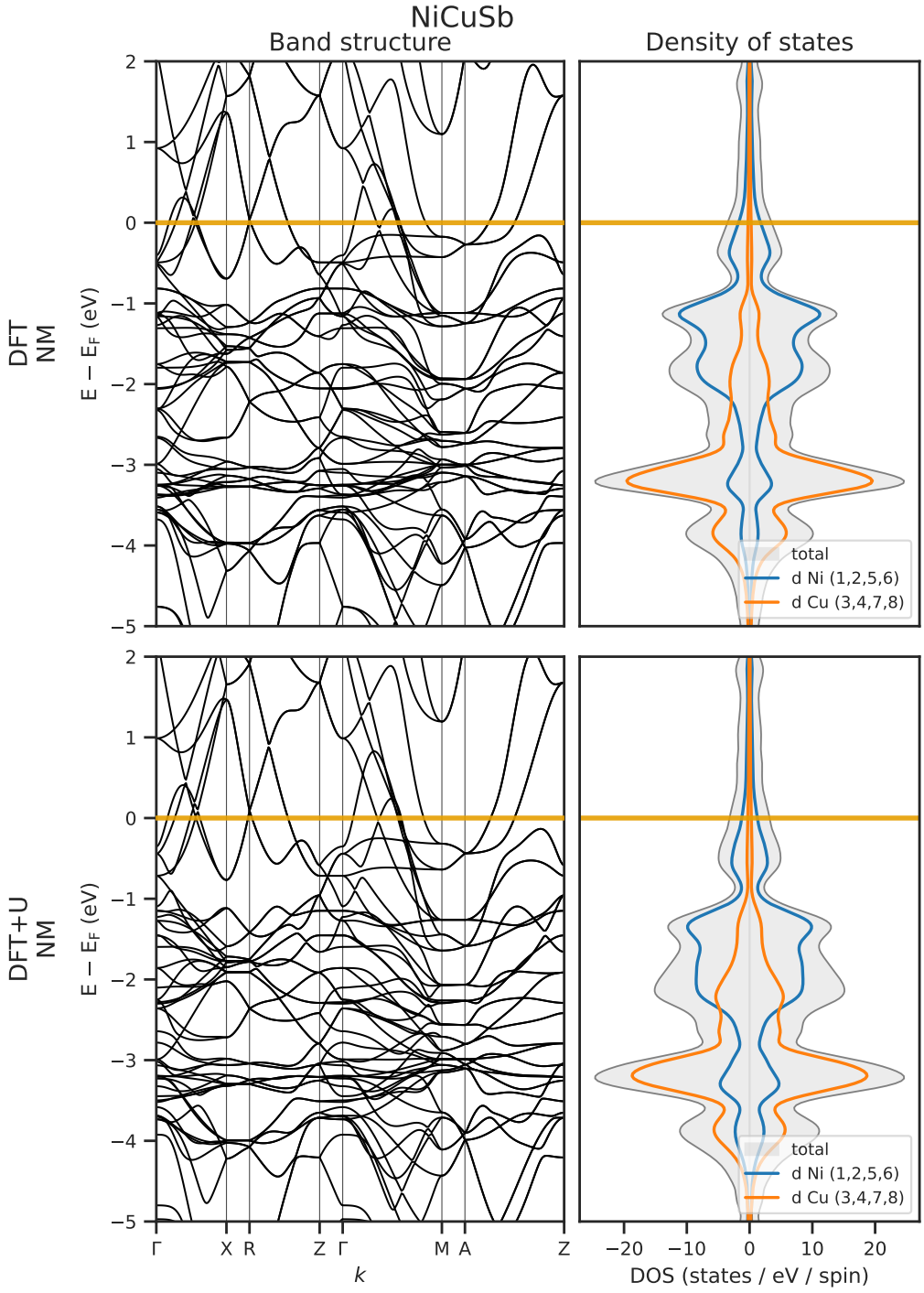


Figure 192: Band structure and Density of states of the lowest in energy calculations.

Configuration: CuNiSb ■ higher-energy

Structure

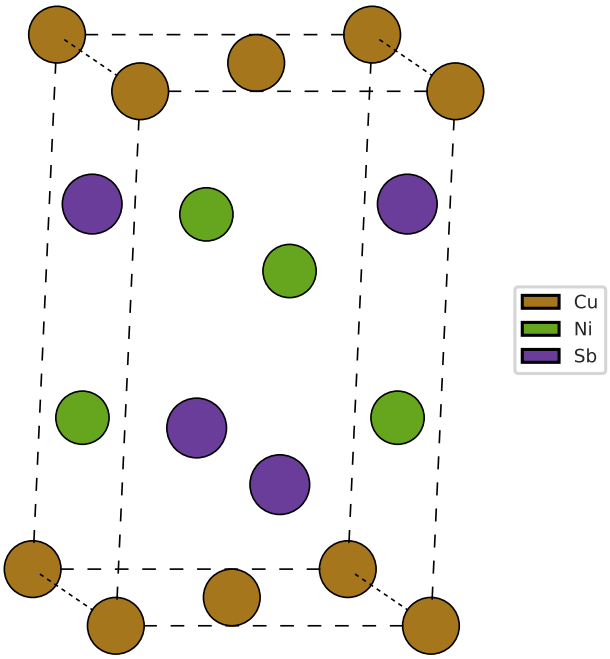


Figure 193: Structure of CuNiSb

a (Å)	c (Å)	z_1	z_2
3.8325	6.4479	0.2699	0.3179

Table 197: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Cu atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-49209.584338	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 198: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

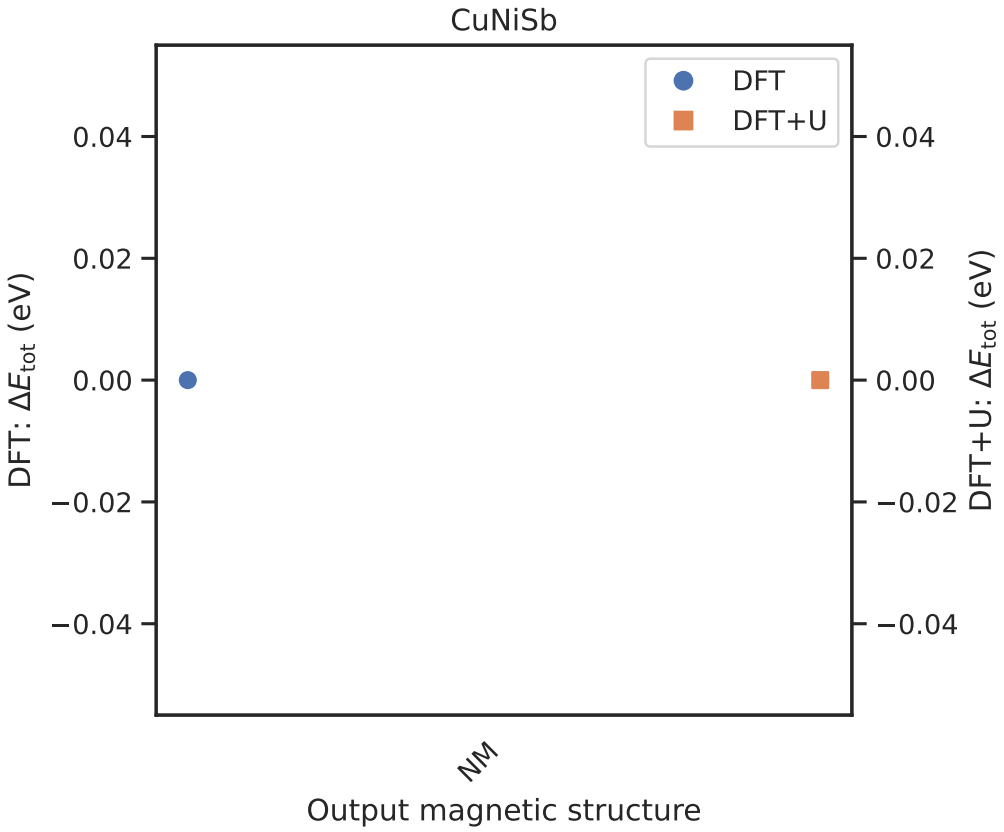


Figure 194: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-49202.728350	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-49202.728322	0.000028	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-49202.728309	0.000041	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-49202.728278	0.000072	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 199: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

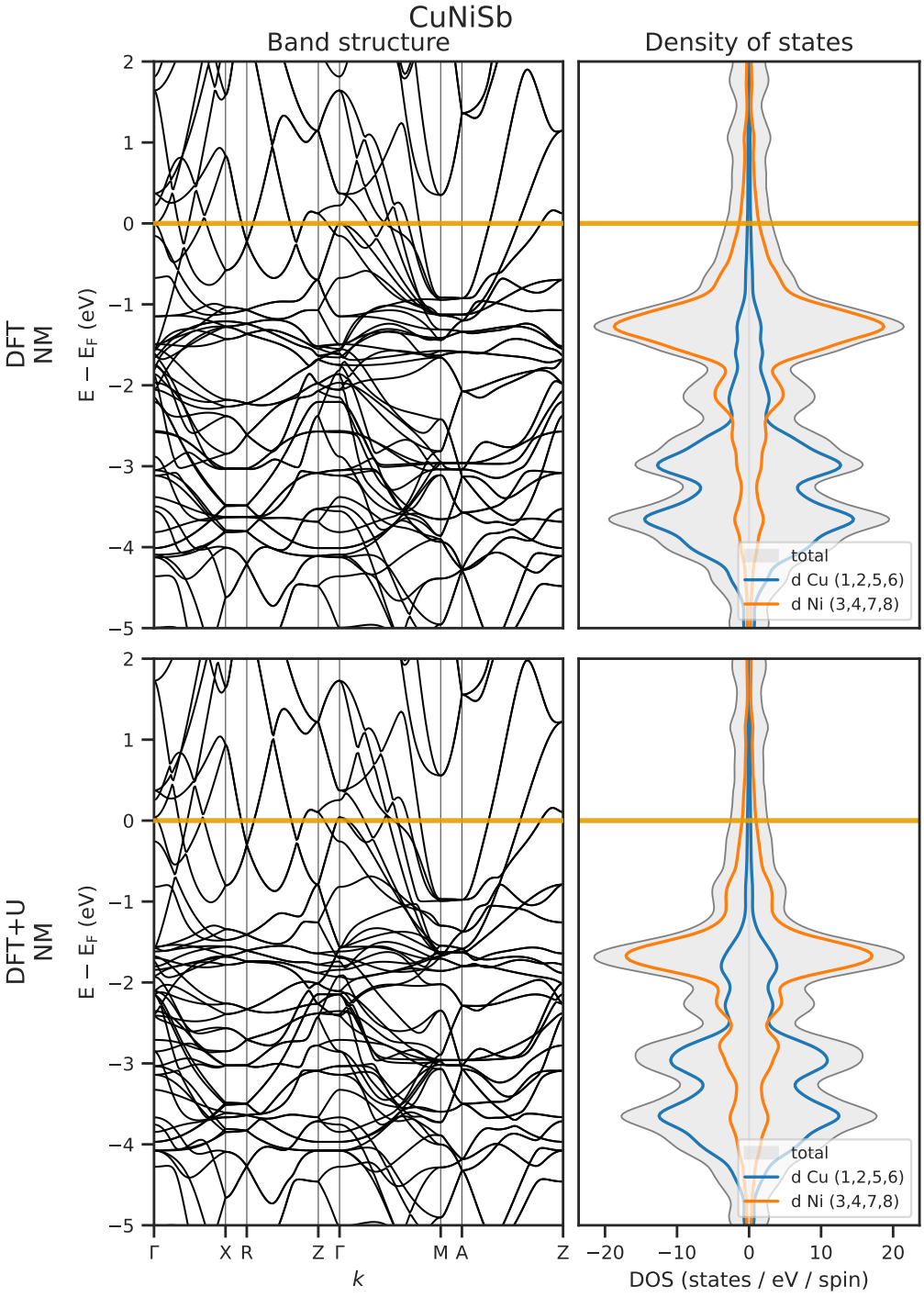


Figure 195: Band structure and Density of states of the lowest in energy calculations.

Material: Fe_2As

Configuration: Fe_2As

Structure

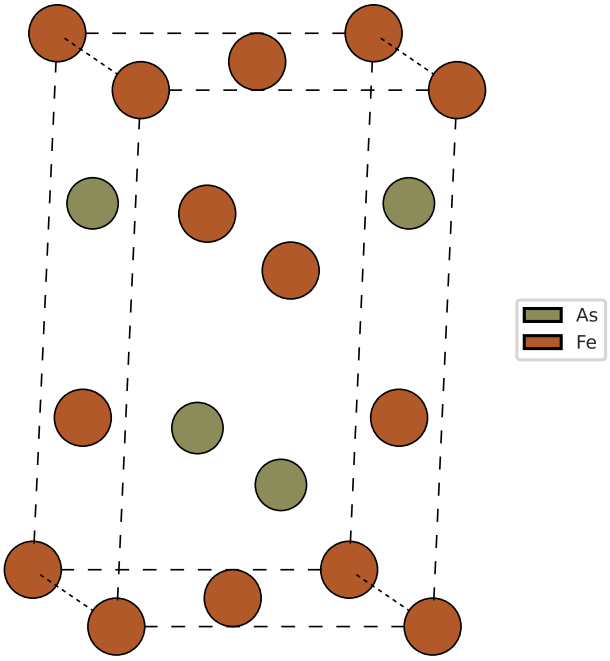


Figure 196: Structure of Fe_2As

a (Å)	c (Å)	z_1	z_2
3.6640	5.8681	0.3238	0.2659

Table 200: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

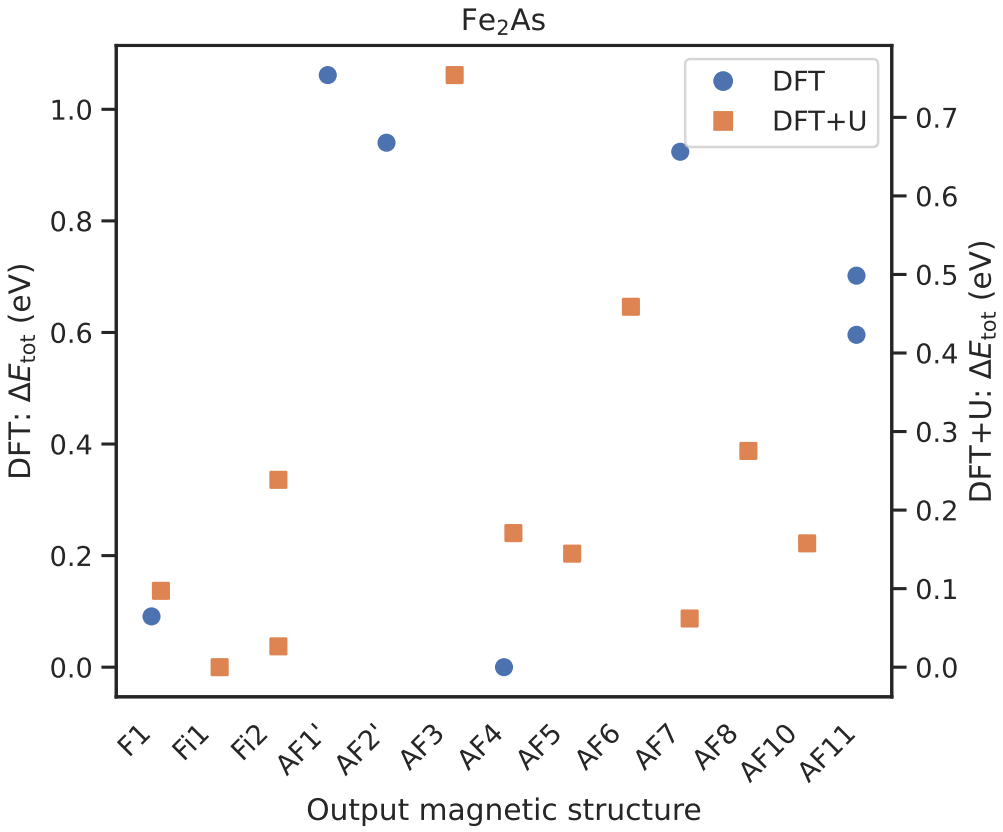


Figure 197: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-38654.549604	0.000000	-1.35, -1.35, -2.51, 2.51, 1.35, 1.35, 2.51, -2.51
F1	-38654.458543	0.091061	-0.96, -0.96, -2.60, -2.60, -0.96, -0.96, -2.60, -2.60
AF11	-38653.953832	0.595772	1.78, 1.78, -2.27, 2.27, -1.78, -1.78, -2.70, 2.70
AF11	-38653.847771	0.701833	1.42, 1.42, 2.76, 2.41, -1.42, -1.42, -2.76, -2.41
AF7	-38653.625680	0.923924	1.52, -1.52, 2.70, 2.70, 1.52, -1.52, -2.70, -2.70
AF2′	-38653.609478	0.940126	0.00, 0.00, -2.53, 2.53, 0.00, 0.00, -2.53, 2.53
AF1′	-38653.488248	1.061356	0.00, 0.00, 2.69, 2.69, -0.00, -0.00, -2.69, -2.69

Table 201: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-38637.335491	0.000000	2.72, 2.72, -3.36, -3.36, 2.72, 2.72, -3.36, -3.36
Fi2	-38637.308975	0.026516	2.67, 2.67, -3.36, 3.10, -2.74, -2.72, -3.18, 3.16
AF7	-38637.273503	0.061987	2.89, -2.89, 3.12, 3.12, 2.89, -2.89, -3.12, -3.12
F1	-38637.238269	0.097221	2.80, 2.80, 3.08, 3.08, 2.80, 2.80, 3.08, 3.08
AF5	-38637.190941	0.144549	2.88, -2.88, -3.05, 3.05, 2.88, -2.88, -3.05, 3.05
AF10	-38637.177831	0.157660	2.85, -2.85, 3.12, 3.12, -2.85, 2.85, -3.12, -3.12
AF4	-38637.164756	0.170734	2.77, 2.77, 3.10, -3.10, -2.77, -2.77, -3.10, 3.10
Fi2	-38637.096948	0.238543	2.78, 2.78, 3.18, 3.38, -2.69, -2.69, -3.08, -3.26
AF8	-38637.060165	0.275326	2.84, -2.84, -3.07, 3.07, -2.84, 2.84, -3.07, 3.07
AF6	-38636.876614	0.458876	2.77, -2.79, -3.09, 3.09, 2.79, -2.77, 3.09, -3.09
AF3	-38636.581666	0.753824	2.72, 2.72, -3.23, 3.23, -2.72, -2.72, 3.23, -3.23

Table 202: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

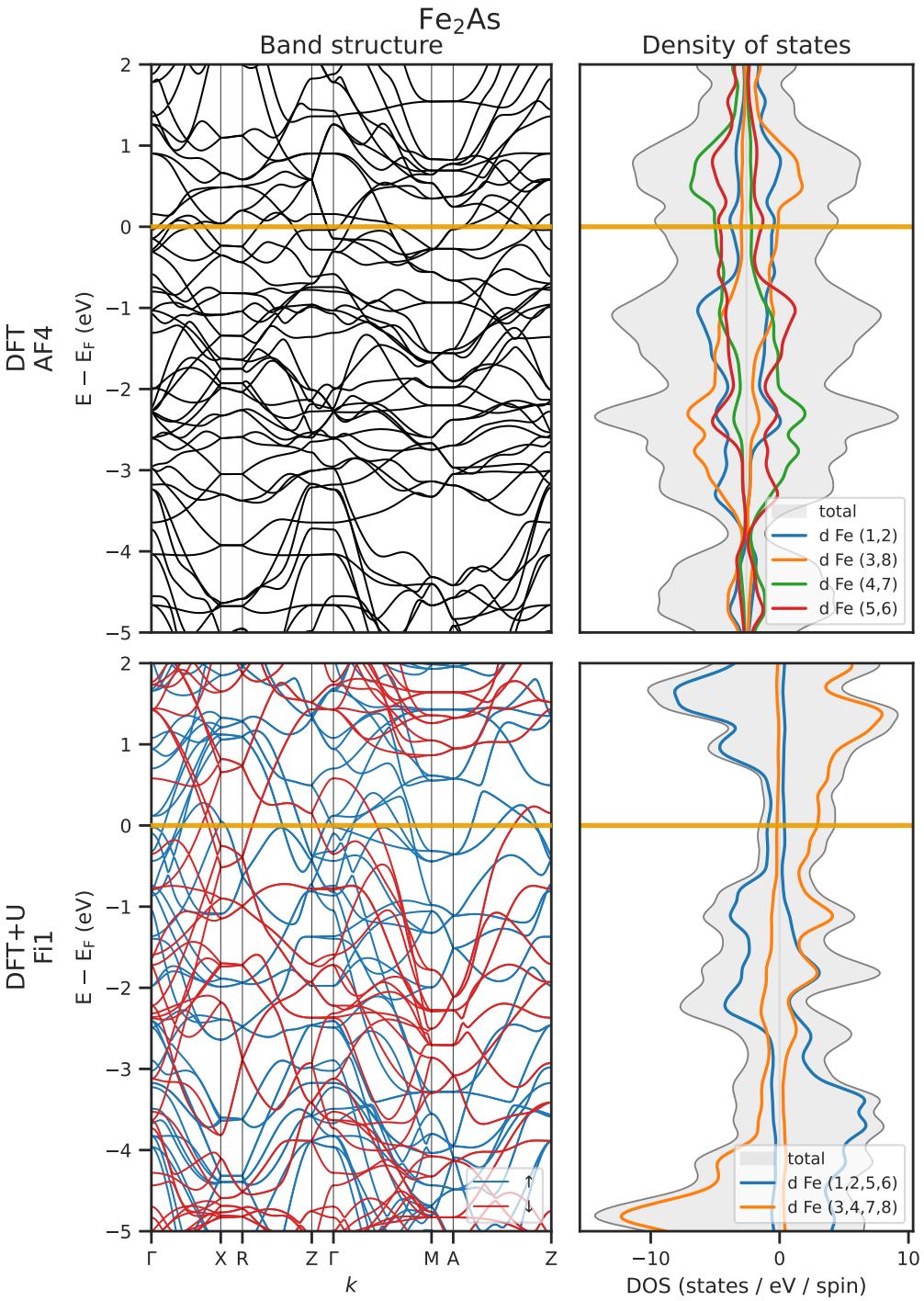


Figure 198: Band structure and Density of states of the lowest in energy calculations.

Material: Fe_2Sb

Configuration: Fe_2Sb

Structure

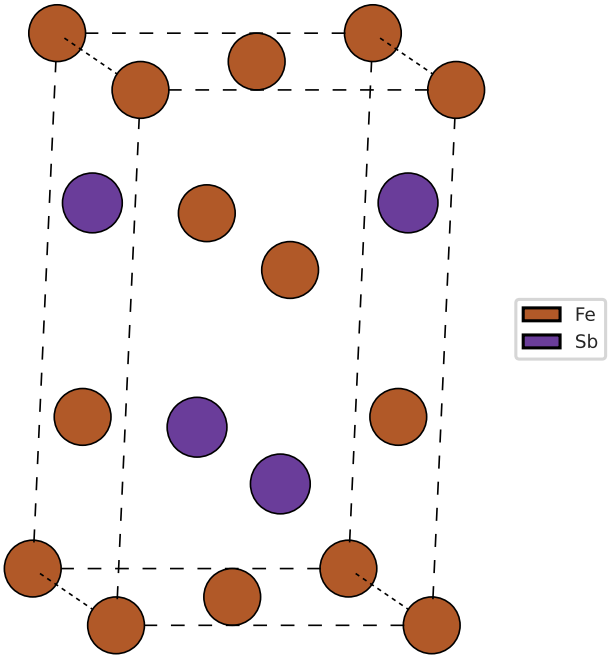


Figure 199: Structure of Fe_2Sb

a (Å)	c (Å)	z_1	z_2
3.9498	6.1559	0.2548	0.2994

Table 203: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of an Sb atom in the unit cell.

Magnetic structure and energy

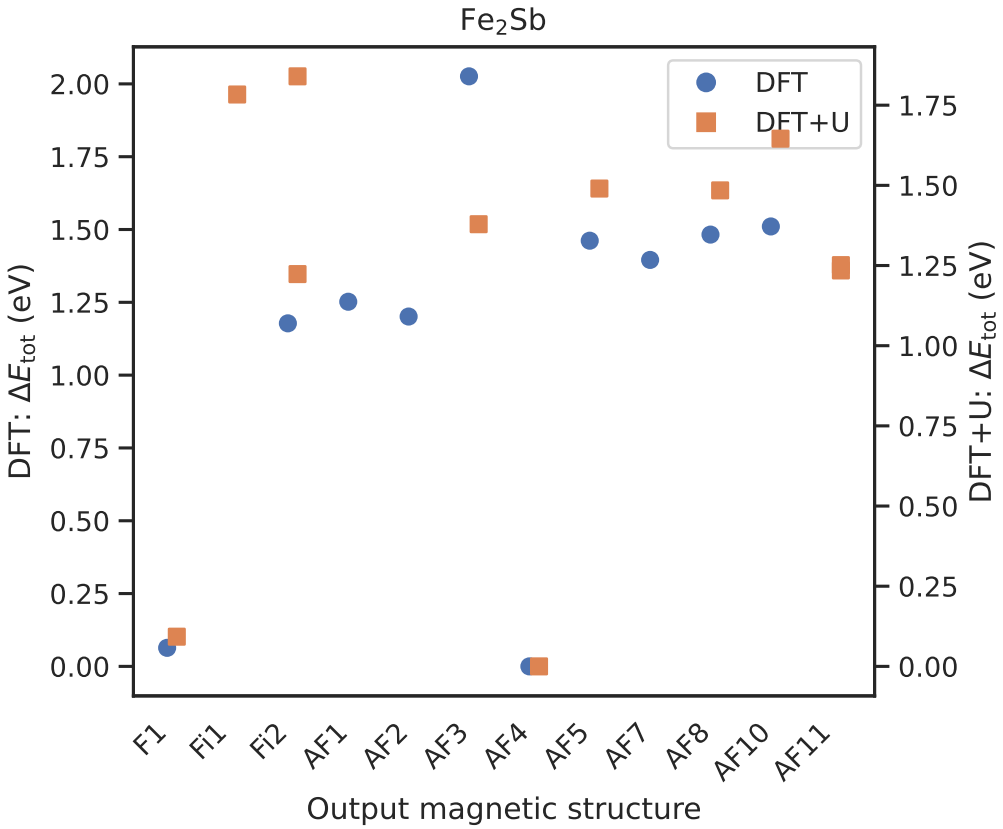


Figure 200: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-36540.880329	0.000000	-2.43, -2.43, -2.68, 2.68, 2.43, 2.43, 2.68, -2.68
F1	-36540.816673	0.063656	2.44, 2.44, 2.71, 2.71, 2.44, 2.44, 2.71, 2.71
Fi2	-36539.702487	1.177841	2.20, 2.20, 2.68, -2.65, 2.20, 2.20, 2.68, -2.65
AF2	-36539.679138	1.201191	2.25, 2.25, -2.62, 2.62, -2.25, -2.25, -2.67, 2.67
AF1	-36539.628319	1.252010	2.25, 2.25, 2.72, 2.66, -2.25, -2.25, -2.72, -2.66
AF7	-36539.484718	1.395610	2.11, -2.11, 2.75, 2.75, 2.11, -2.11, -2.75, -2.75
AF5	-36539.418736	1.461593	2.06, -2.06, -2.72, 2.72, 2.06, -2.06, -2.72, 2.72
AF8	-36539.397776	1.482553	2.03, -2.03, -2.72, 2.72, -2.03, 2.03, -2.72, 2.72
AF10	-36539.369827	1.510502	2.01, -2.01, 2.73, 2.73, -2.01, 2.01, -2.73, -2.73
AF3	-36538.854389	2.025939	2.07, 2.07, -2.63, 2.63, -2.07, -2.07, 2.63, -2.63

Table 204: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-36524.986120	0.000000	2.95, 2.95, 3.00, -3.00, -2.95, -2.95, -3.00, 3.00
F1	-36524.893498	0.092622	2.95, 2.95, 3.05, 3.05, 2.95, 2.95, 3.05, 3.05
Fi2	-36523.762806	1.223314	3.18, -2.92, -3.04, 3.24, -2.95, 3.03, 3.24, -3.04
AF11	-36523.751411	1.234709	3.05, -3.05, 3.24, 3.06, 3.11, -3.11, -3.06, -3.24
AF11	-36523.734859	1.251260	3.09, 3.09, 3.12, 2.93, -3.09, -3.09, -3.12, -2.93
AF3	-36523.607279	1.378841	2.97, 2.97, -3.17, 3.17, -2.97, -2.97, 3.17, -3.17
AF8	-36523.501784	1.484336	3.01, -3.01, -3.19, 3.25, -3.06, 3.06, -3.25, 3.19
AF5	-36523.496055	1.490065	3.07, -3.07, -3.23, 3.23, 3.07, -3.07, -3.23, 3.23
AF10	-36523.340514	1.645606	3.06, -3.06, 3.21, 3.21, -3.06, 3.06, -3.21, -3.21
Fi1	-36523.202782	1.783338	2.95, 2.95, -3.20, -3.20, 2.95, 2.95, -3.20, -3.20
Fi2	-36523.146152	1.839968	-3.04, 3.08, 1.26, -3.19, -2.94, 2.94, 3.06, 3.02

Table 205: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

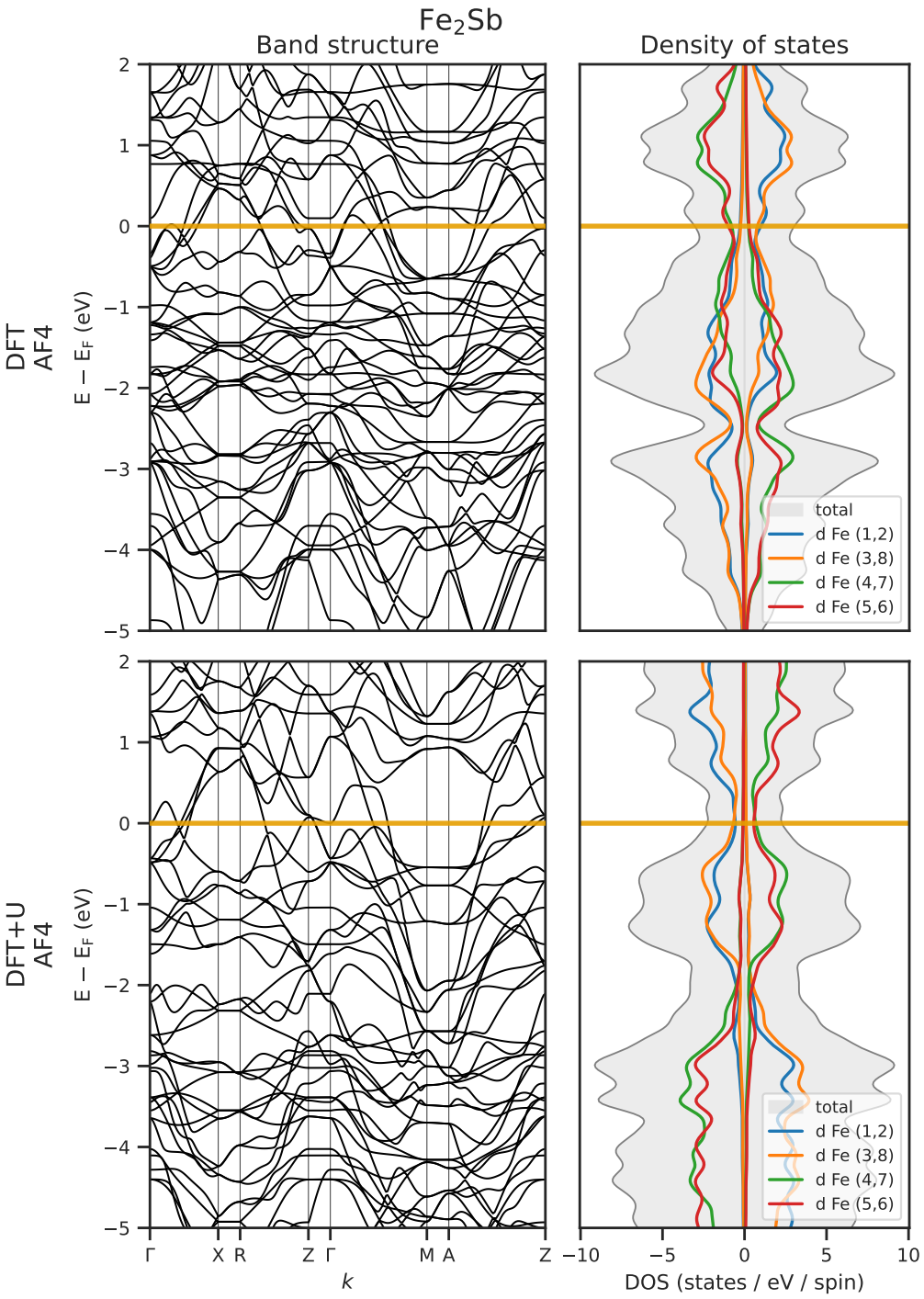


Figure 201: Band structure and Density of states of the lowest in energy calculations.

Material: FeGaAs

Configuration: FeGaAs ■ lower-energy

Structure

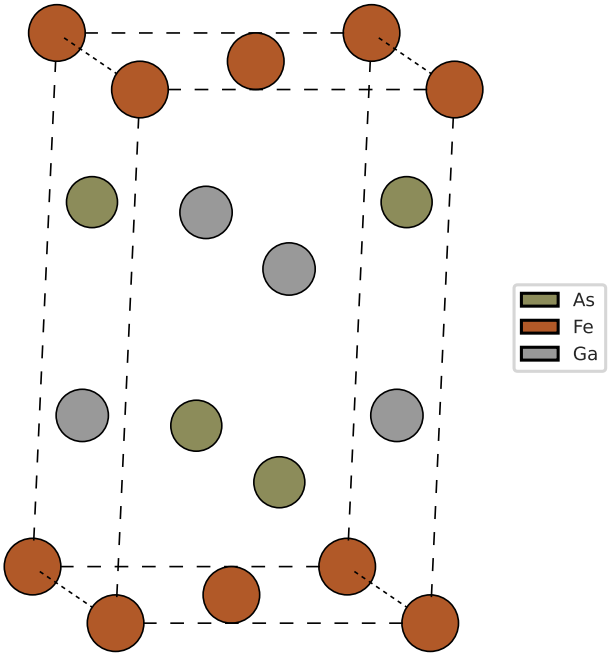


Figure 202: Structure of FeGaAs

a (Å)	c (Å)	z_1	z_2
4.0600	5.5209	0.2816	0.2574

Table 206: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1″	-33462.179265	0.000000	0.17, 0.17, -0.02, -0.02, 0.16, 0.17, -0.02, -0.02
AF5″	-33462.172374	0.006890	0.71, -0.71, 0.00, 0.00, 0.71, -0.71, 0.00, 0.00
AF1″	-33462.171106	0.008159	0.16, 0.16, -0.01, 0.01, -0.16, -0.16, 0.01, -0.01
AF8″	-33462.165959	0.013306	0.17, -0.17, 0.00, 0.00, -0.17, 0.17, 0.00, 0.00

Table 207: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

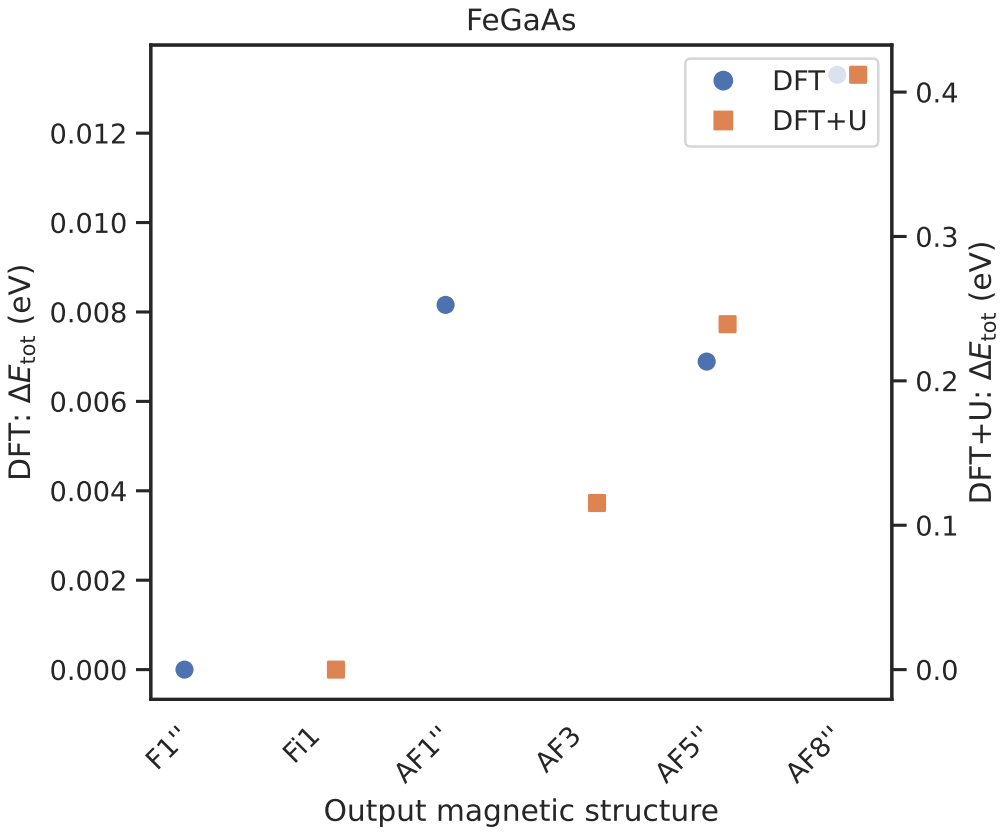


Figure 203: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
Fi1	-33453.198360	0.000000	2.50, 2.50, -0.19, -0.19, 2.50, 2.50, -0.19, -0.19
AF3	-33453.082965	0.115395	2.50, 2.50, -0.21, 0.21, -2.50, -2.50, 0.21, -0.21
AF5″	-33452.959100	0.239260	2.58, -2.58, 0.00, 0.00, 2.58, -2.58, 0.00, 0.00
AF8″	-33452.786372	0.411988	2.62, -2.62, 0.00, 0.00, -2.66, 2.66, 0.00, 0.00

Table 208: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

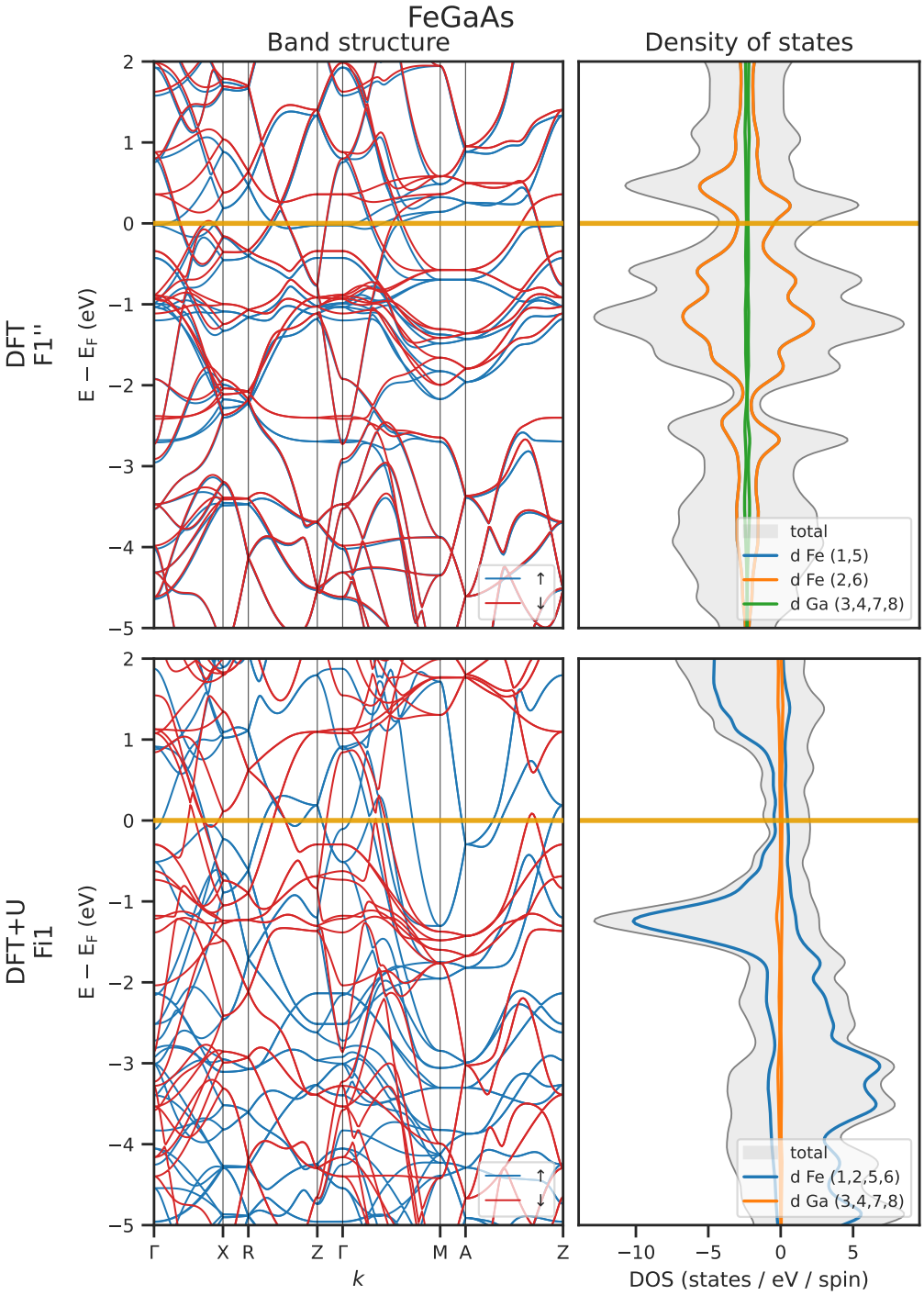


Figure 204: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaFeAs ■ higher-energy

Structure

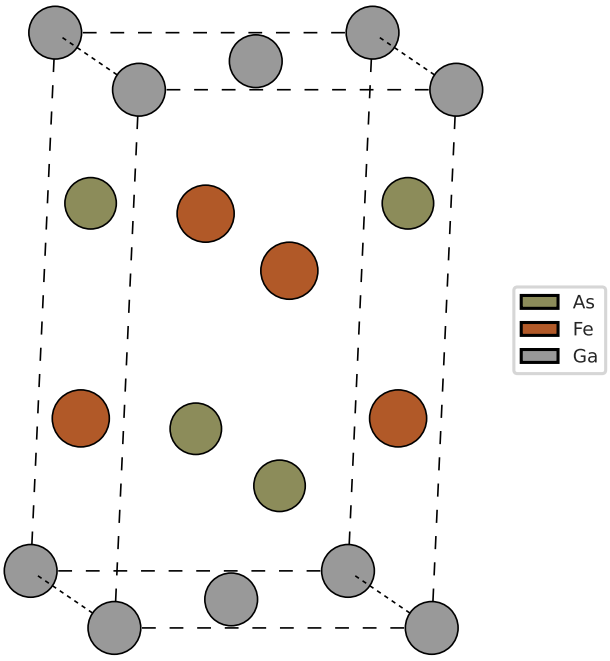


Figure 205: Structure of GaFeAs

a (Å)	c (Å)	z_1	z_2
3.5658	7.1169	0.2612	0.3800

Table 209: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1′	-33461.843791	0.000000	0.00, 0.00, 2.23, 2.23, 0.00, 0.00, -2.23, -2.23
Fi1	-33461.757980	0.085811	-0.16, -0.16, 2.14, 2.14, -0.16, -0.16, 2.14, 2.14
AF2′	-33461.649288	0.194503	0.00, 0.00, -2.17, 2.17, 0.00, 0.00, -2.17, 2.17
AF3	-33461.577951	0.265840	0.17, 0.17, -2.05, 2.04, -0.17, -0.17, 2.05, -2.05

Table 210: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

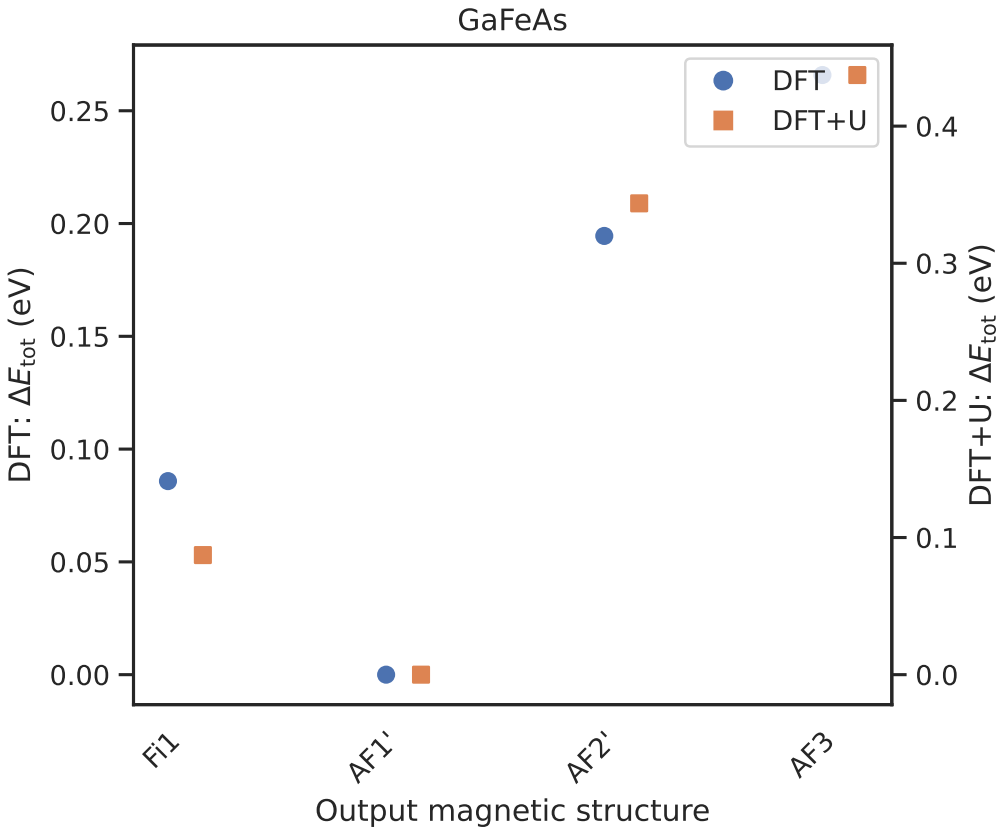


Figure 206: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1′	-33453.544019	0.000000	0.00, 0.00, 2.90, 2.90, 0.00, 0.00, -2.90, -2.90
Fi1	-33453.456820	0.087199	-0.24, -0.24, 2.77, 2.77, -0.24, -0.24, 2.77, 2.77
AF2′	-33453.200327	0.343692	0.00, 0.00, -2.94, 2.94, 0.00, 0.00, -2.94, 2.94
AF3	-33453.106755	0.437264	0.23, 0.23, -2.87, 2.87, -0.23, -0.23, 2.87, -2.87

Table 211: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

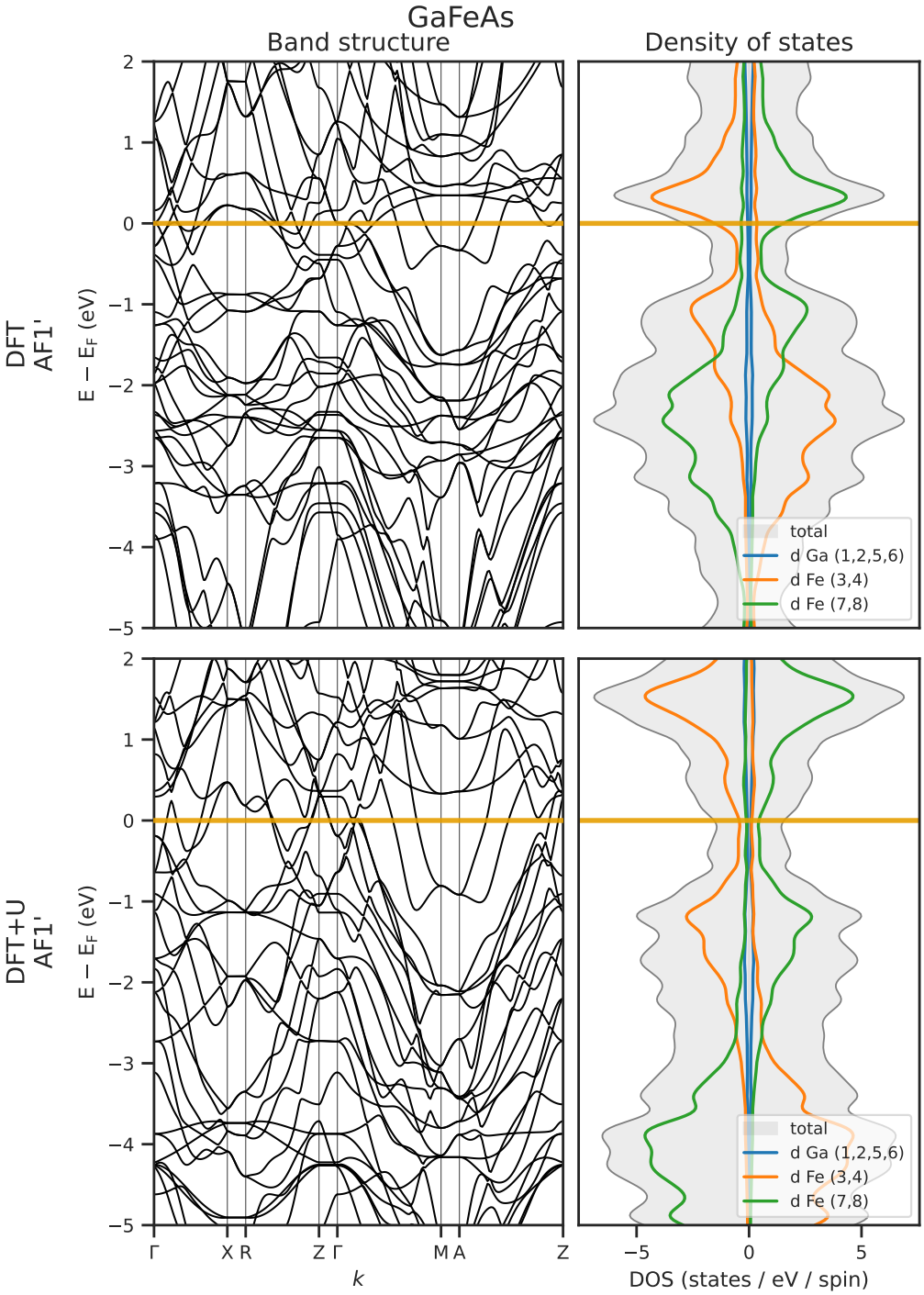


Figure 207: Band structure and Density of states of the lowest in energy calculations.

Material: FeGaSb

Configuration: FeGaSb ■ lower-energy

Structure

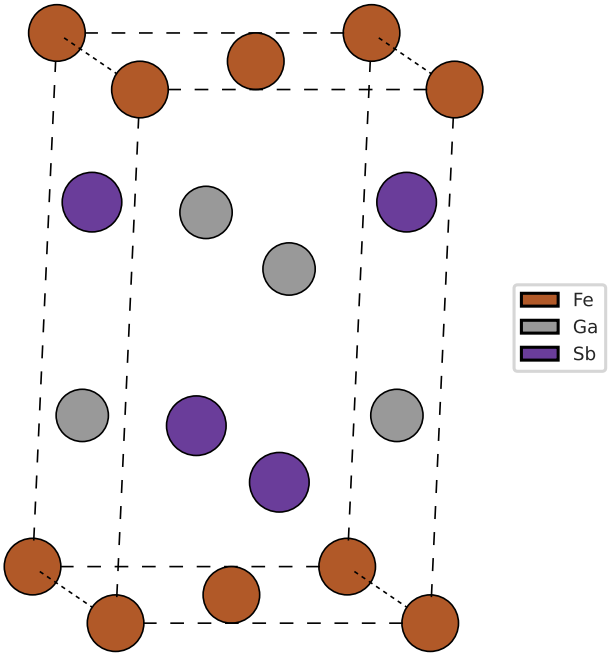


Figure 208: Structure of FeGaSb

a (Å)	c (Å)	z_1	z_2
4.2909	5.9006	0.2434	0.2812

Table 212: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-31348.184244	0.000000	1.73, -1.74, 0.00, 0.00, 1.74, -1.74, 0.00, 0.00
AF3	-31348.153959	0.030285	1.71, 1.71, -0.11, 0.11, -1.71, -1.71, 0.11, -0.11
AF8″	-31348.152701	0.031543	1.68, -1.68, 0.00, 0.00, -1.68, 1.68, 0.00, 0.00
Fi1	-31348.143420	0.040824	1.85, 1.85, -0.13, -0.13, 1.85, 1.85, -0.13, -0.13

Table 213: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

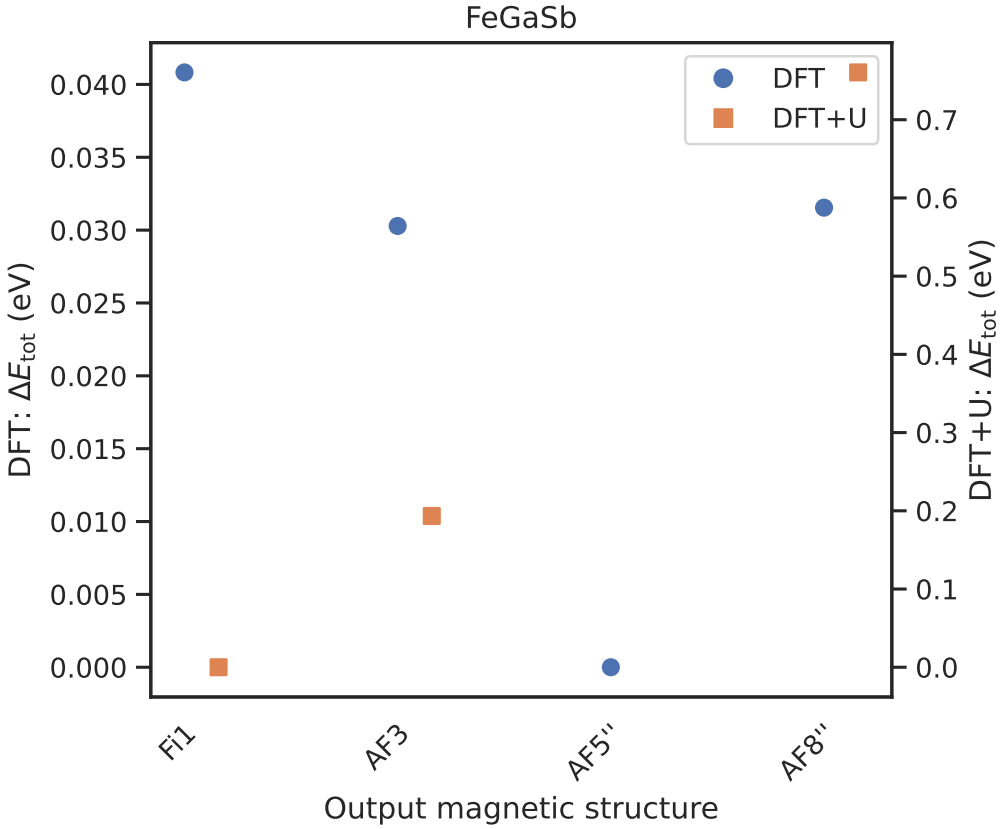


Figure 209: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-31340.194156	0.000000	2.65, 2.65, -0.22, -0.22, 2.65, 2.65, -0.22, -0.22
AF3	-31340.000771	0.193385	2.66, 2.67, -0.22, 0.22, -2.66, -2.67, 0.22, -0.22
AF8″	-31339.433671	0.760485	2.83, -2.83, 0.00, 0.00, -2.83, 2.83, 0.00, 0.00

Table 214: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

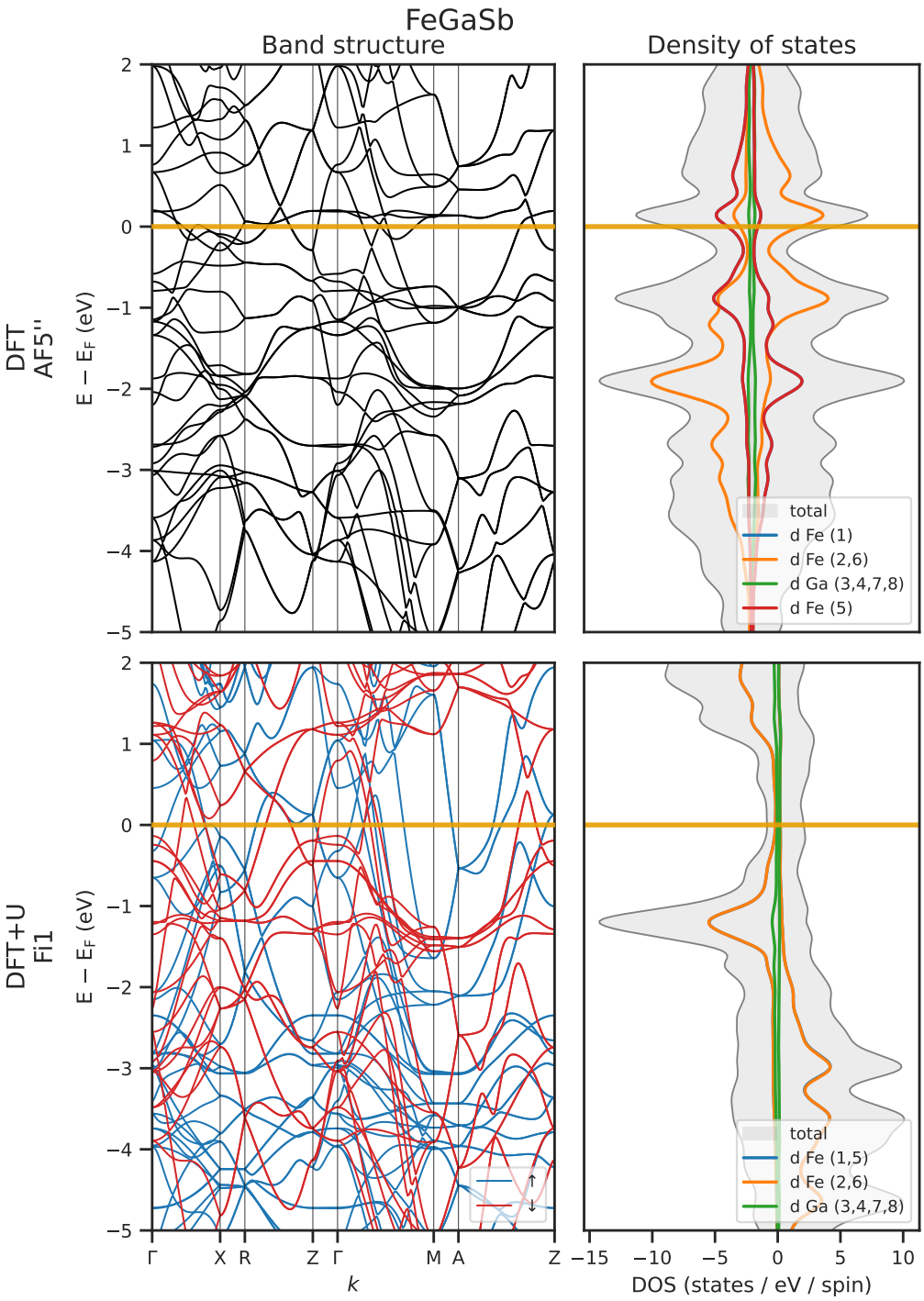


Figure 210: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaFeSb ■ higher-energy

Structure

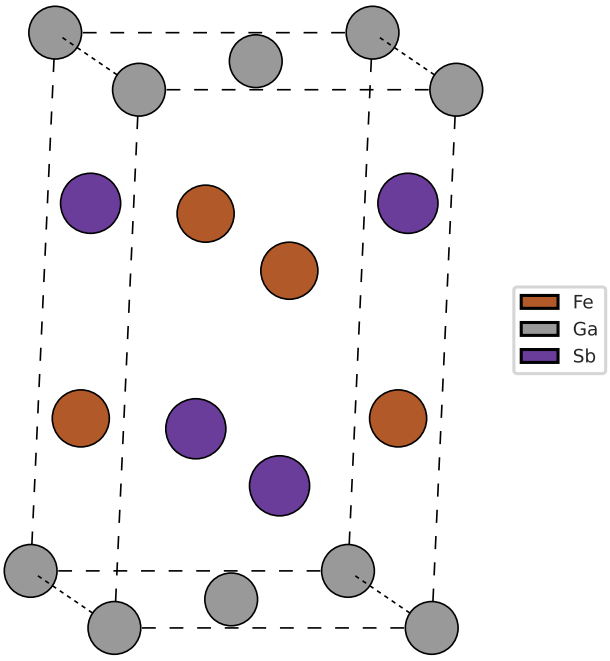


Figure 211: Structure of GaFeSb

a (Å)	c (Å)	z_1	z_2
3.6415	9.2790	0.4209	0.3032

Table 215: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-31344.502199	0.000000	0.00, 0.00, -2.80, 2.80, -0.00, -0.00, 2.80, -2.80
AF2′	-31344.488916	0.013284	0.00, 0.00, -2.80, 2.80, 0.00, 0.00, -2.80, 2.80
F1′	-31344.462208	0.039992	0.05, 0.05, 2.73, 2.73, 0.05, 0.05, 2.73, 2.73
AF1′	-31344.450582	0.051618	0.00, 0.00, 2.80, 2.80, 0.00, 0.00, -2.80, -2.80

Table 216: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

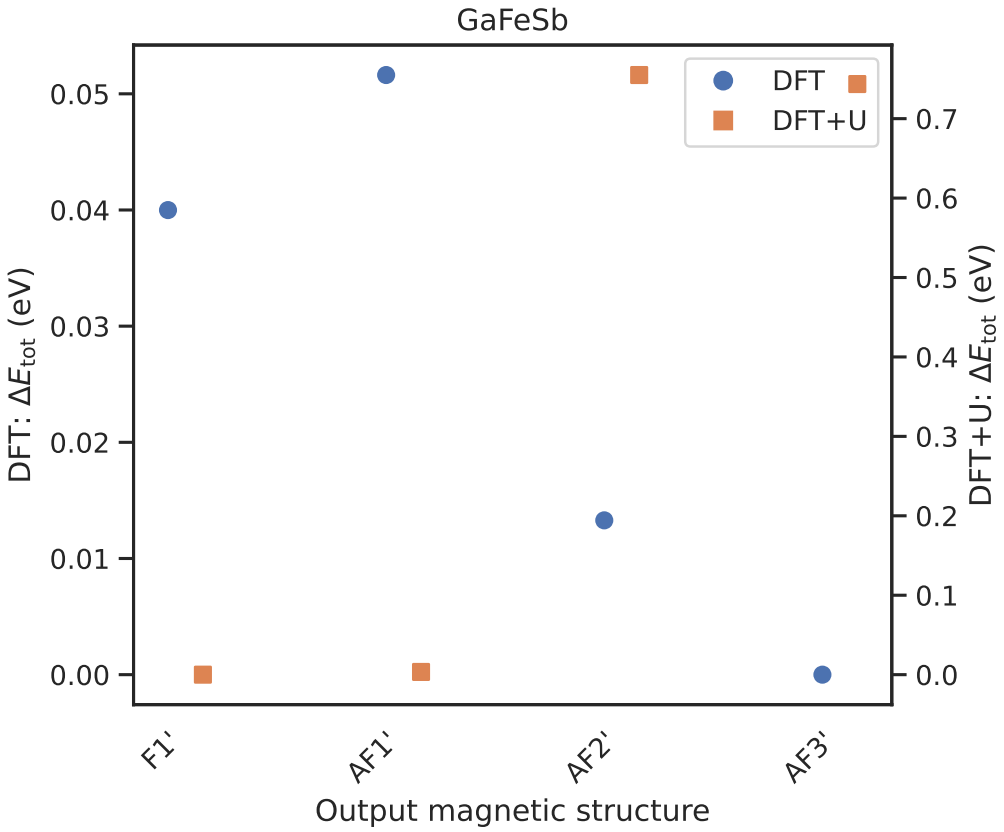


Figure 212: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1′	-31337.871886	0.000000	0.04, 0.04, 3.26, 3.26, 0.04, 0.04, 3.26, 3.26
AF1′	-31337.868455	0.003430	0.00, 0.00, 3.30, 3.30, 0.00, 0.00, -3.30, -3.30
AF3′	-31337.128319	0.743566	-0.02, -0.02, -3.33, 3.33, 0.02, 0.02, 3.33, -3.33
AF2′	-31337.116960	0.754925	0.00, 0.00, -3.33, 3.33, 0.00, 0.00, -3.33, 3.33

Table 217: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

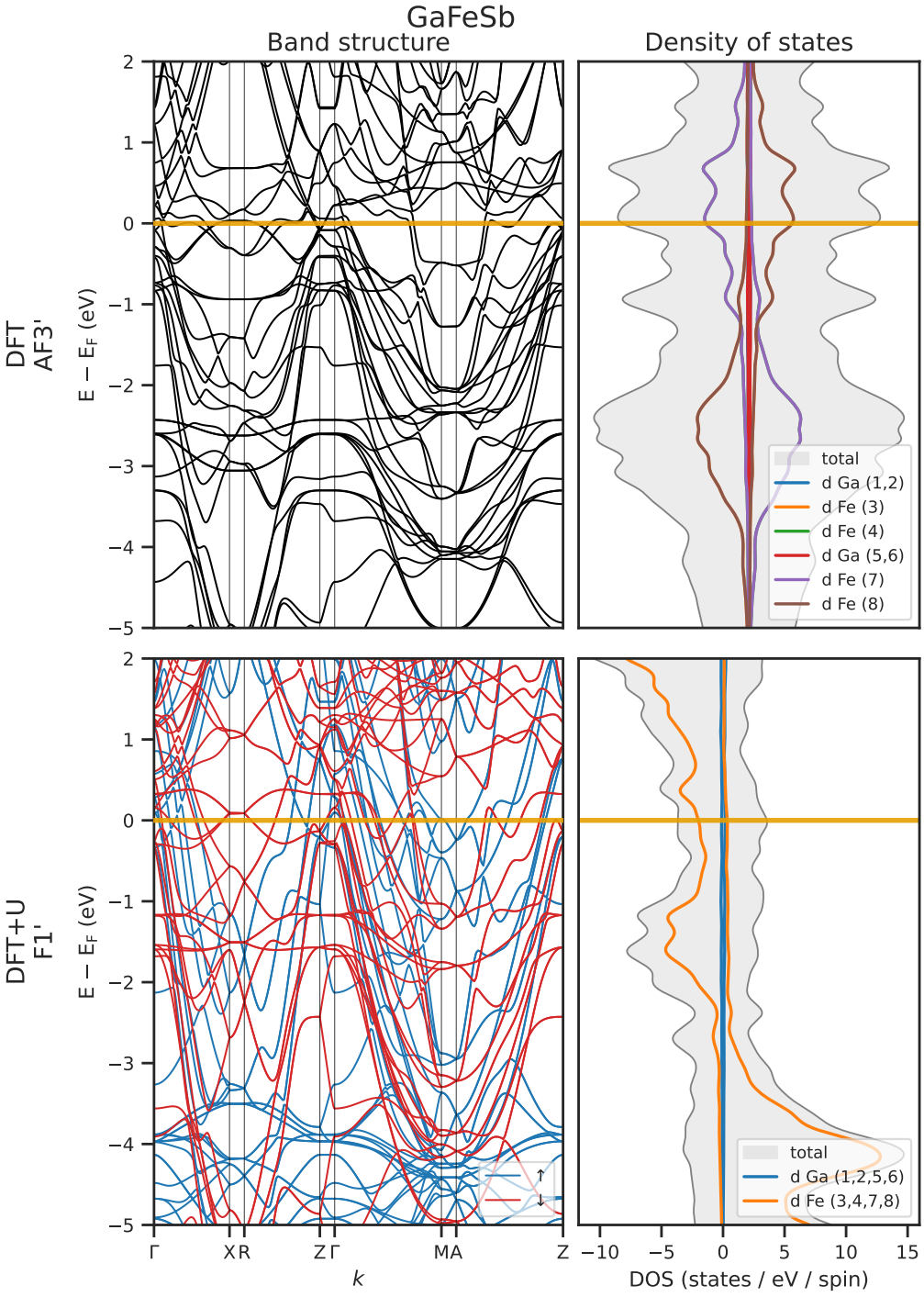


Figure 213: Band structure and Density of states of the lowest in energy calculations.

Material: FeMnAs

Configuration: FeMnAs ■ lower-energy

Structure

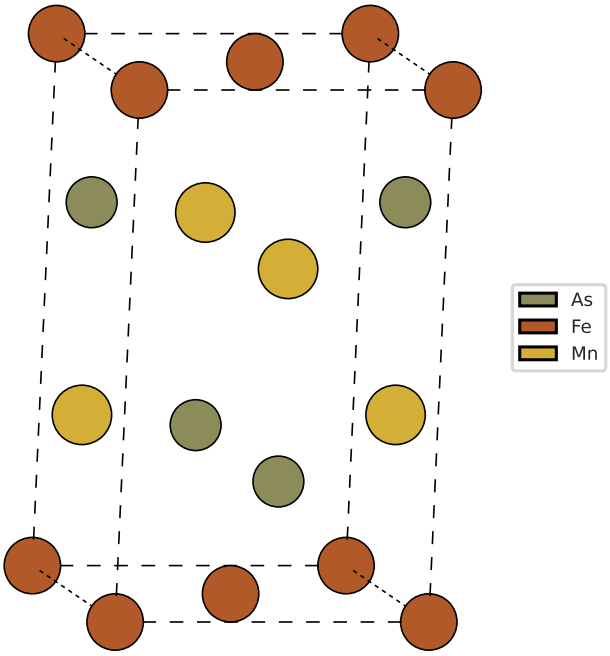


Figure 214: Structure of FeMnAs

a (Å)	c (Å)	z_1	z_2
3.7734	5.8402	0.3264	0.2506

Table 218: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-36526.806608	0.000000	-0.12, -0.12, 3.79, -3.79, 0.12, 0.12, -3.79, 3.79
AF2′	-36526.483512	0.323095	0.00, 0.00, -3.79, 3.79, 0.00, 0.00, -3.79, 3.79
Fi1	-36526.266793	0.539814	-1.55, -1.55, 3.78, 3.78, -1.55, -1.55, 3.78, 3.78
AF1′	-36525.978736	0.827872	0.00, 0.00, 3.66, 3.66, 0.00, 0.00, -3.66, -3.66
AF1′	-36525.978629	0.827978	-0.00, 0.00, 3.66, 3.66, 0.00, -0.00, -3.66, -3.66

Table 219: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

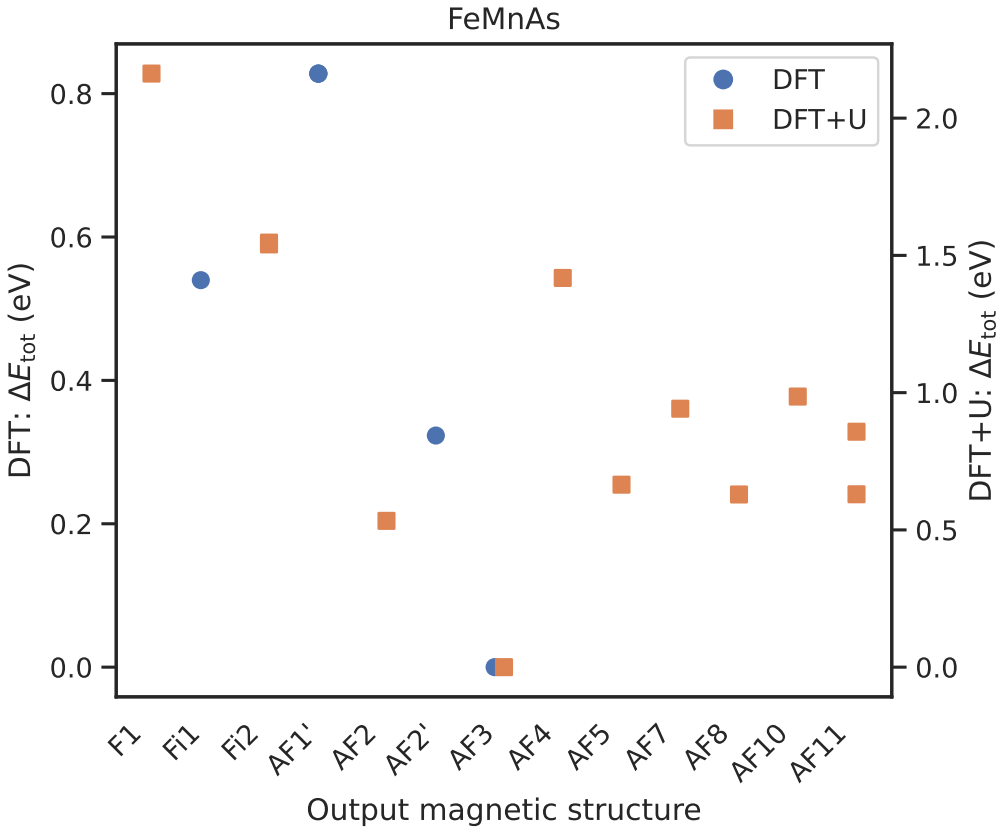


Figure 215: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-36511.981605	0.000000	2.81, 2.81, -4.72, 4.72, -2.81, -2.81, 4.72, -4.72
AF2	-36511.448645	0.532960	2.79, 2.79, -4.69, 4.69, -2.79, -2.79, -4.61, 4.61
AF8	-36511.352545	0.629060	2.67, -2.67, -4.63, 4.63, -2.67, 2.67, -4.63, 4.63
AF11	-36511.351801	0.629804	-2.67, 2.67, -4.63, 4.63, 2.67, -2.67, -4.63, 4.63
AF5	-36511.316836	0.664769	2.67, -2.67, -4.63, 4.63, 2.67, -2.67, -4.63, 4.63
AF11	-36511.123905	0.857700	2.68, 2.68, 4.55, 4.69, -2.68, -2.68, -4.55, -4.69
AF7	-36511.040045	0.941560	2.70, -2.70, 4.60, 4.60, 2.70, -2.70, -4.60, -4.60
AF10	-36510.995820	0.985785	2.70, -2.70, 4.56, 4.56, -2.70, 2.70, -4.56, -4.56
AF4	-36510.563739	1.417866	2.72, 2.72, 4.59, -4.59, -2.72, -2.72, -4.59, 4.59
Fi2	-36510.441493	1.540112	2.80, -2.20, -4.58, 4.58, -2.68, 1.97, 4.58, -4.58
Fi2	-36510.435028	1.546577	2.81, -2.15, -4.59, 4.59, 1.82, -2.67, 4.59, -4.59
F1	-36509.819247	2.162358	2.66, 2.66, 4.56, 4.56, 2.66, 2.66, 4.56, 4.56

Table 220: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

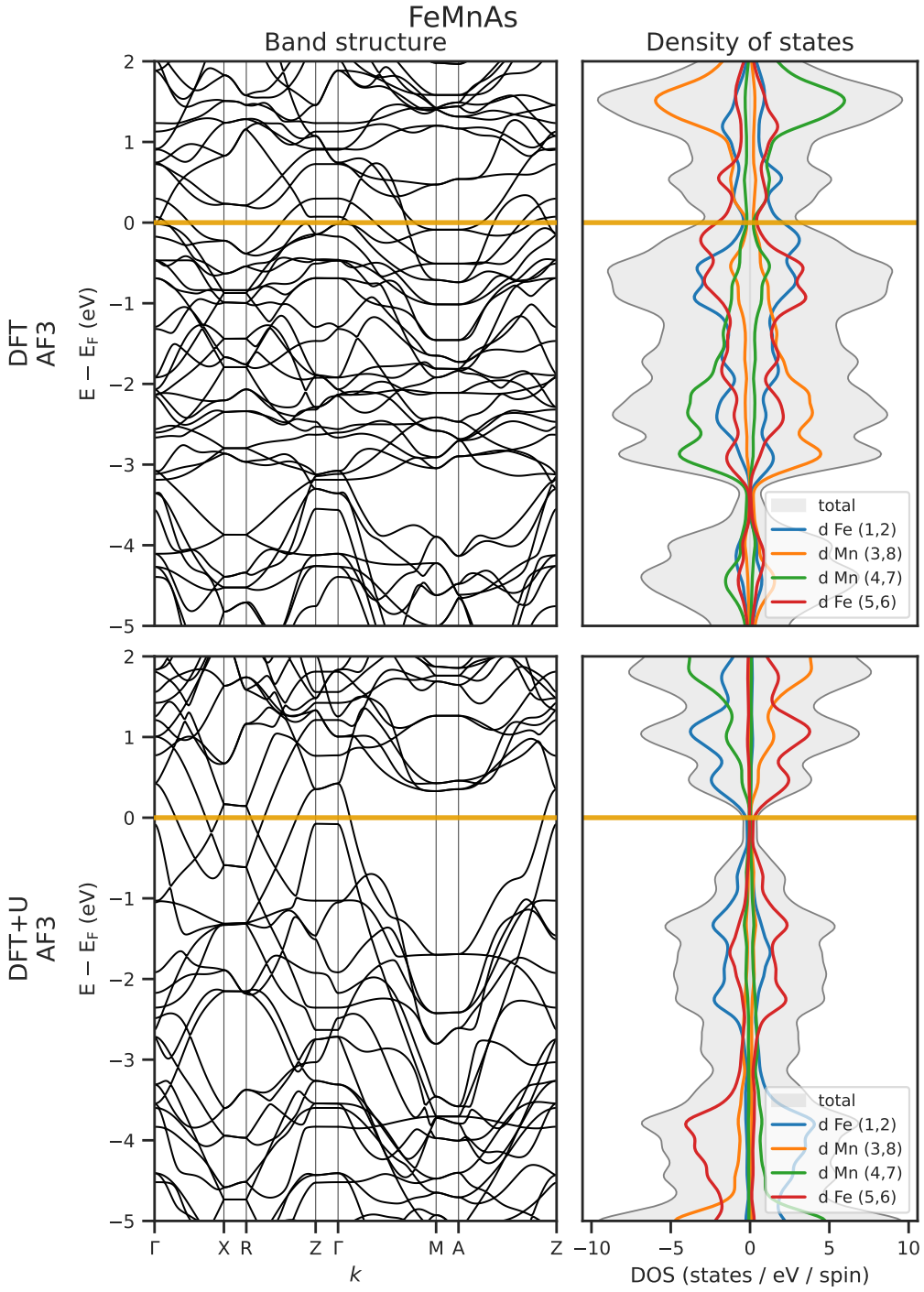


Figure 216: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnFeAs ■ higher-energy

Structure

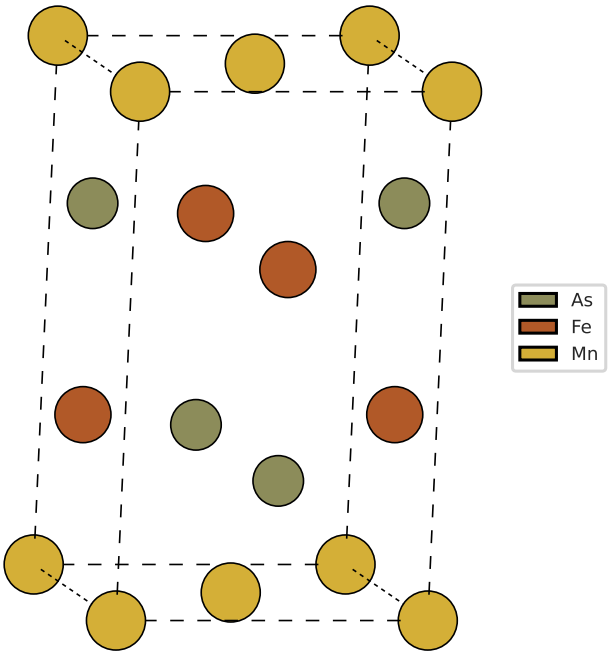


Figure 217: Structure of MnFeAs

a (Å)	c (Å)	z_1	z_2
3.7016	6.0122	0.3016	0.2862

Table 221: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

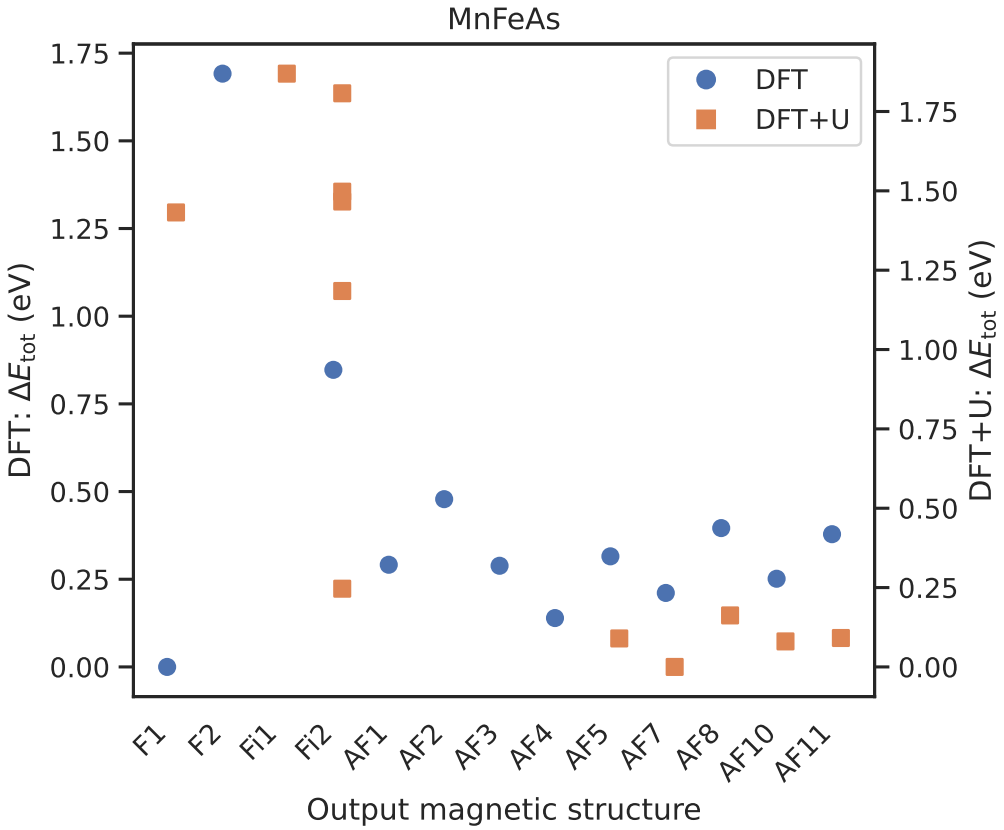


Figure 218: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-36524.960008	0.000000	2.22, 2.22, 2.44, 2.44, 2.22, 2.22, 2.44, 2.44
AF4	-36524.820662	0.139346	2.19, 2.19, 2.37, -2.37, -2.19, -2.19, -2.37, 2.37
AF7	-36524.749073	0.210935	2.60, -2.60, 2.55, 2.55, 2.60, -2.60, -2.55, -2.55
AF10	-36524.708584	0.251424	2.62, -2.62, 2.39, 2.39, -2.62, 2.62, -2.39, -2.39
AF3	-36524.671569	0.288439	1.64, 1.64, -2.77, 2.77, -1.64, -1.64, 2.77, -2.77
AF1	-36524.668679	0.291329	2.23, 2.23, 2.62, 2.58, -2.23, -2.23, -2.62, -2.58
AF5	-36524.644694	0.315314	2.52, -2.52, -2.40, 2.40, 2.53, -2.53, -2.40, 2.40
AF11	-36524.581553	0.378455	2.54, -0.99, -2.54, 2.54, -2.54, 1.01, 2.55, -2.55
AF8	-36524.564131	0.395877	2.29, -2.29, -2.40, 2.40, -2.29, 2.29, -2.40, 2.40
AF2	-36524.481669	0.478339	2.18, 2.18, -2.59, 2.59, -2.19, -2.19, -2.59, 2.58
Fi2	-36524.112936	0.847072	0.48, -2.60, -2.48, 0.07, 0.09, -2.79, -2.55, -2.61
F2	-36523.268409	1.691598	0.25, 0.25, -0.03, -0.04, 0.12, 0.12, 0.04, 2.49

Table 222: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF7	-36508.925721	0.000000	4.25, -4.25, 2.98, 2.98, 4.25, -4.25, -2.98, -2.98
AF10	-36508.845319	0.080402	4.25, -4.25, 2.99, 2.99, -4.25, 4.25, -2.99, -2.99
AF5	-36508.835963	0.089758	4.25, -4.25, -2.93, 2.93, 4.25, -4.25, -2.93, 2.93
AF11	-36508.834575	0.091146	4.31, -4.21, -2.92, 2.92, -4.31, 4.21, 2.92, -2.92
AF8	-36508.763437	0.162284	4.26, -4.26, -2.96, 2.96, -4.26, 4.26, -2.96, 2.96
Fi2	-36508.679233	0.246488	4.24, -4.27, -3.09, 2.88, 4.19, -4.33, 2.86, -2.92
Fi2	-36507.741253	1.184468	4.15, 4.15, -3.02, 3.30, -4.13, -4.13, -2.95, 2.91
F1	-36507.493732	1.431989	3.91, 3.91, 2.88, 2.89, 3.91, 3.91, 2.89, 2.88
Fi2	-36507.459319	1.466402	4.30, 4.29, -3.04, 3.00, -4.24, -4.26, 3.34, -2.92
Fi2	-36507.428294	1.497427	4.00, 4.00, 3.05, 3.21, -4.13, -4.13, -3.04, -3.40
Fi2	-36507.118353	1.807368	3.91, 3.91, 2.98, -2.86, -3.92, -3.92, -2.90, 2.93
Fi1	-36507.056451	1.869270	4.05, 4.05, -3.29, -3.29, 4.05, 4.05, -3.29, -3.29

Table 223: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

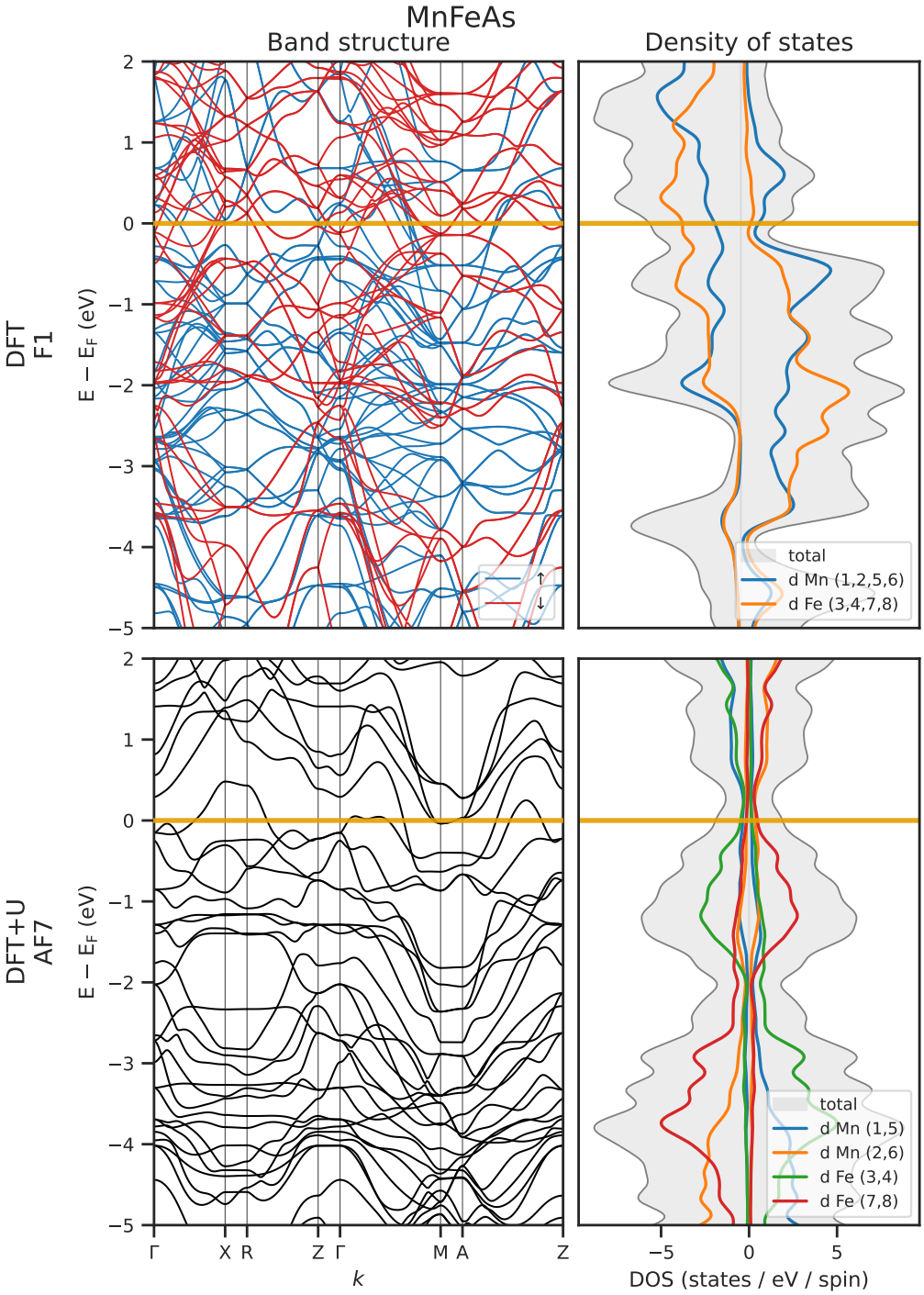


Figure 219: Band structure and Density of states of the lowest in energy calculations.

Material: FeMnSb

Configuration: FeMnSb ■ lower-energy

Structure

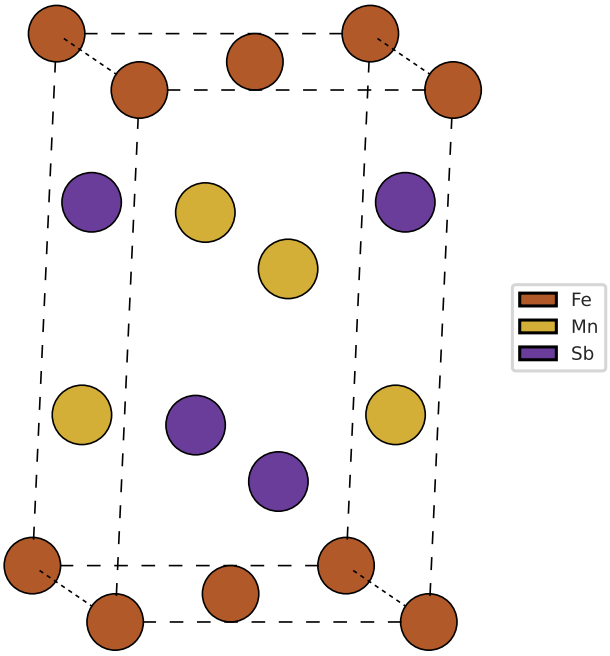


Figure 220: Structure of FeMnSb

a (Å)	c (Å)	z_1	z_2
4.0518	6.1251	0.2566	0.2800

Table 224: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-34411.301357	0.000000	0.52, 0.52, 3.78, 3.78, 0.52, 0.52, 3.78, 3.78
AF4	-34411.236956	0.064401	-0.32, -0.32, -3.77, 3.77, 0.32, 0.32, 3.77, -3.77
AF2′	-34411.155933	0.145424	0.00, 0.00, -3.88, 3.88, 0.00, 0.00, -3.88, 3.88
AF1′	-34411.153788	0.147569	0.00, 0.00, 3.92, 3.92, 0.00, 0.00, -3.92, -3.92
Fi1	-34410.950808	0.350549	1.20, 1.20, -3.96, -3.96, 1.20, 1.20, -3.96, -3.96

Table 225: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

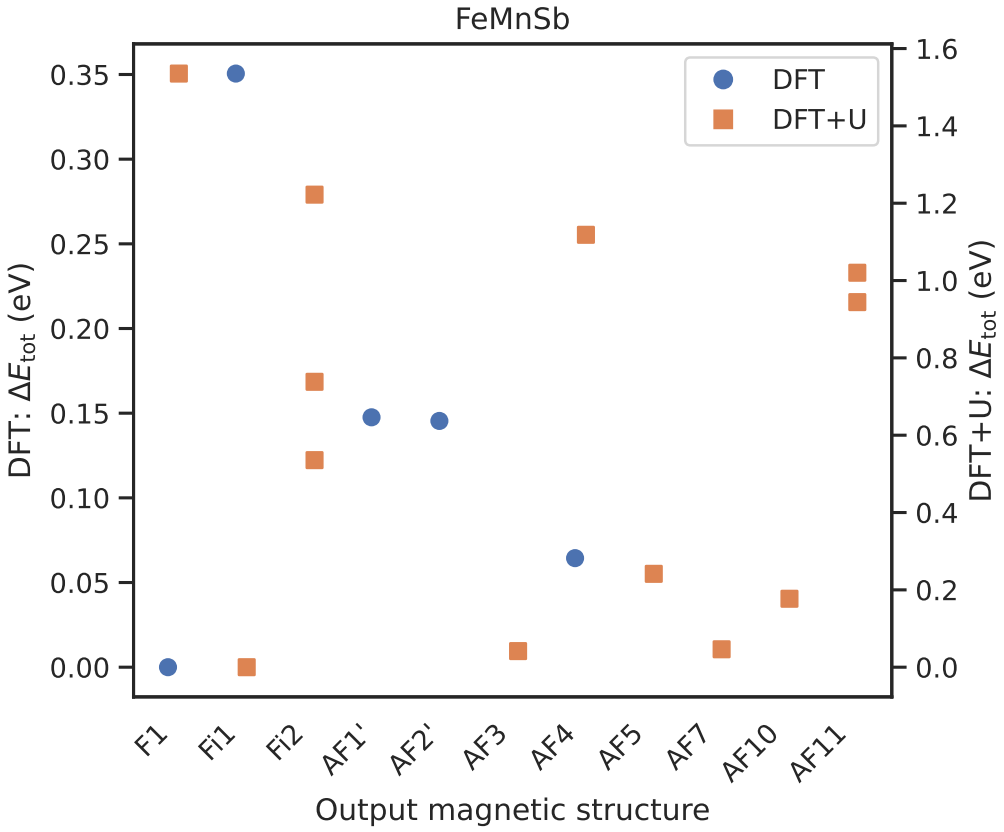


Figure 221: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-34397.336558	0.000000	2.89, 2.89, -4.84, -4.84, 2.89, 2.89, -4.84, -4.84
AF3	-34397.294920	0.041638	2.93, 2.93, -4.78, 4.78, -2.93, -2.93, 4.78, -4.78
AF7	-34397.290227	0.046331	2.75, -2.75, 4.65, 4.65, 2.75, -2.75, -4.65, -4.65
AF10	-34397.159531	0.177027	2.75, -2.75, 4.65, 4.65, -2.75, 2.75, -4.65, -4.65
AF5	-34397.095090	0.241468	2.75, -2.75, -4.64, 4.64, 2.75, -2.75, -4.64, 4.64
Fi2	-34396.801024	0.535534	2.63, 2.63, 4.52, 4.82, -2.81, -2.81, -4.53, -4.81
Fi2	-34396.598449	0.738109	2.79, 2.79, -4.80, 4.80, -2.63, -2.63, -4.51, 4.53
AF11	-34396.392352	0.944205	2.76, -2.58, -4.60, 4.60, 2.58, -2.76, 4.60, -4.60
AF11	-34396.316356	1.020202	2.74, -2.58, -4.60, 4.60, -2.74, 2.58, 4.60, -4.60
AF4	-34396.218245	1.118313	2.65, 2.65, 4.50, -4.50, -2.65, -2.65, -4.50, 4.50
Fi2	-34396.114400	1.222158	2.88, 2.88, -4.85, -4.74, 0.76, 0.76, -4.74, -4.85
F1	-34395.801252	1.535306	2.81, 2.81, 4.52, 4.52, 2.81, 2.81, 4.52, 4.52

Table 226: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

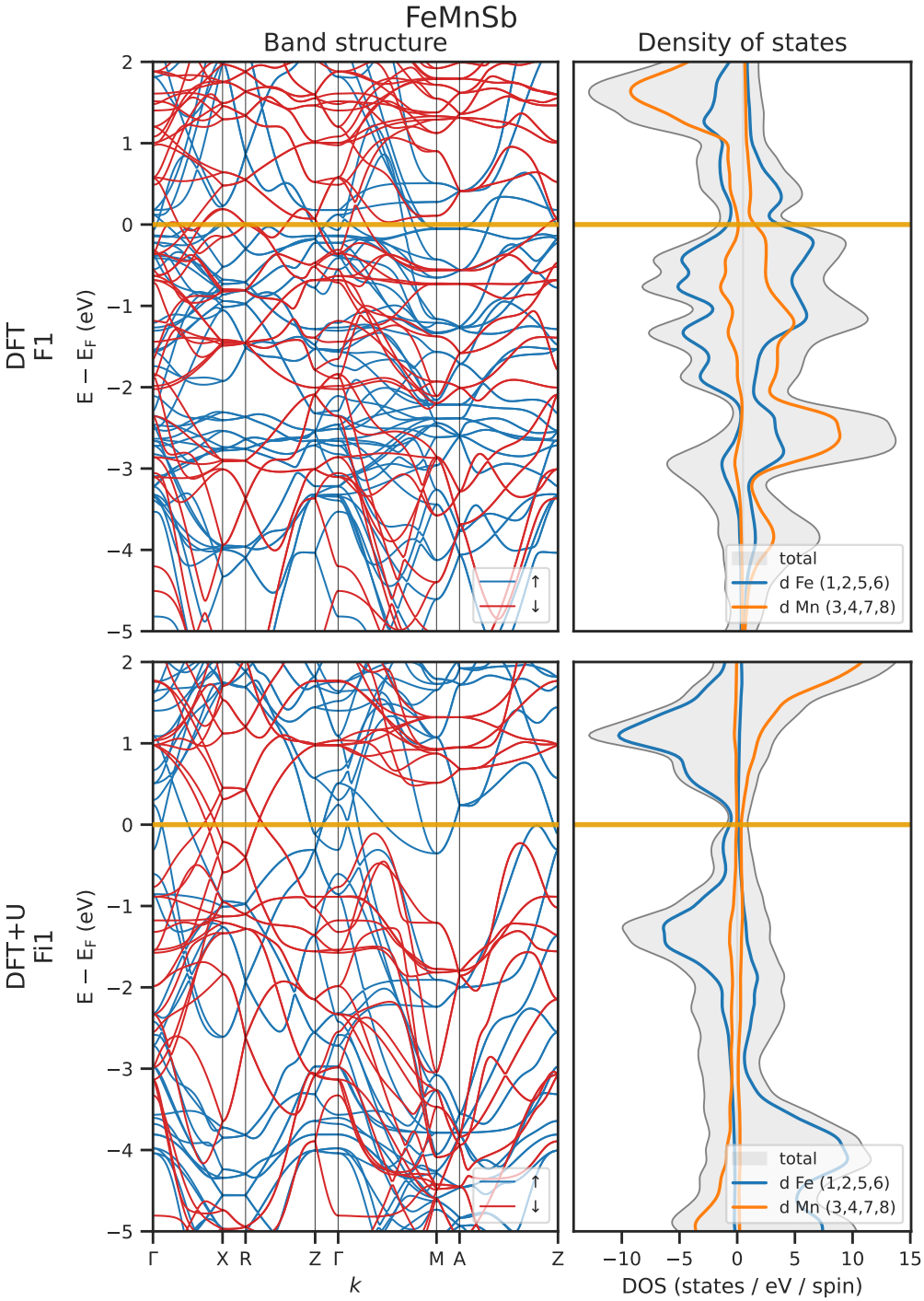


Figure 222: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnFeSb ■ higher-energy

Structure

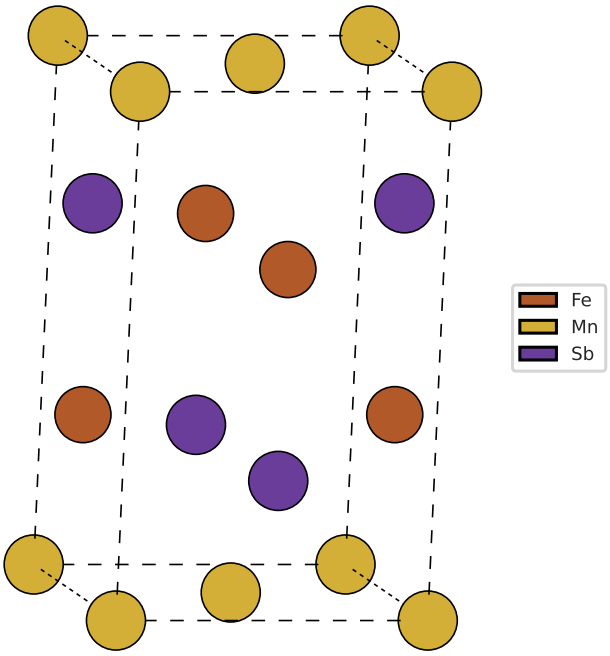


Figure 223: Structure of MnFeSb

a (Å)	c (Å)	z_1	z_2
3.8876	6.4134	0.2560	0.3133

Table 227: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

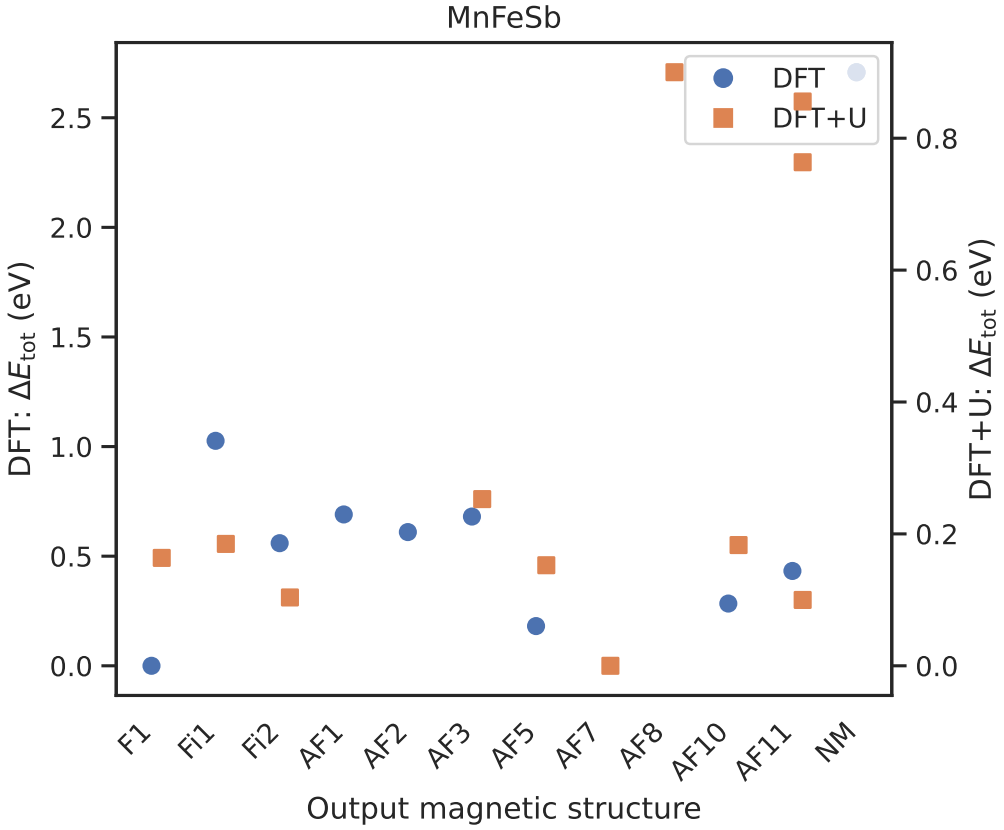


Figure 224: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
F1	-34410.396659	0.000000	2.65, 2.65, 2.19, 2.18, 2.65, 2.65, 2.18, 2.19
AF5	-34410.215477	0.181183	2.82, -2.82, -2.30, 2.30, 2.82, -2.82, -2.30, 2.30
AF10	-34410.112754	0.283905	2.87, -2.87, 2.32, 2.32, -2.87, 2.87, -2.32, -2.32
AF11	-34409.964071	0.432589	3.05, -2.62, -2.31, 2.31, -3.06, 2.62, 2.31, -2.31
Fi2	-34409.837312	0.559347	2.85, -2.82, -2.31, -0.13, -2.83, 3.15, -2.25, 2.32
AF2	-34409.786679	0.609980	2.90, 2.90, -2.32, 2.32, -2.90, -2.90, -2.26, 2.26
AF3	-34409.715834	0.680825	1.98, 1.98, -2.73, 2.73, -1.98, -1.98, 2.73, -2.73
AF1	-34409.706252	0.690407	2.91, 2.91, 2.28, 2.30, -2.91, -2.91, -2.28, -2.30
Fi1	-34409.370407	1.026252	1.89, 1.89, -2.70, -2.70, 1.89, 1.89, -2.70, -2.70
NM	-34407.689289	2.707371	0.00, 0.00, 0.00, 0.00, -0.00, 0.00, 0.00, 0.00
NM	-34407.688906	2.707753	0.00, 0.00, 0.00, 0.00, 0.00, -0.00, 0.00, 0.00

Table 228: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF7	-34395.033585	0.000000	4.43, -4.43, 2.85, 2.85, 4.43, -4.43, -2.85, -2.85
AF11	-34394.933740	0.099844	4.28, 4.28, -2.99, 2.99, -4.28, -4.28, -2.84, 2.84
Fi2	-34394.929955	0.103630	-4.31, 4.55, -2.81, -2.83, -4.29, -4.29, 2.95, -2.81
AF5	-34394.881092	0.152493	4.42, -4.42, -2.85, 2.85, 4.42, -4.42, -2.85, 2.85
F1	-34394.869966	0.163619	4.14, 4.14, 2.77, 2.77, 4.14, 4.14, 2.77, 2.77
AF10	-34394.850510	0.183075	4.43, -4.43, 2.86, 2.86, -4.43, 4.43, -2.86, -2.86
Fi1	-34394.848763	0.184822	4.40, 4.40, -3.01, -3.01, 4.40, 4.40, -3.01, -3.01
AF3	-34394.780808	0.252776	4.42, 4.42, -2.89, 2.89, -4.42, -4.42, 2.89, -2.89
AF11	-34394.270007	0.763578	4.60, -4.26, -2.90, 2.90, -4.60, 4.26, 2.97, -2.97
AF11	-34394.177894	0.855690	4.21, 4.21, 2.72, 2.92, -4.21, -4.21, -2.72, -2.92
AF8	-34394.133489	0.900096	4.39, -4.39, -3.03, 3.03, -4.39, 4.39, -3.03, 3.03

Table 229: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

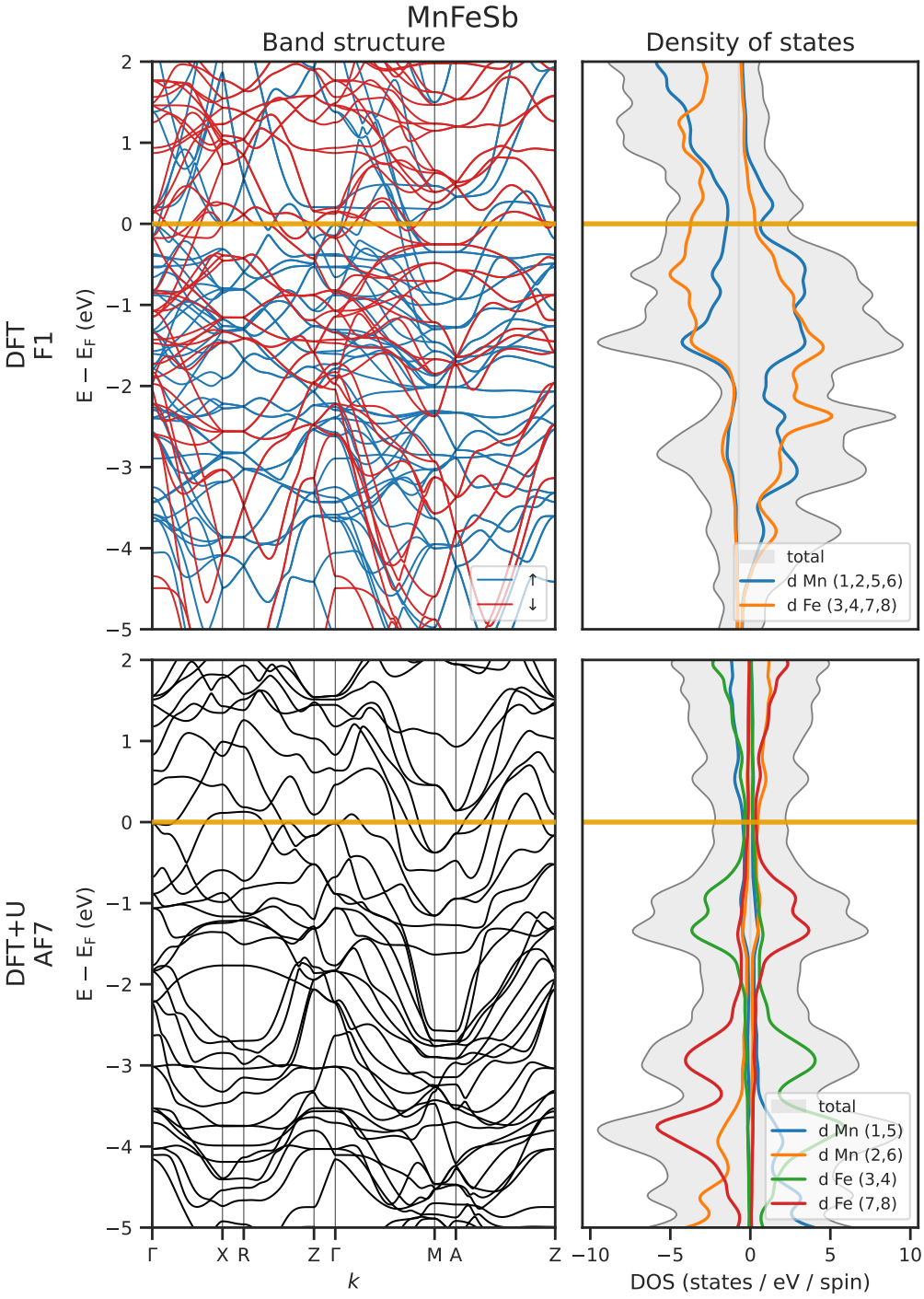


Figure 225: Band structure and Density of states of the lowest in energy calculations.

Material: FeNiAs

Configuration: FeNiAs ■ lower-energy

Structure

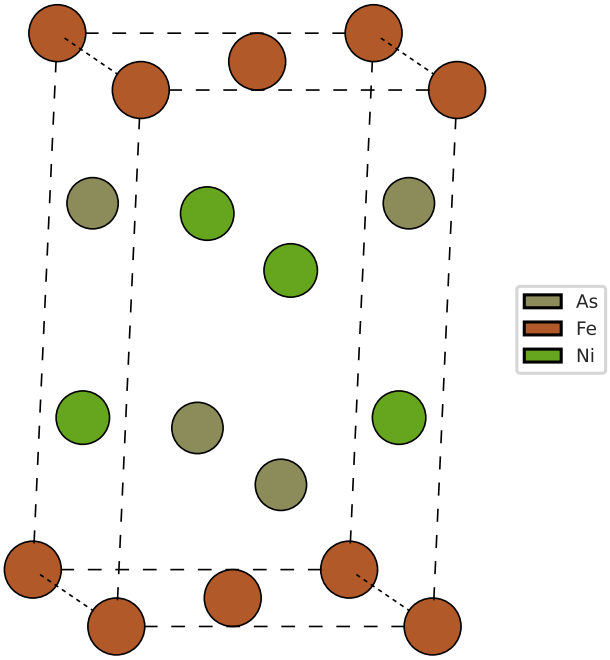


Figure 226: Structure of FeNiAs

a (Å)	c (Å)	z_1	z_2
3.6593	5.8840	0.3128	0.2828

Table 230: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1″	-43357.953838	0.000000	1.83, 1.83, 0.06, -0.06, -1.83, -1.83, -0.06, 0.06
F1″	-43357.902181	0.051657	1.89, 1.89, 0.02, 0.02, 1.88, 1.88, 0.02, 0.02
AF5″	-43357.222761	0.731077	2.09, -2.09, 0.00, 0.00, 2.09, -2.09, 0.00, 0.00
AF8″	-43357.086206	0.867632	1.85, -1.85, 0.00, 0.00, -1.84, 1.84, 0.00, 0.00
AF11″	-43357.028056	0.925782	0.09, -0.09, 0.00, 0.00, 2.07, -2.07, 0.00, 0.00

Table 231: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

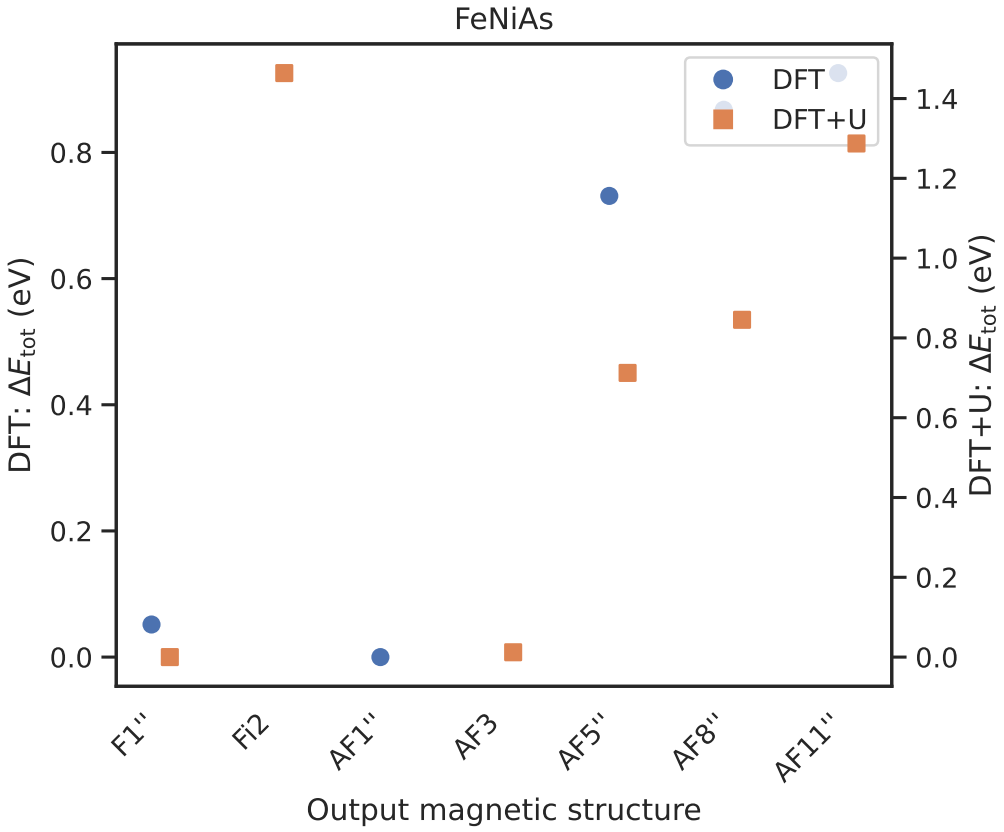


Figure 227: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
F1″	-43341.994703	0.000000	2.94, 2.94, -0.03, -0.02, 2.95, 2.95, -0.02, -0.03
F1″	-43341.994701	0.000001	2.94, 2.94, -0.03, -0.02, 2.95, 2.95, -0.02, -0.03
AF3	-43341.982622	0.012080	2.88, 2.88, -0.13, 0.13, -2.88, -2.88, 0.13, -0.13
AF3	-43341.982621	0.012081	2.88, 2.88, -0.13, 0.13, -2.88, -2.88, 0.13, -0.13
AF3	-43341.982620	0.012082	2.88, 2.88, -0.13, 0.13, -2.88, -2.88, 0.13, -0.13
AF3	-43341.982608	0.012095	2.88, 2.88, -0.13, 0.13, -2.88, -2.88, 0.13, -0.13
AF5″	-43341.282398	0.712305	3.10, -3.10, 0.00, 0.00, 3.10, -3.10, 0.00, 0.00
AF5″	-43341.282398	0.712305	3.10, -3.10, 0.00, 0.00, 3.10, -3.10, 0.00, 0.00
AF8″	-43341.149283	0.845419	3.09, -3.09, 0.00, 0.00, -3.09, 3.09, 0.00, 0.00
AF8″	-43341.149282	0.845420	3.09, -3.09, 0.00, 0.00, -3.09, 3.09, 0.00, 0.00
AF11″	-43340.707311	1.287391	2.96, -2.96, 0.00, 0.00, -3.08, 3.08, 0.00, 0.00
Fi2	-43340.530879	1.463824	3.12, -3.07, -0.01, 0.27, 3.03, -1.05, 0.27, -0.01

Table 232: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

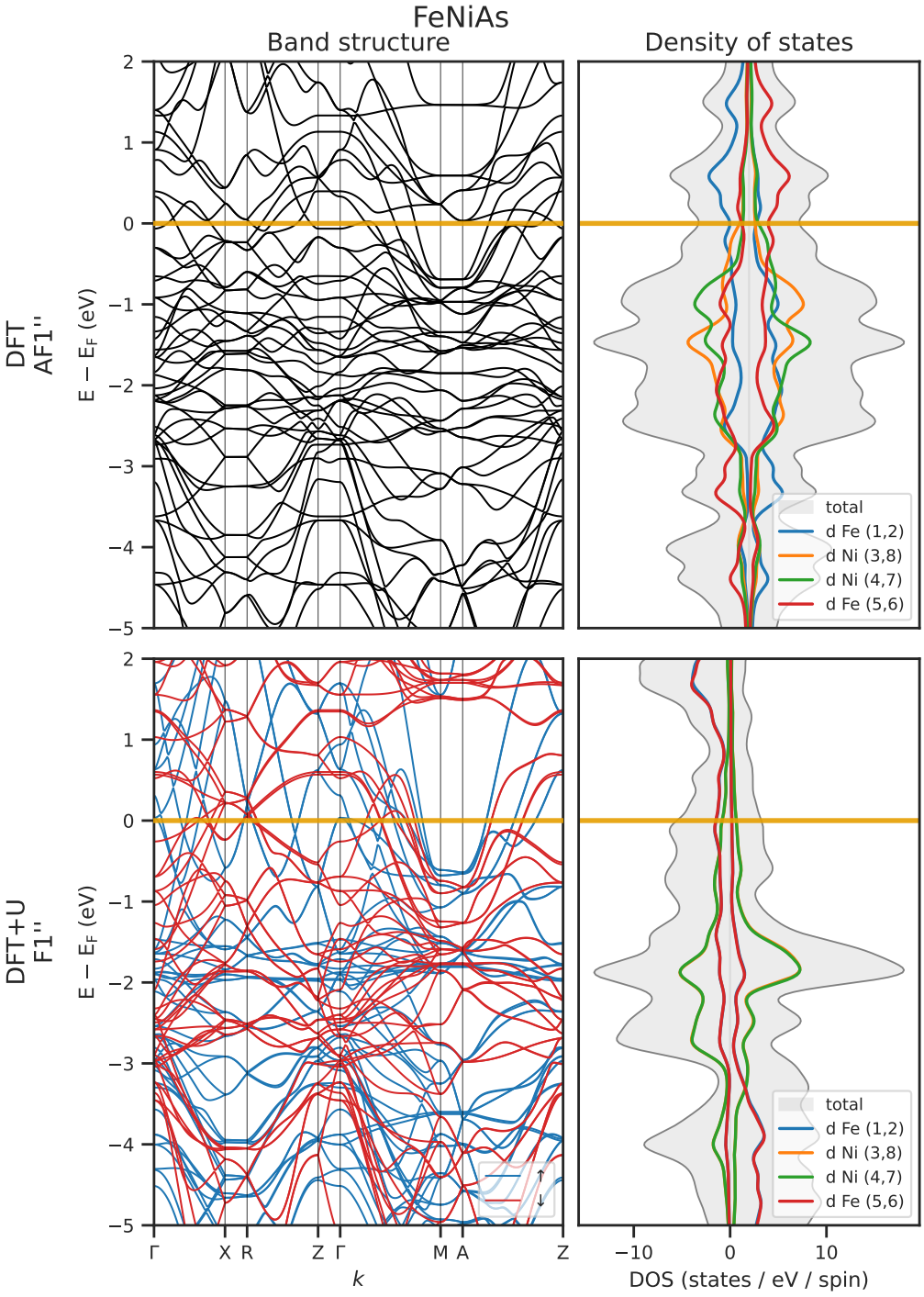


Figure 228: Band structure and Density of states of the lowest in energy calculations.

Configuration: NiFeAs ■ higher-energy

Structure

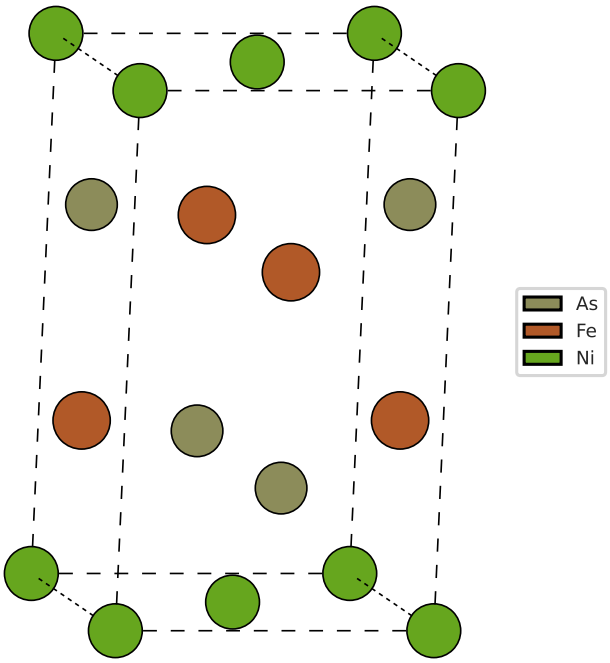


Figure 229: Structure of NiFeAs

a (Å)	c (Å)	z_1	z_2
3.5822	6.1204	0.3520	0.2634

Table 233: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-43357.621418	0.000000	0.00, 0.00, -2.52, 2.52, 0.00, 0.00, -2.52, 2.52
AF3′	-43357.383178	0.238241	0.08, 0.08, -2.38, 2.38, -0.08, -0.08, 2.38, -2.38
AF1′	-43357.255401	0.366018	0.00, 0.00, 2.41, 2.41, 0.00, 0.00, -2.41, -2.41
F1′	-43357.122659	0.498759	-0.08, -0.08, 2.35, 2.35, -0.08, -0.08, 2.35, 2.35

Table 234: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

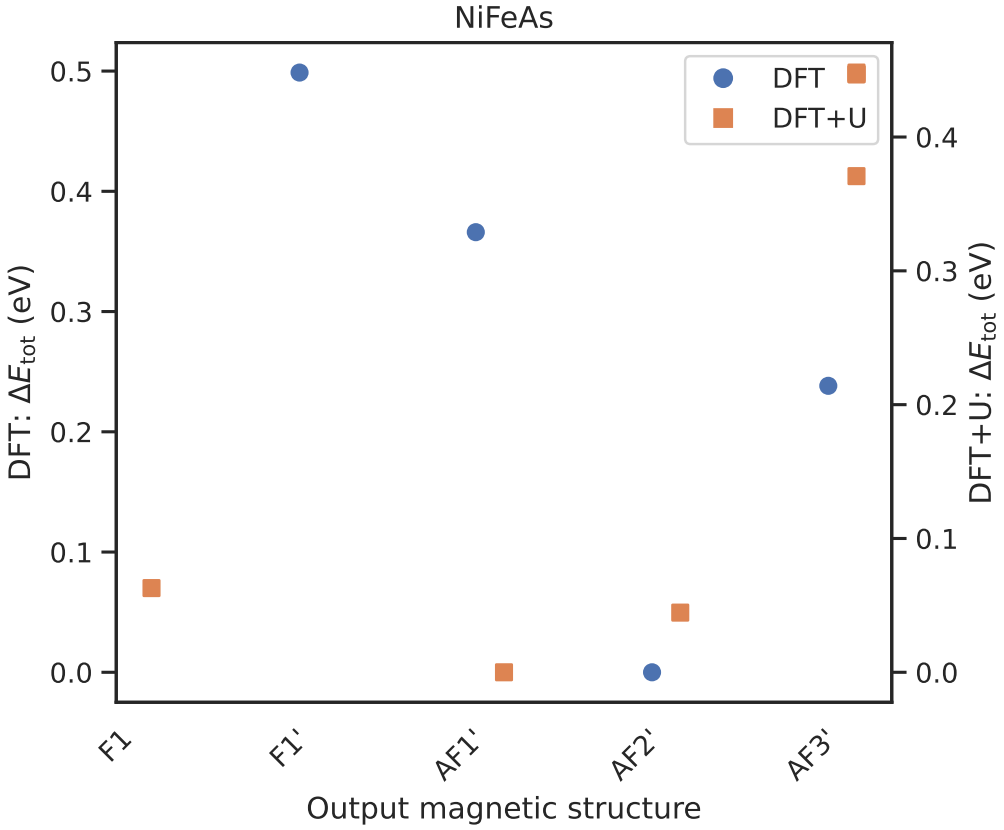


Figure 230: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF1′	-43342.217562	0.000000	0.00, 0.00, 3.22, 3.22, 0.00, 0.00, -3.22, -3.22
AF1′	-43342.217561	0.000001	0.00, 0.00, 3.22, 3.22, 0.00, 0.00, -3.22, -3.22
AF1′	-43342.217561	0.000001	0.00, 0.00, 3.22, 3.22, 0.00, 0.00, -3.22, -3.22
AF2′	-43342.172962	0.044600	0.00, 0.00, -3.16, 3.16, 0.00, 0.00, -3.16, 3.16
AF2′	-43342.172962	0.044600	0.00, 0.00, -3.16, 3.16, 0.00, 0.00, -3.16, 3.16
AF2′	-43342.172961	0.044601	0.00, 0.00, -3.16, 3.16, 0.00, 0.00, -3.16, 3.16
F1	-43342.154634	0.062928	-0.12, -0.12, -3.21, -3.21, -0.12, -0.12, -3.21, -3.21
AF3′	-43341.846790	0.370772	0.02, 0.05, -3.16, 3.16, -0.02, -0.05, 3.16, -3.16
AF3′	-43341.770671	0.446891	-0.08, -0.08, 3.17, -3.20, 0.08, 0.08, -3.17, 3.20
AF3′	-43341.770643	0.446919	0.08, 0.08, -3.20, 3.17, -0.08, -0.08, 3.20, -3.17
AF3′	-43341.769391	0.448171	0.06, 0.06, -3.20, 3.20, -0.06, -0.06, 3.18, -3.19

Table 235: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

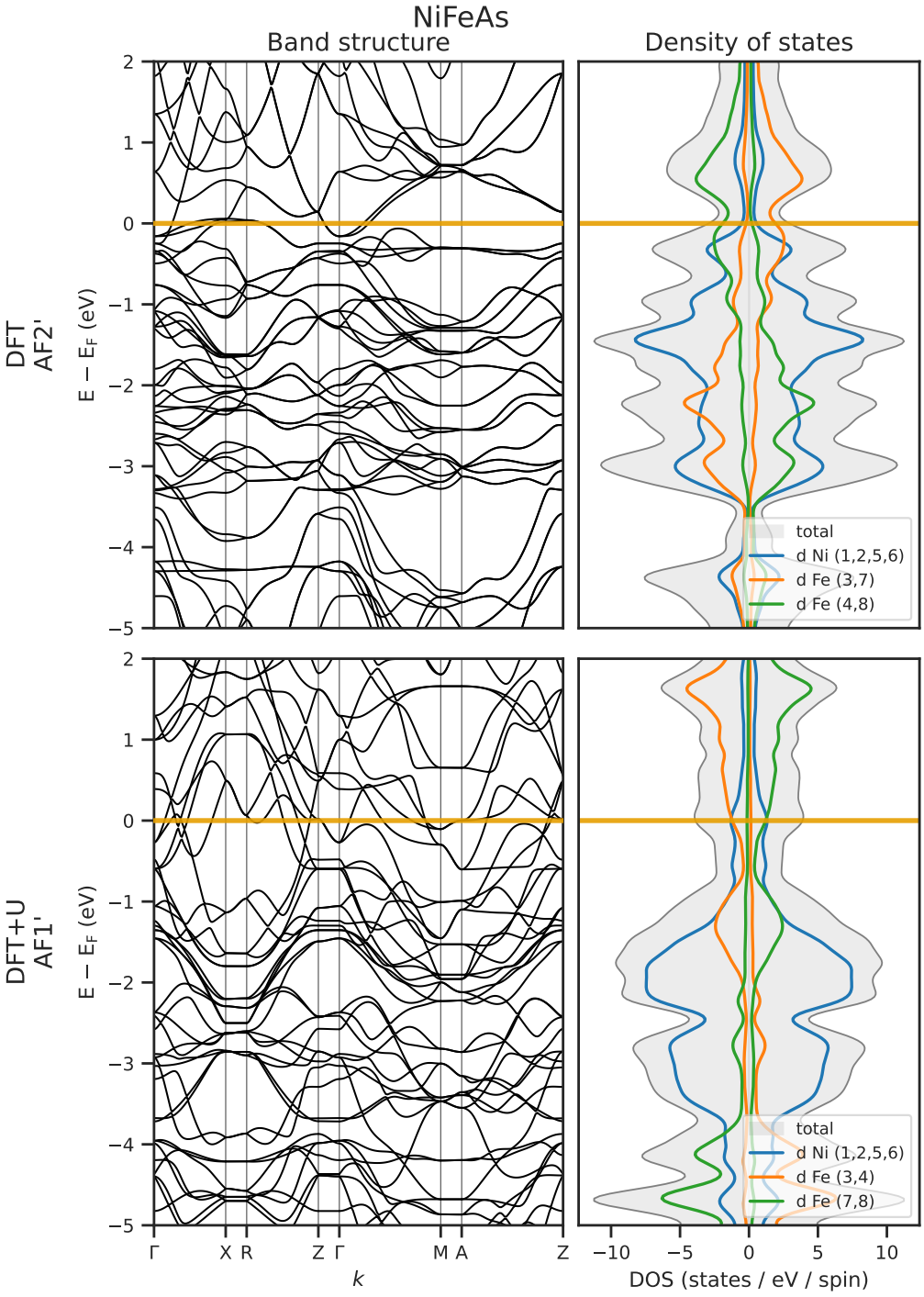


Figure 231: Band structure and Density of states of the lowest in energy calculations.

Material: FeNiSb

Configuration: FeNiSb ■ lower-energy

Structure

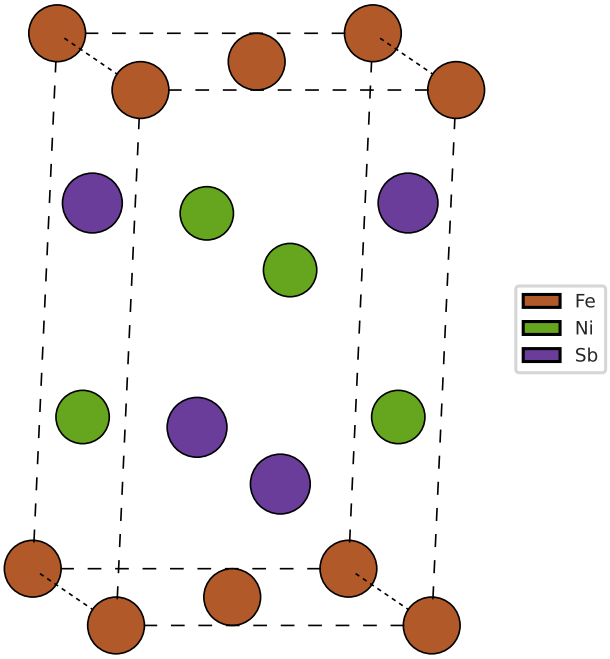


Figure 232: Structure of FeNiSb

a (Å)	c (Å)	z_1	z_2
3.8438	6.2041	0.2633	0.3091

Table 236: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Fe atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-41244.099643	0.000000	2.51, 2.51, 0.21, 0.21, 2.51, 2.51, 0.21, 0.21
AF4	-41244.067992	0.031652	2.51, 2.51, 0.19, -0.19, -2.51, -2.51, -0.19, 0.19
AF5″	-41243.512577	0.587066	2.41, -2.41, 0.00, 0.00, 2.41, -2.41, 0.00, 0.00
AF8″	-41243.340909	0.758734	2.30, -2.30, 0.00, 0.00, -2.30, 2.30, 0.00, 0.00
AF11″	-41242.955412	1.144231	0.05, -0.05, 0.00, 0.00, 2.41, -2.41, 0.00, 0.00

Table 237: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

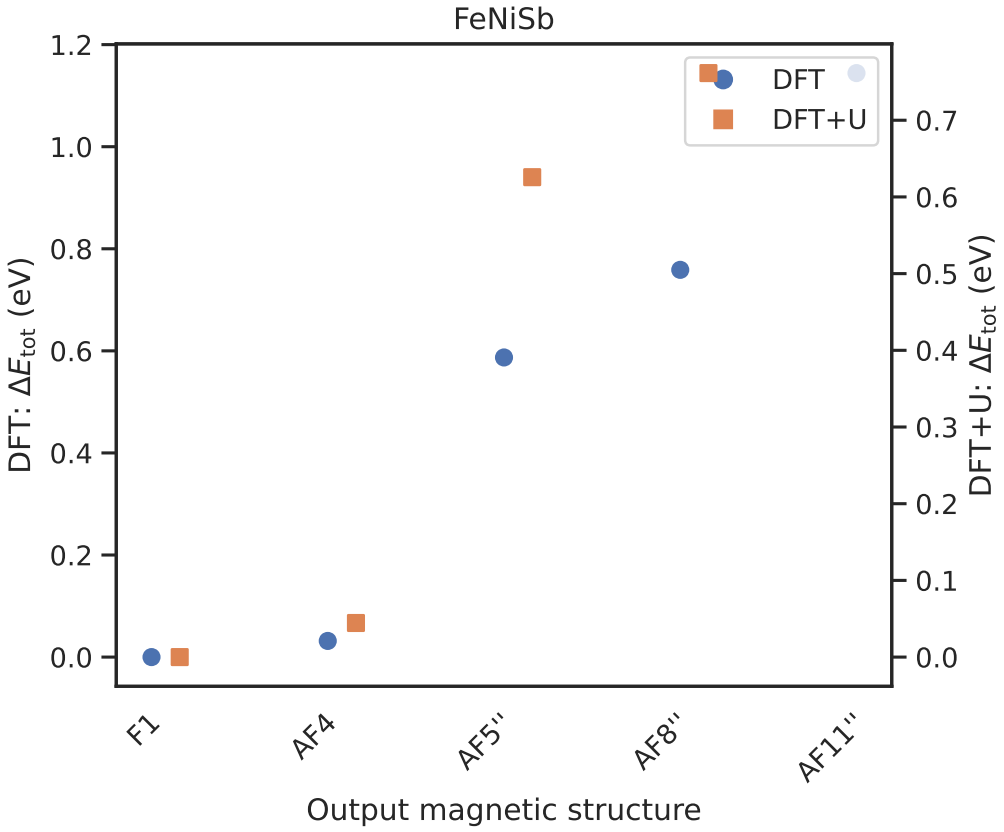


Figure 233: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
F1	-41229.169871	0.000000	3.16, 3.16, 0.30, 0.30, 3.16, 3.16, 0.30, 0.30
F1	-41229.169870	0.000001	-3.16, -3.16, -0.30, -0.30, -3.16, -3.16, -0.30, -0.30
F1	-41229.169868	0.000003	3.16, 3.16, 0.30, 0.30, 3.16, 3.16, 0.30, 0.30
AF4	-41229.125411	0.044460	3.17, 3.17, 0.28, -0.28, -3.17, -3.17, -0.28, 0.28
AF4	-41229.125410	0.044461	3.17, 3.17, 0.28, -0.28, -3.17, -3.17, -0.28, 0.28
AF4	-41229.125409	0.044462	3.17, 3.17, 0.28, -0.28, -3.17, -3.17, -0.28, 0.28
AF4	-41229.125404	0.044467	3.17, 3.17, 0.28, -0.28, -3.17, -3.17, -0.28, 0.28
AF5″	-41228.544110	0.625761	3.24, -3.24, 0.00, 0.00, 3.24, -3.24, 0.00, 0.00
AF5″	-41228.544109	0.625763	3.24, -3.24, 0.00, 0.00, 3.24, -3.24, 0.00, 0.00
AF5″	-41228.544107	0.625764	3.24, -3.24, 0.00, 0.00, 3.24, -3.24, 0.00, 0.00
AF8″	-41228.408392	0.761479	3.21, -3.21, 0.00, 0.00, -3.21, 3.21, 0.00, 0.00
AF8″	-41228.408392	0.761480	3.21, -3.21, 0.00, 0.00, -3.21, 3.21, 0.00, 0.00

Table 238: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

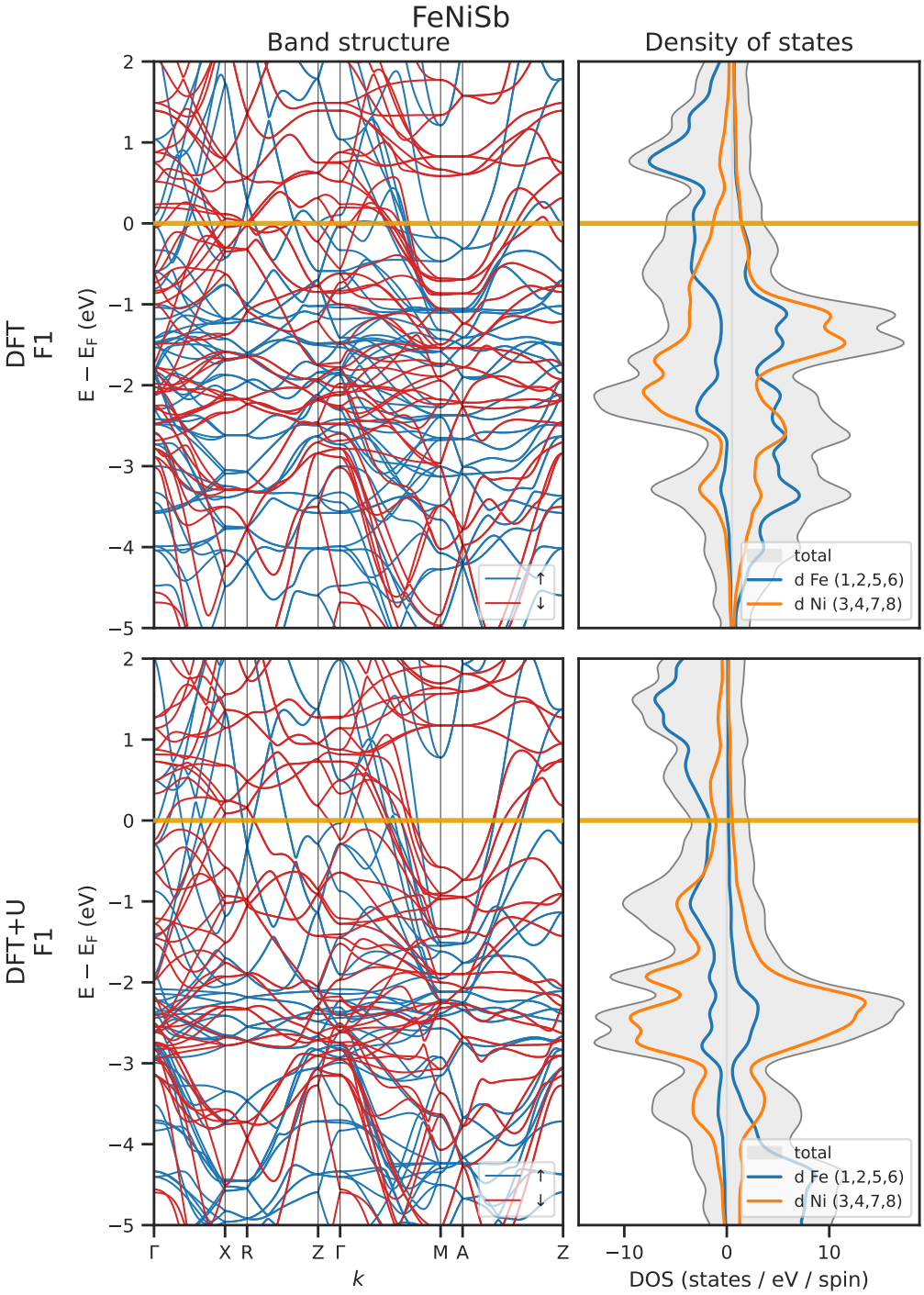


Figure 234: Band structure and Density of states of the lowest in energy calculations.

Configuration: NiFeSb ■ higher-energy

Structure

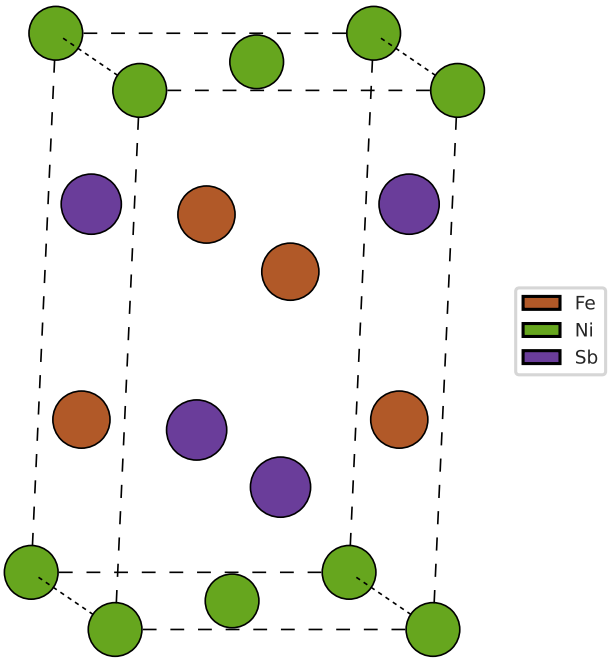


Figure 235: Structure of NiFeSb

a (Å)	c (Å)	z_1	z_2
4.0061	6.0253	0.2602	0.2890

Table 239: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of an Fe atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF4	-41242.780656	0.000000	-0.23, -0.23, -2.95, 2.95, 0.23, 0.23, 2.95, -2.95
AF2′	-41242.762261	0.018394	0.00, 0.00, -2.93, 2.93, 0.00, 0.00, -2.93, 2.93
AF1′	-41242.681915	0.098740	0.00, 0.00, 3.04, 3.04, 0.00, 0.00, -3.04, -3.04
F1	-41242.656145	0.124510	-0.29, -0.29, -3.00, -3.00, -0.29, -0.29, -3.00, -3.00
F2	-41241.456906	1.323750	-0.27, -0.27, -2.98, -0.01, -0.17, -0.17, -0.01, -2.98

Table 240: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

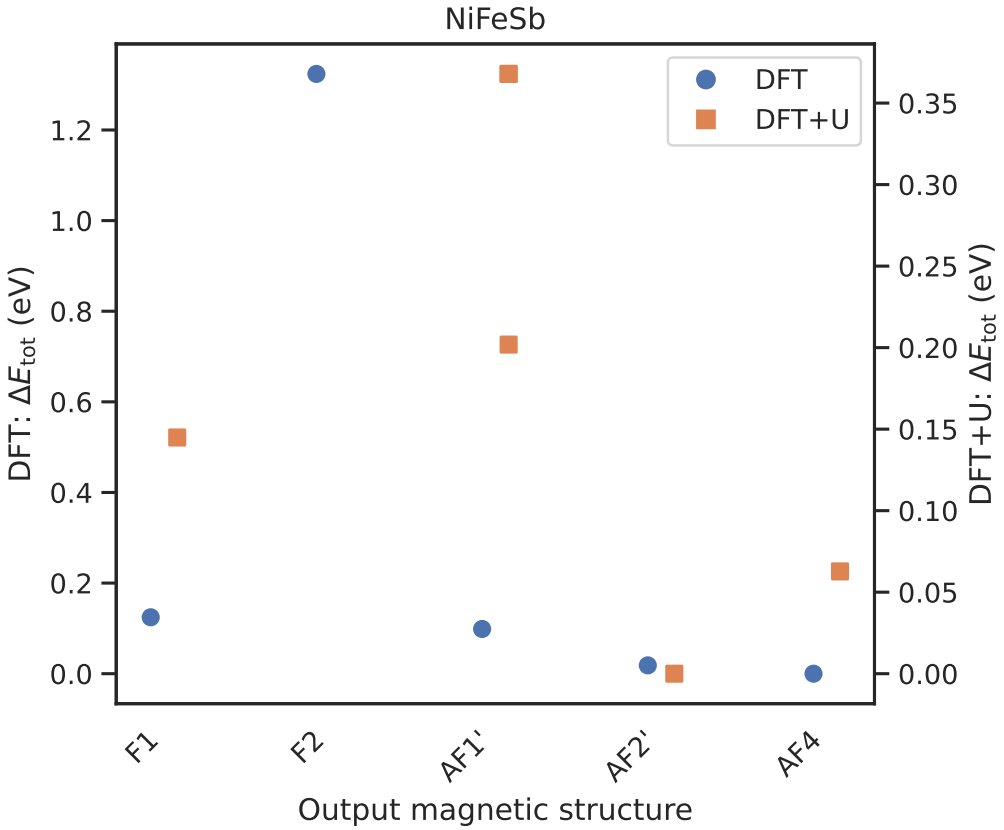


Figure 236: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
AF2′	-41228.789540	0.000000	0.00, 0.00, -3.24, 3.24, 0.00, 0.00, -3.24, 3.24
AF2′	-41228.789539	0.000001	0.00, 0.00, -3.24, 3.24, 0.00, 0.00, -3.24, 3.24
AF2′	-41228.789539	0.000001	0.00, 0.00, -3.24, 3.24, 0.00, 0.00, -3.24, 3.24
AF4	-41228.726793	0.062746	0.20, 0.20, 3.29, -3.29, -0.20, -0.20, -3.29, 3.29
AF4	-41228.726793	0.062746	-0.20, -0.20, -3.29, 3.29, 0.20, 0.20, 3.29, -3.29
AF4	-41228.726793	0.062747	-0.20, -0.20, -3.29, 3.29, 0.20, 0.20, 3.29, -3.29
AF4	-41228.726792	0.062748	-0.20, -0.20, -3.29, 3.29, 0.20, 0.20, 3.29, -3.29
F1	-41228.644661	0.144878	-0.24, -0.24, -3.31, -3.31, -0.24, -0.24, -3.31, -3.31
F1	-41228.644655	0.144885	0.24, 0.24, 3.31, 3.31, 0.24, 0.24, 3.30, 3.30
AF1′	-41228.587670	0.201869	0.04, -0.02, 3.33, 3.33, 0.03, 0.03, -3.30, -3.43
AF1′	-41228.421654	0.367885	0.00, 0.00, 3.32, 3.32, 0.00, 0.00, -3.32, -3.32
AF1′	-41228.421654	0.367886	0.00, 0.00, 3.32, 3.32, 0.00, 0.00, -3.32, -3.32

Table 241: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

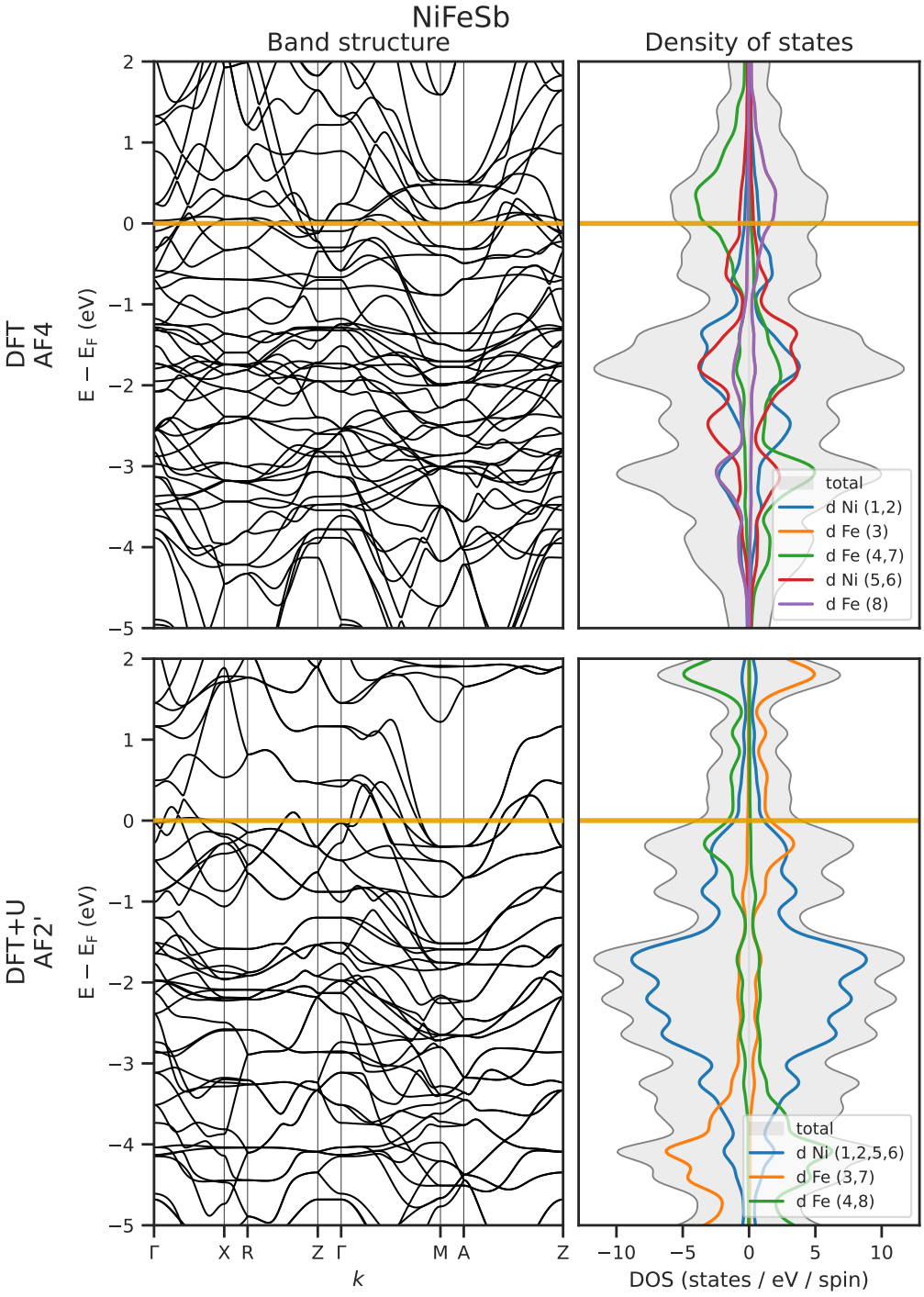


Figure 237: Band structure and Density of states of the lowest in energy calculations.

Material: Ga_2As

Configuration: Ga_2As

Structure

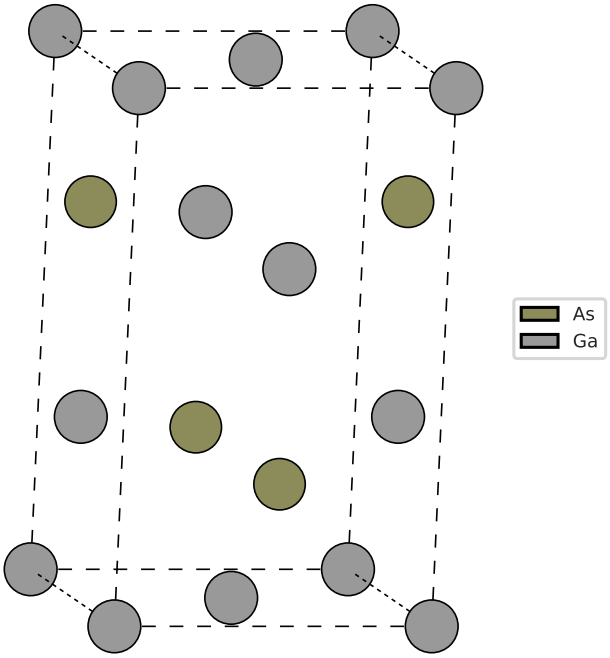


Figure 238: Structure of Ga_2As

a (Å)	c (Å)	z_1	z_2
3.9055	7.9650	0.3617	0.3006

Table 242: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-28268.683297	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 243: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

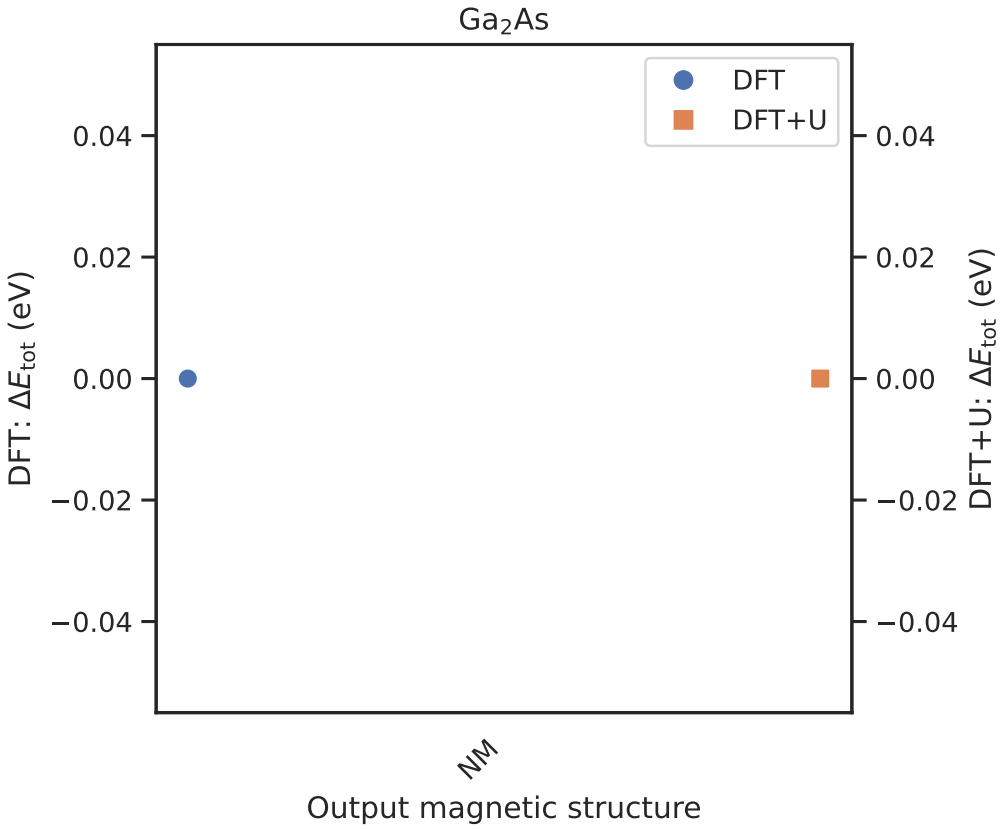


Figure 239: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-28268.683308	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 244: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

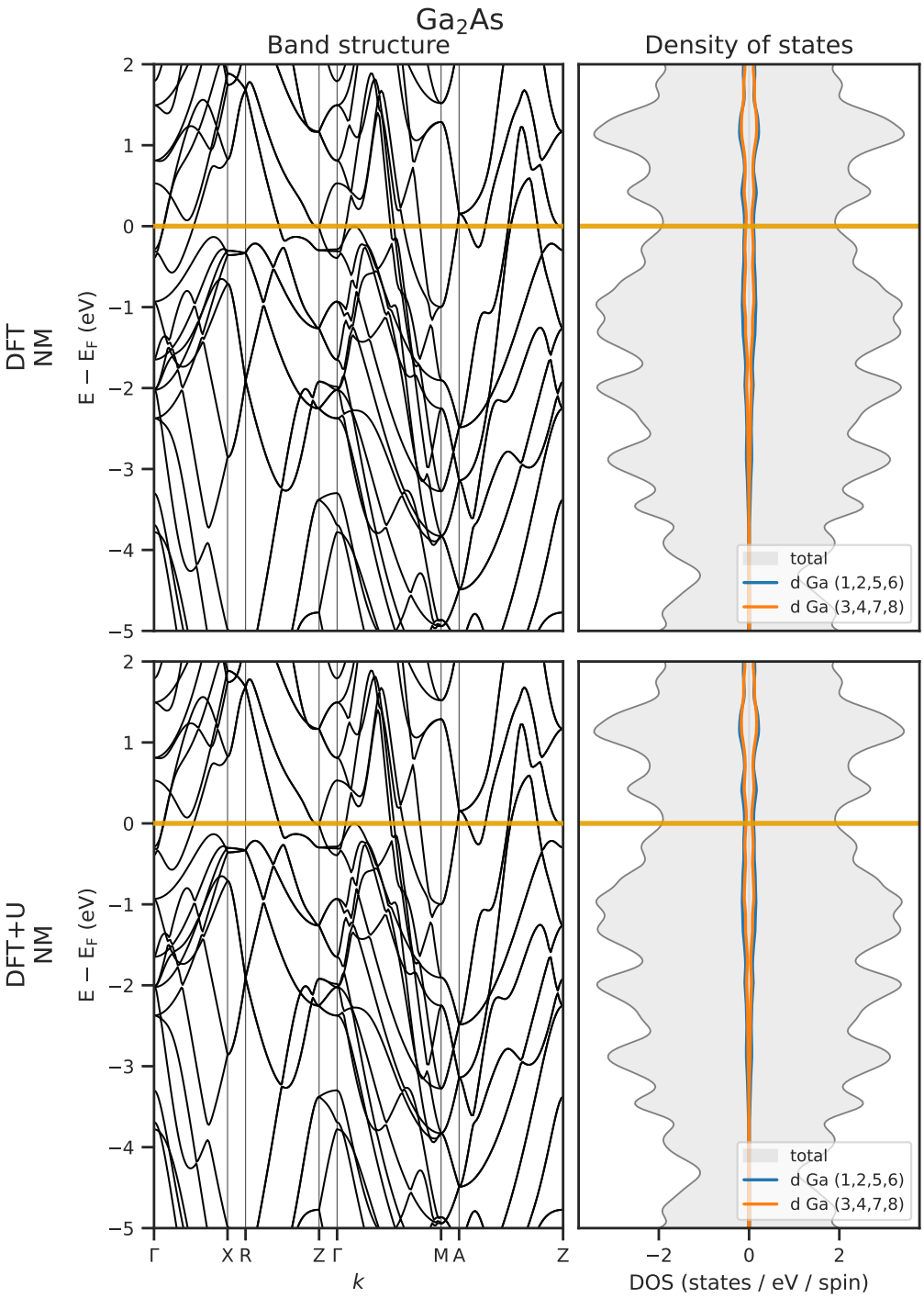


Figure 240: Band structure and Density of states of the lowest in energy calculations.

Material: Ga_2Sb

Configuration: Ga_2Sb

Structure

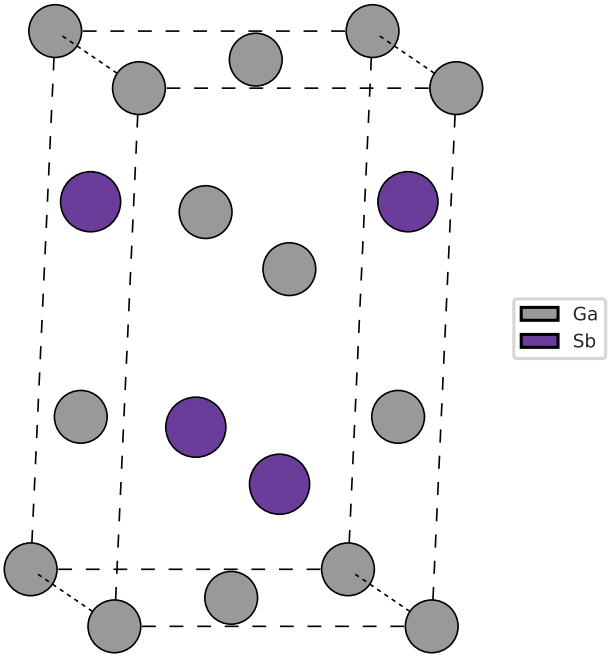


Figure 241: Structure of Ga_2Sb

a (Å)	c (Å)	z_1	z_2
4.2215	7.9296	0.3211	0.3111

Table 245: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of an Sb atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-26155.362290	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 246: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

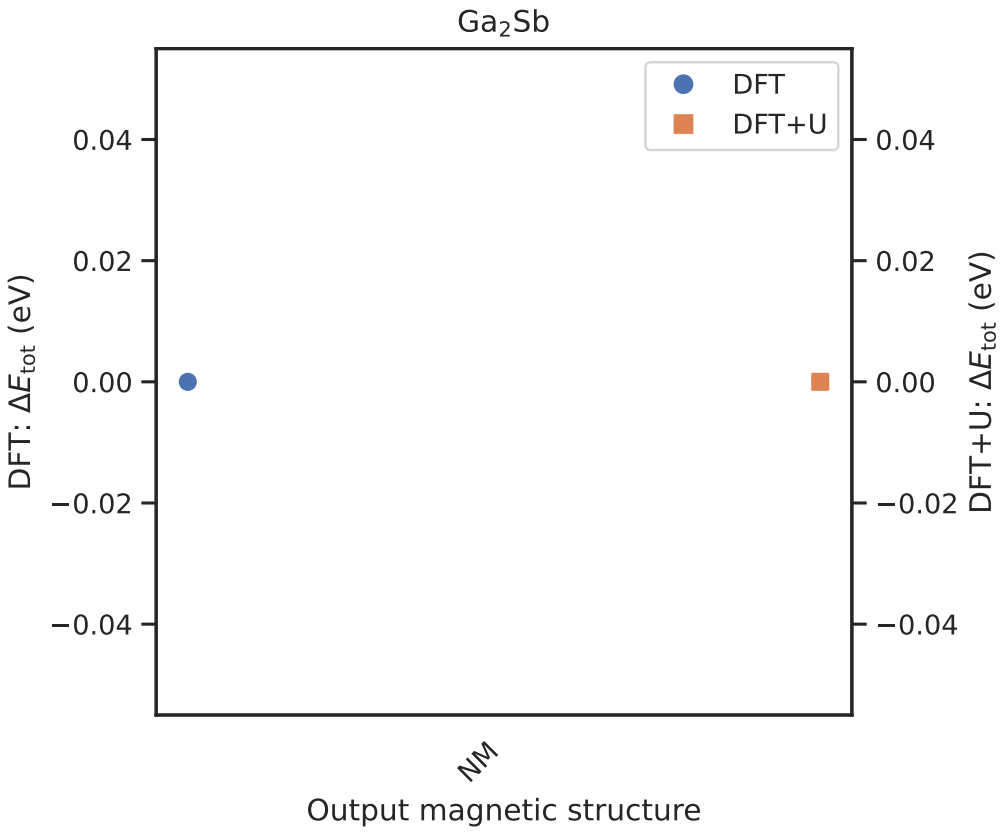


Figure 242: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-26155.361965	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 247: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

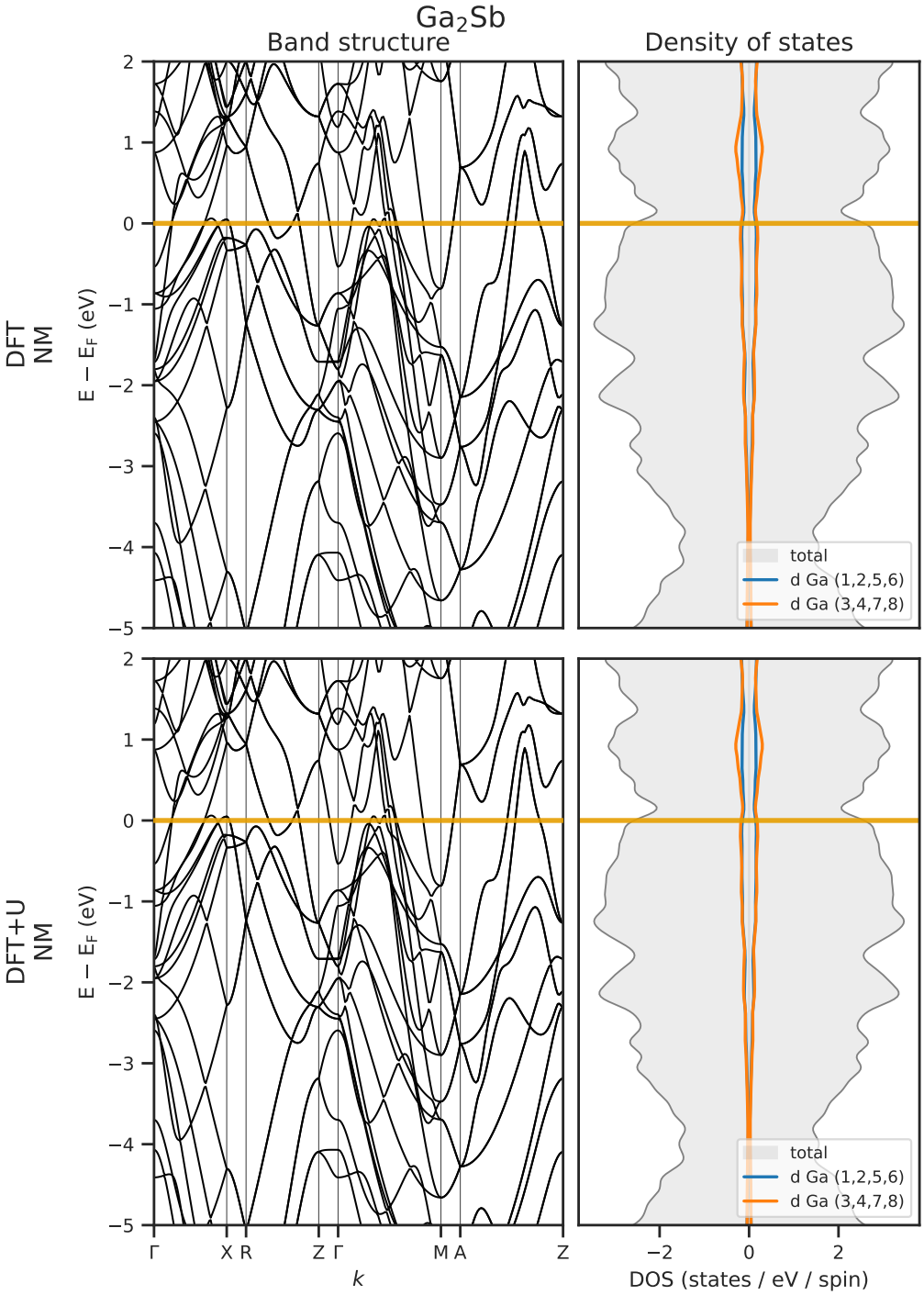


Figure 243: Band structure and Density of states of the lowest in energy calculations.

Material: GaMnAs

Configuration: GaMnAs ■ lower-energy

Structure

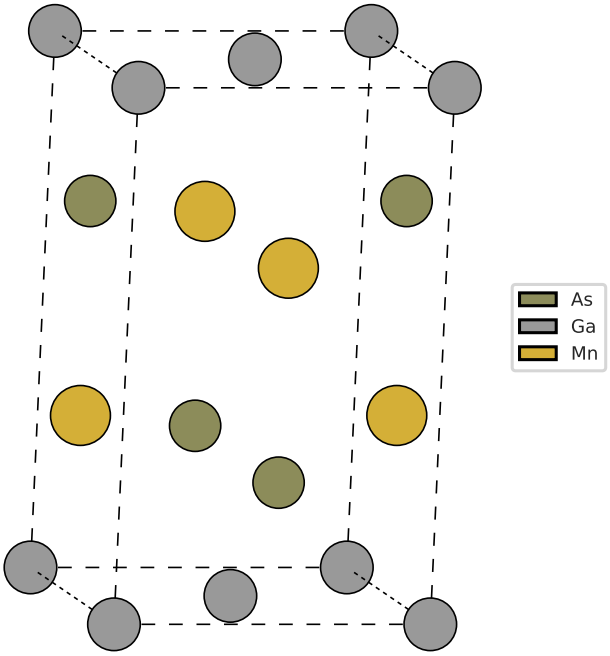


Figure 244: Structure of GaMnAs

a (Å)	c (Å)	z_1	z_2
3.5988	7.3030	0.2715	0.3733

Table 248: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-31333.440743	0.000000	0.00, 0.00, -3.09, 3.09, 0.00, 0.00, -3.09, 3.09
AF1′	-31333.355458	0.085284	0.00, 0.00, 3.12, 3.12, 0.00, 0.00, -3.12, -3.12
AF3	-31333.204430	0.236313	0.30, 0.30, -2.91, 2.91, -0.30, -0.30, 2.91, -2.91
Fi1	-31332.891920	0.548822	-0.27, -0.27, 2.75, 2.75, -0.27, -0.27, 2.75, 2.75

Table 249: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

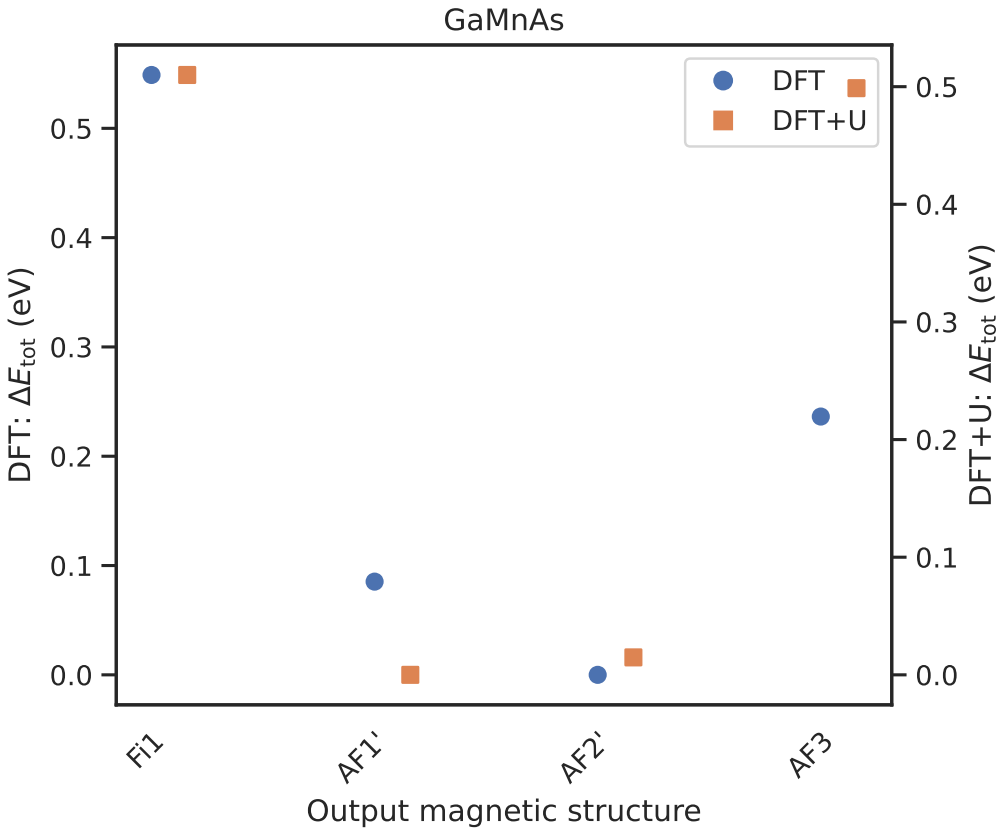


Figure 245: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF1′	-31325.838491	0.000000	0.00, 0.00, 4.40, 4.40, 0.00, 0.00, -4.40, -4.40
AF2′	-31325.823656	0.014835	0.00, 0.00, -4.40, 4.40, 0.00, 0.00, -4.40, 4.40
AF3	-31325.339756	0.498735	0.34, 0.34, -4.35, 4.35, -0.34, -0.34, 4.35, -4.35
Fi1	-31325.328545	0.509946	-0.22, -0.22, 4.42, 4.42, -0.22, -0.22, 4.42, 4.42

Table 250: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

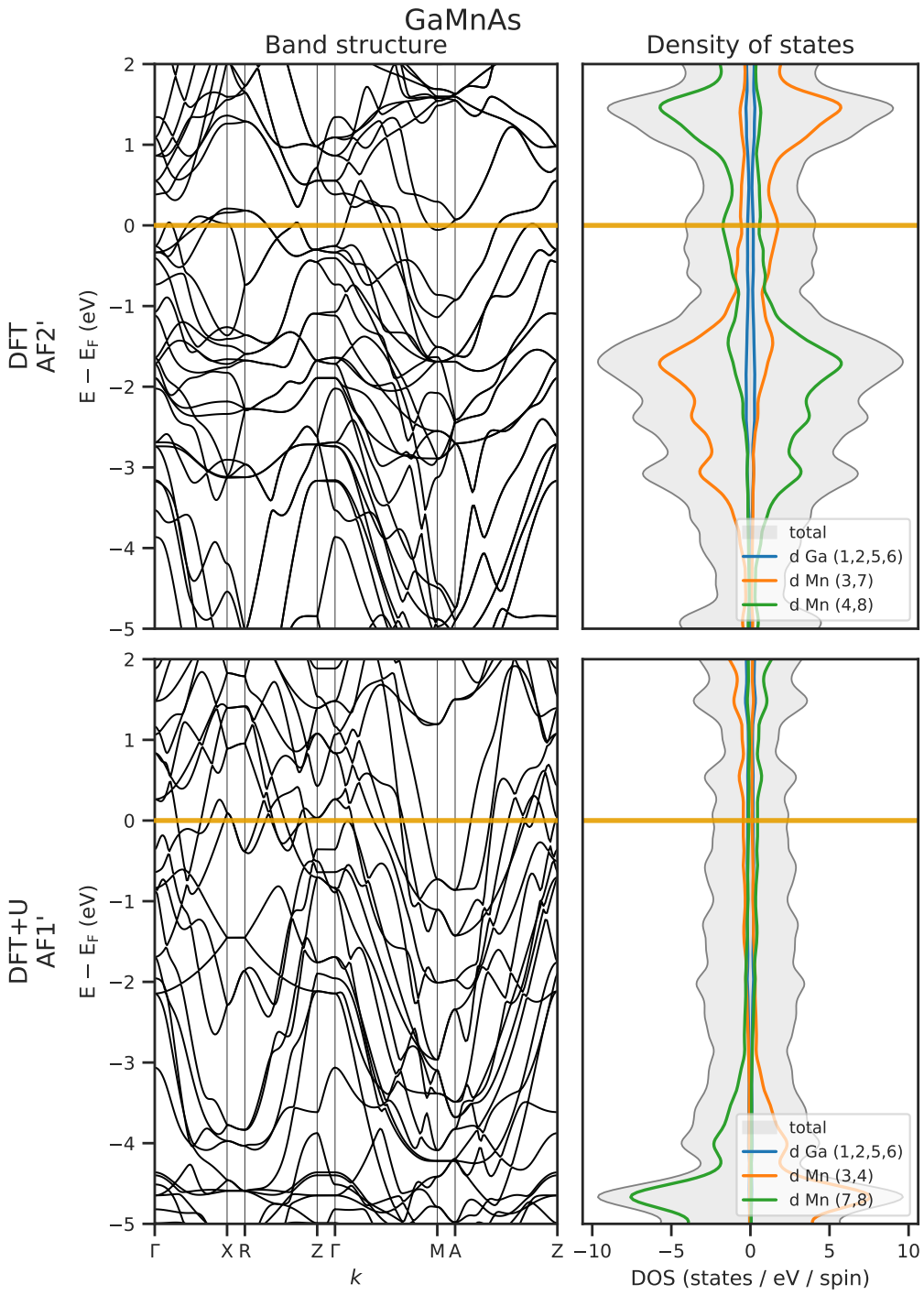


Figure 246: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnGaAs ■ higher-energy

Structure

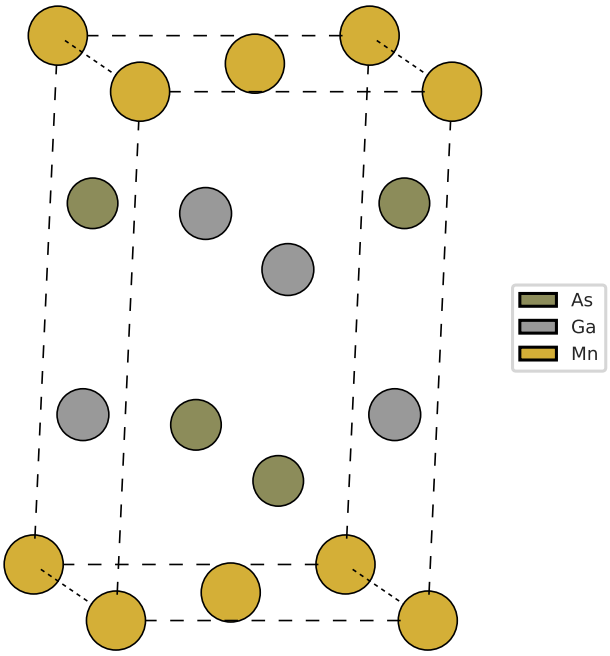


Figure 247: Structure of MnGaAs

a (Å)	c (Å)	z_1	z_2
4.1978	5.9236	0.2984	0.2647

Table 251: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-31333.393641	0.000000	3.65, -3.65, 0.00, 0.00, 3.65, -3.65, 0.00, 0.00
Fi2	-31333.109132	0.284509	3.41, 3.42, -0.12, 0.01, 3.66, -3.58, 0.01, -0.12
AF3	-31333.067280	0.326361	3.47, 3.47, -0.11, 0.11, -3.47, -3.47, 0.11, -0.11
Fi1	-31332.903771	0.489870	3.39, 3.39, -0.12, -0.12, 3.39, 3.39, -0.12, -0.12

Table 252: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

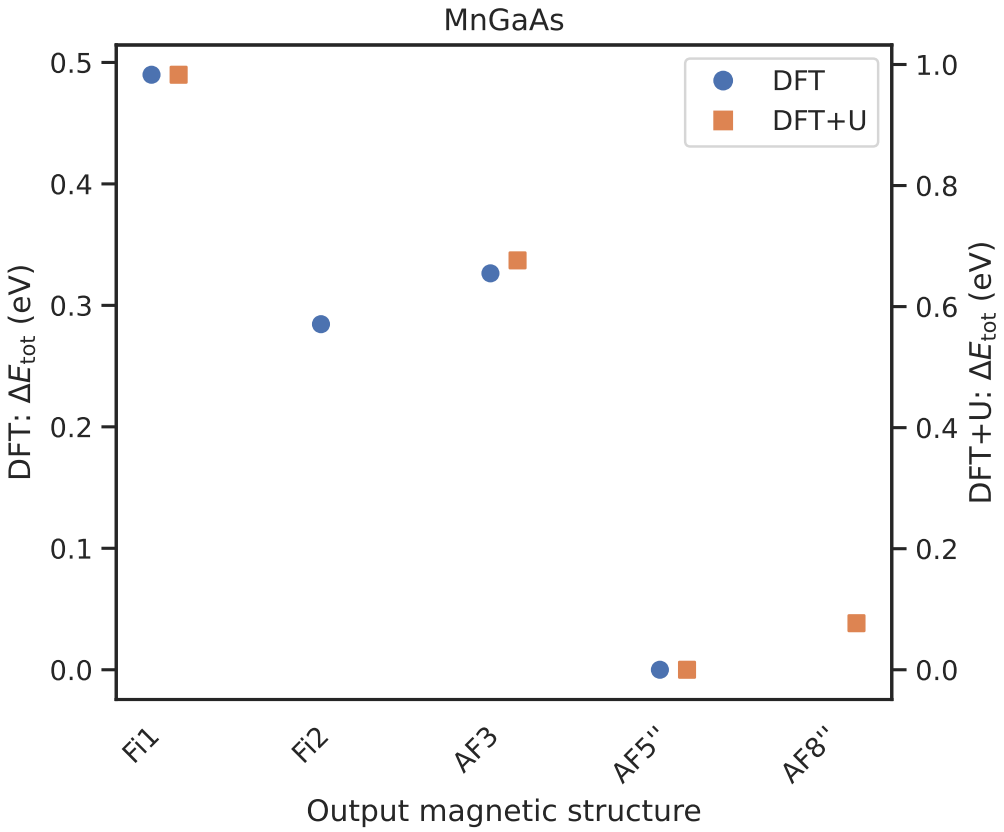


Figure 248: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-31327.160256	0.000000	4.54, -4.54, 0.00, 0.00, 4.54, -4.54, 0.00, 0.00
AF8″	-31327.083353	0.076903	4.56, -4.56, 0.00, 0.00, -4.56, 4.56, 0.00, 0.00
AF3	-31326.483898	0.676358	4.46, 4.46, -0.19, 0.19, -4.46, -4.46, 0.19, -0.19
Fi1	-31326.177188	0.983068	4.45, 4.45, -0.16, -0.16, 4.45, 4.45, -0.16, -0.16

Table 253: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

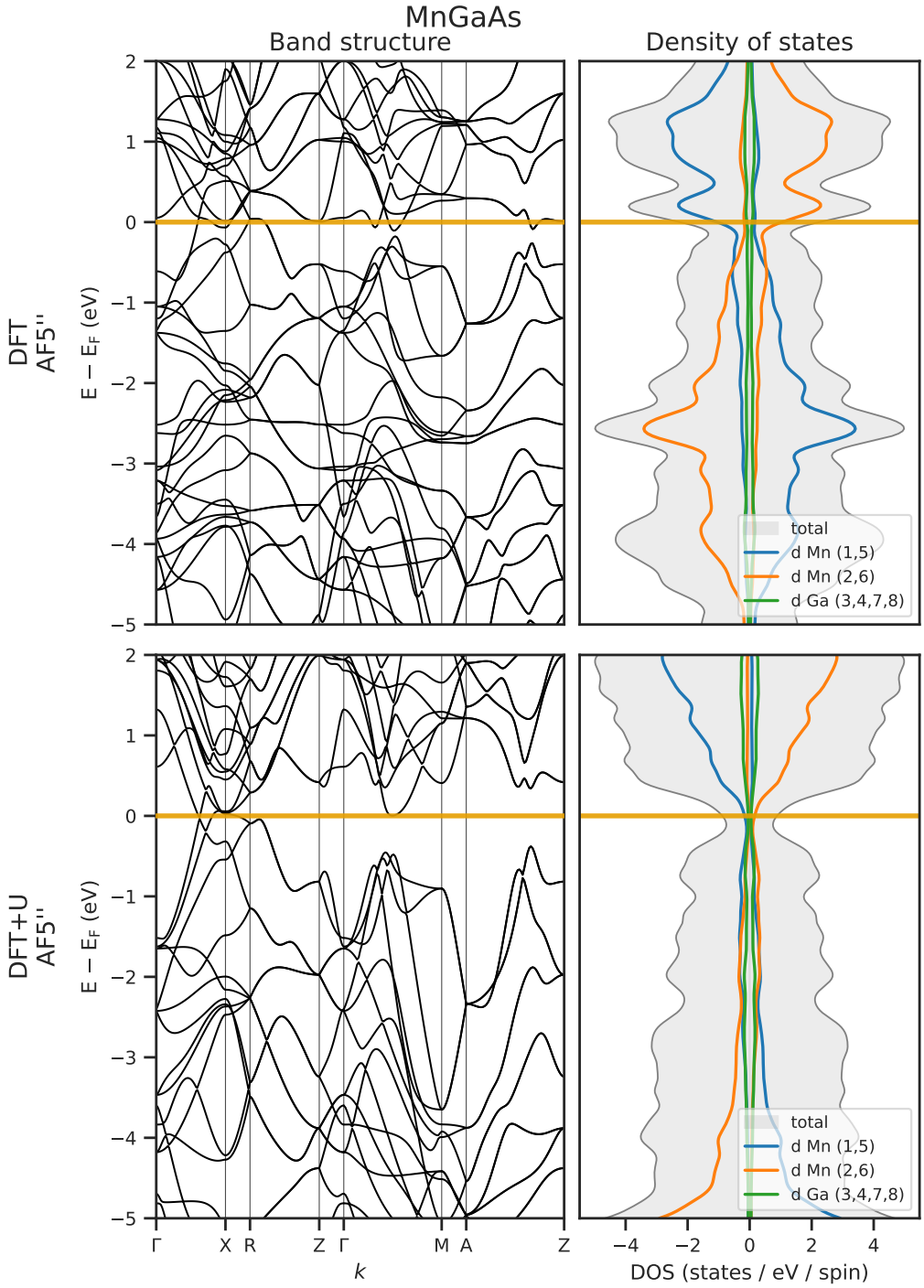


Figure 249: Band structure and Density of states of the lowest in energy calculations.

Material: GaMnSb

Configuration: GaMnSb ■ lower-energy

Structure

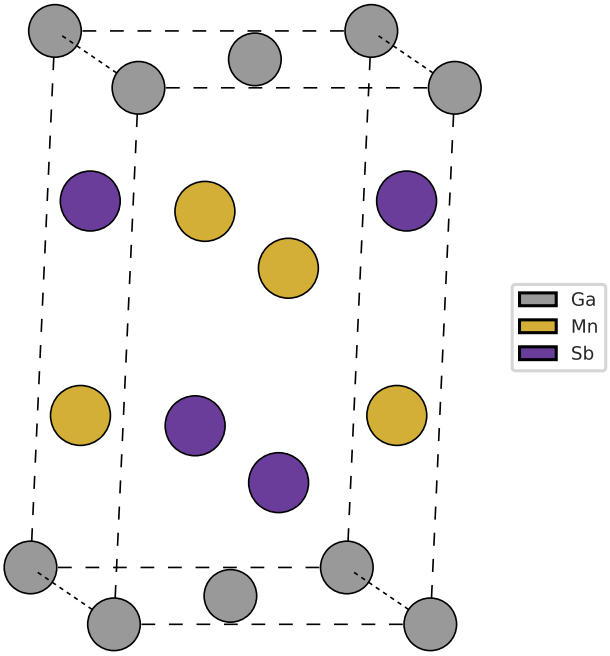


Figure 250: Structure of GaMnSb

a (Å)	c (Å)	z_1	z_2
3.7519	7.7348	0.2517	0.3680

Table 254: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-29220.045230	0.000000	0.00, 0.00, -3.27, 3.27, 0.00, 0.00, -3.27, 3.27
AF1′	-29219.876326	0.168904	0.00, 0.00, 3.24, 3.24, 0.00, 0.00, -3.24, -3.24
AF3	-29219.719835	0.325395	0.29, 0.29, -3.06, 3.06, -0.29, -0.29, 3.06, -3.06
Fi1	-29219.325417	0.719813	-0.29, -0.29, 2.81, 2.81, -0.29, -0.29, 2.81, 2.81

Table 255: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

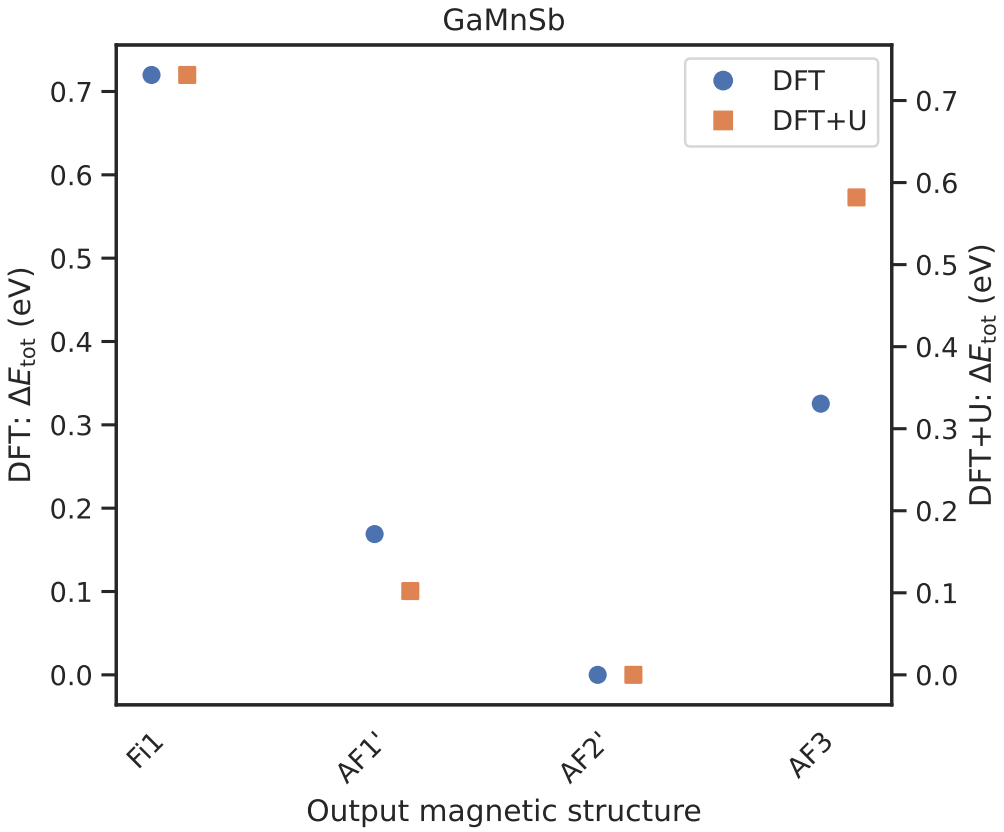


Figure 251: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF2′	-29212.817456	0.000000	0.00, 0.00, -4.47, 4.47, 0.00, 0.00, -4.47, 4.47
AF1′	-29212.715325	0.102131	0.00, 0.00, 4.48, 4.48, 0.00, 0.00, -4.48, -4.48
AF3	-29212.235540	0.581916	0.31, 0.31, -4.44, 4.44, -0.31, -0.31, 4.44, -4.44
Fi1	-29212.086305	0.731150	-0.25, -0.25, 4.48, 4.48, -0.25, -0.25, 4.48, 4.48

Table 256: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

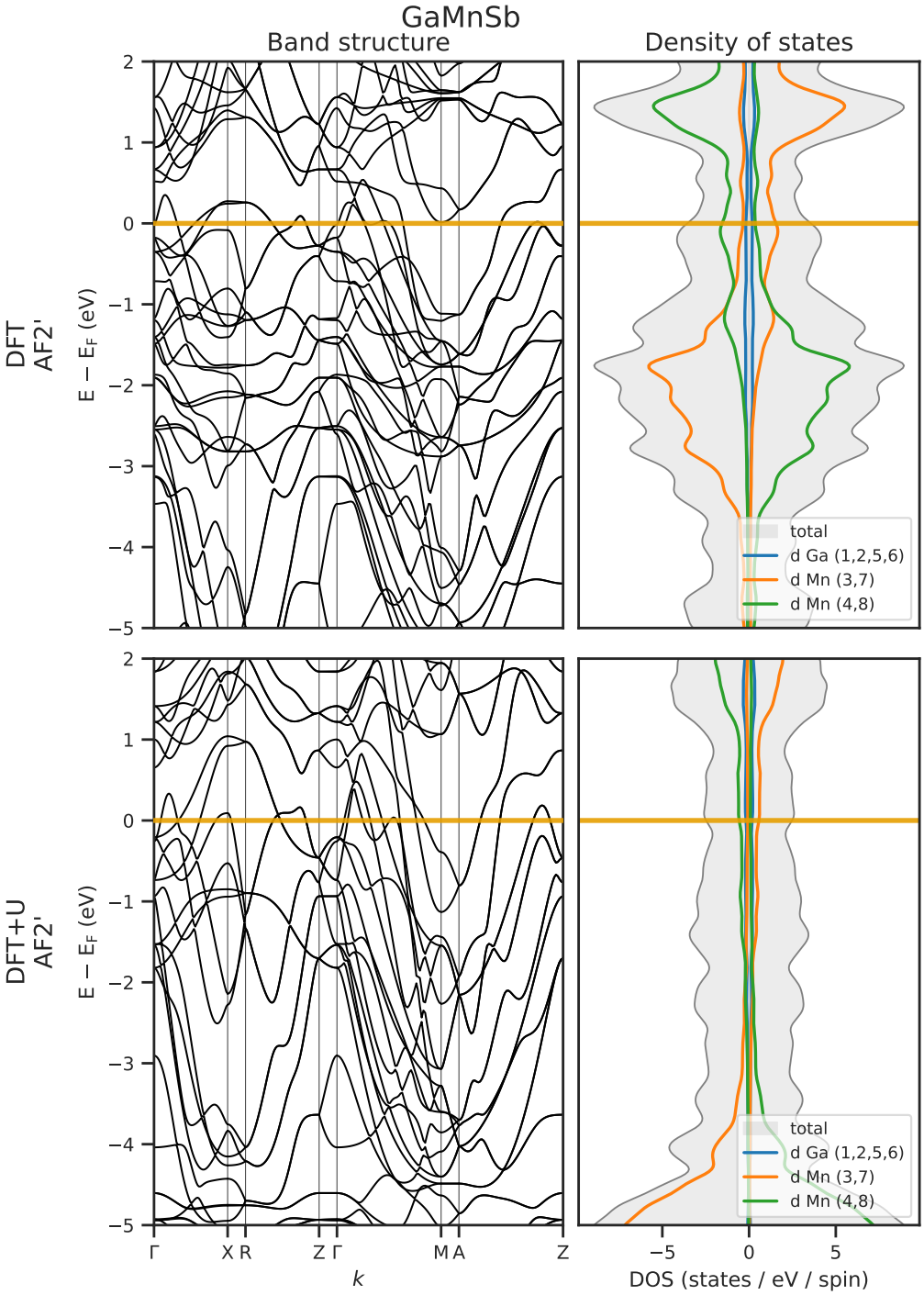


Figure 252: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnGaSb ■ higher-energy

Structure

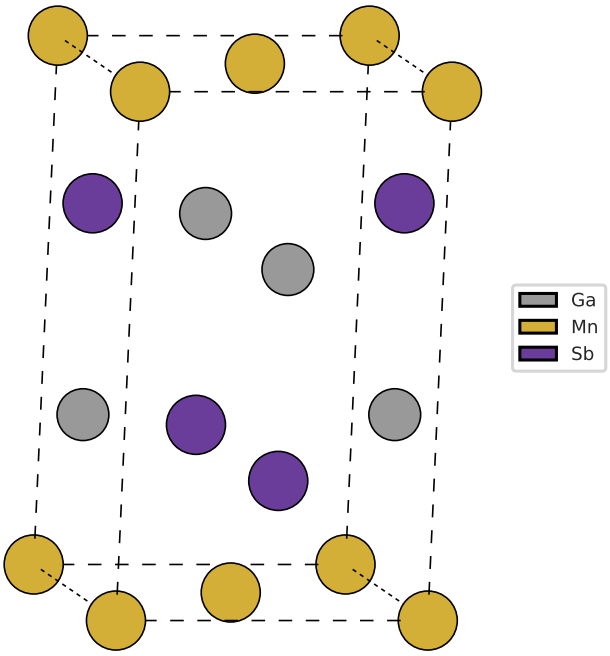


Figure 253: Structure of MnGaSb

a (Å)	c (Å)	z_1	z_2
4.4182	6.2404	0.2655	0.2830

Table 257: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-29219.324111	0.000000	3.79, -3.79, 0.00, 0.00, 3.79, -3.79, 0.00, 0.00
AF8″	-29219.188229	0.135883	3.80, -3.80, 0.00, -0.00, -3.80, 3.80, -0.00, 0.00
Fi2	-29219.075983	0.248129	3.60, 3.60, -0.15, -0.00, -3.75, 3.79, -0.00, -0.15
Fi1	-29218.934401	0.389710	3.60, 3.60, -0.17, -0.17, 3.60, 3.60, -0.17, -0.17

Table 258: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

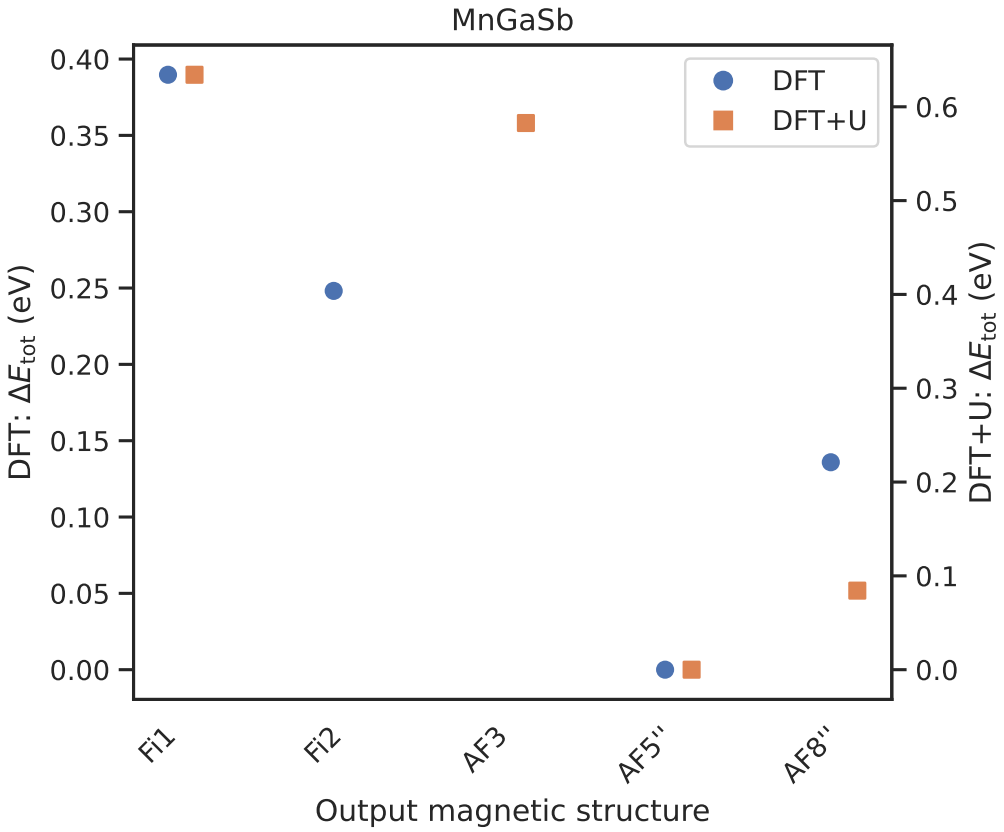


Figure 254: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-29213.566501	0.000000	4.58, -4.58, 0.00, 0.00, 4.58, -4.58, 0.00, 0.00
AF8″	-29213.482234	0.084267	4.59, -4.59, 0.00, 0.00, -4.59, 4.59, 0.00, 0.00
AF3	-29212.983798	0.582703	4.56, 4.56, -0.20, 0.20, -4.56, -4.56, 0.20, -0.20
Fi1	-29212.932365	0.634137	4.58, 4.58, -0.20, -0.20, 4.58, 4.58, -0.20, -0.20

Table 259: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

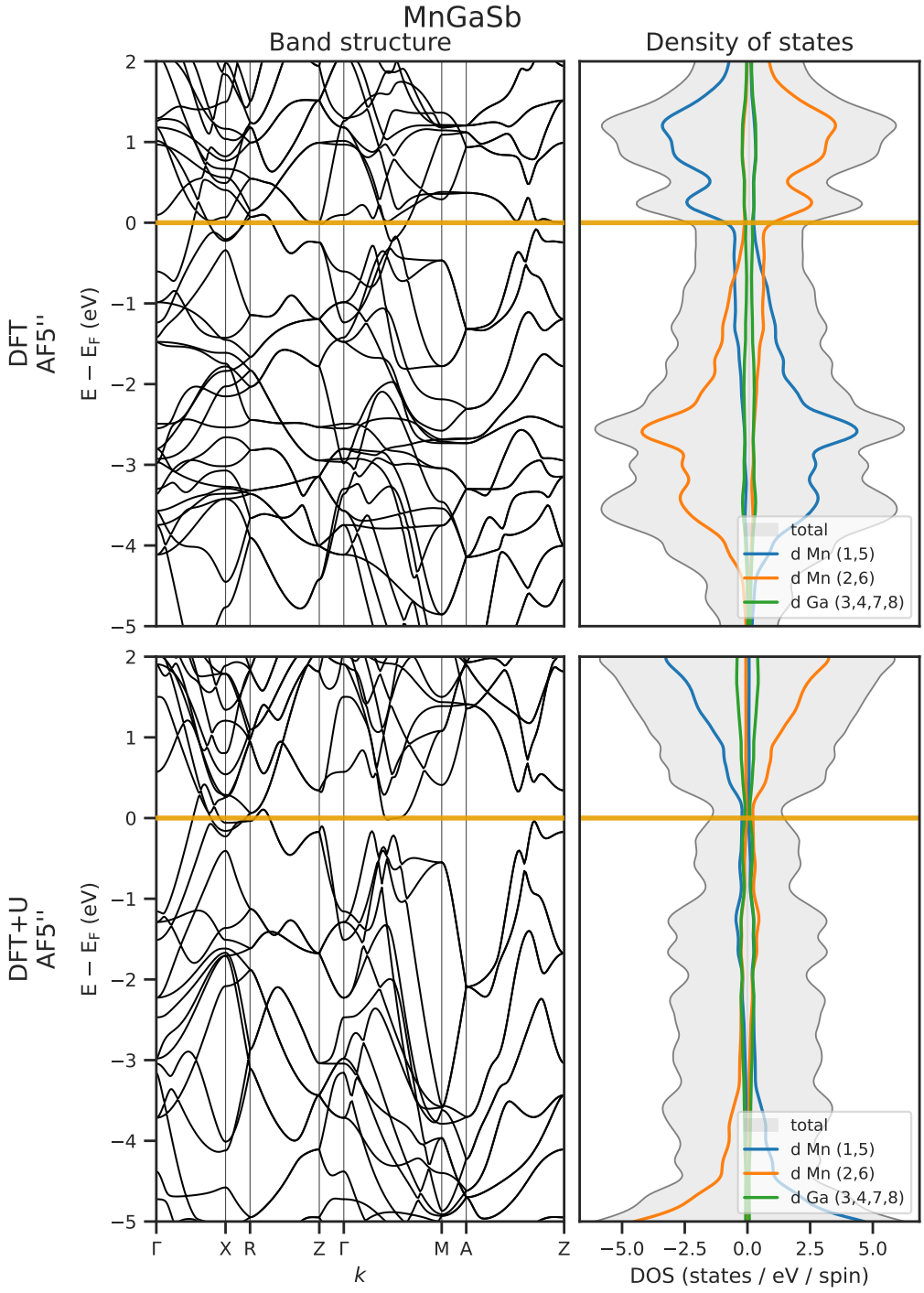


Figure 255: Band structure and Density of states of the lowest in energy calculations.

Material: NiGaAs

Configuration: NiGaAs ■ lower-energy

Structure

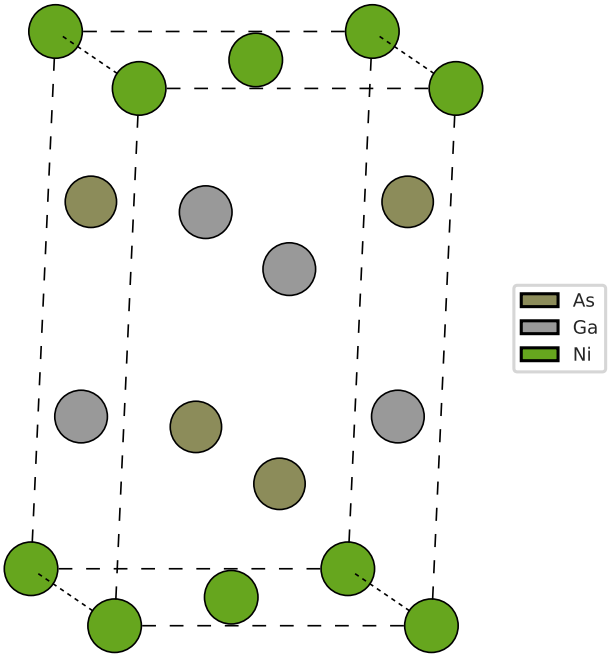


Figure 256: Structure of NiGaAs

a (Å)	c (Å)	z_1	z_2
4.1514	5.5974	0.2715	0.2633

Table 260: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-38166.130252	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 261: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

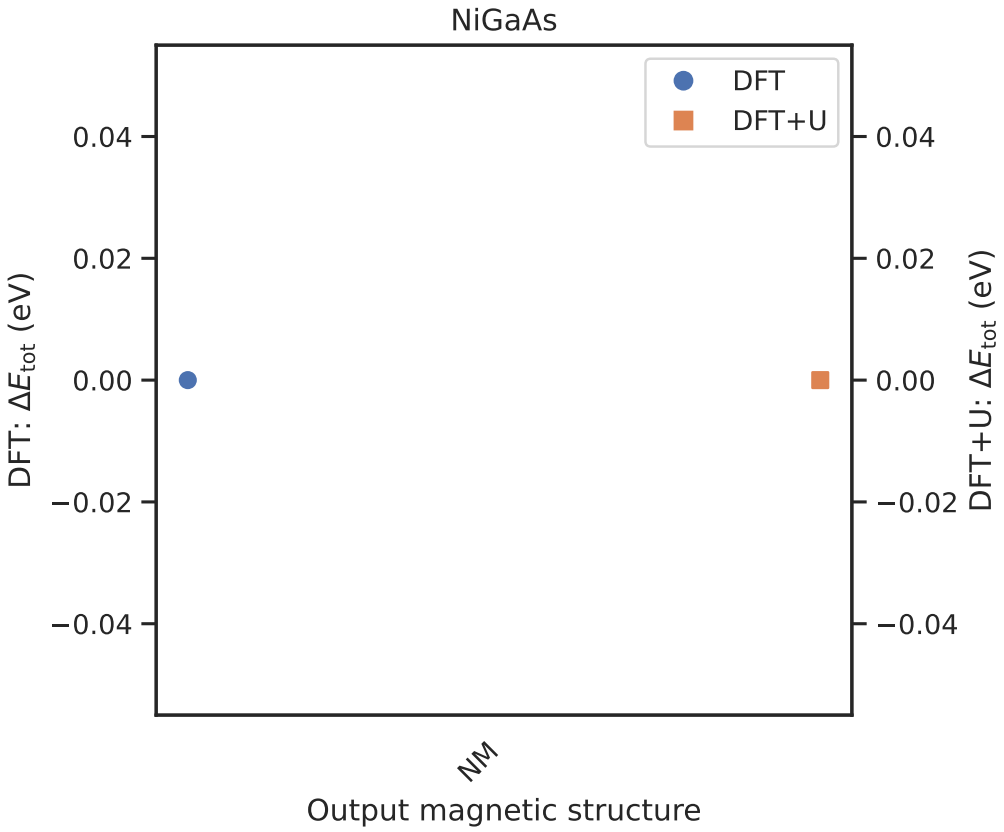


Figure 257: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-38159.033652	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-38159.033652	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-38159.033650	0.000002	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-38159.033650	0.000002	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 262: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

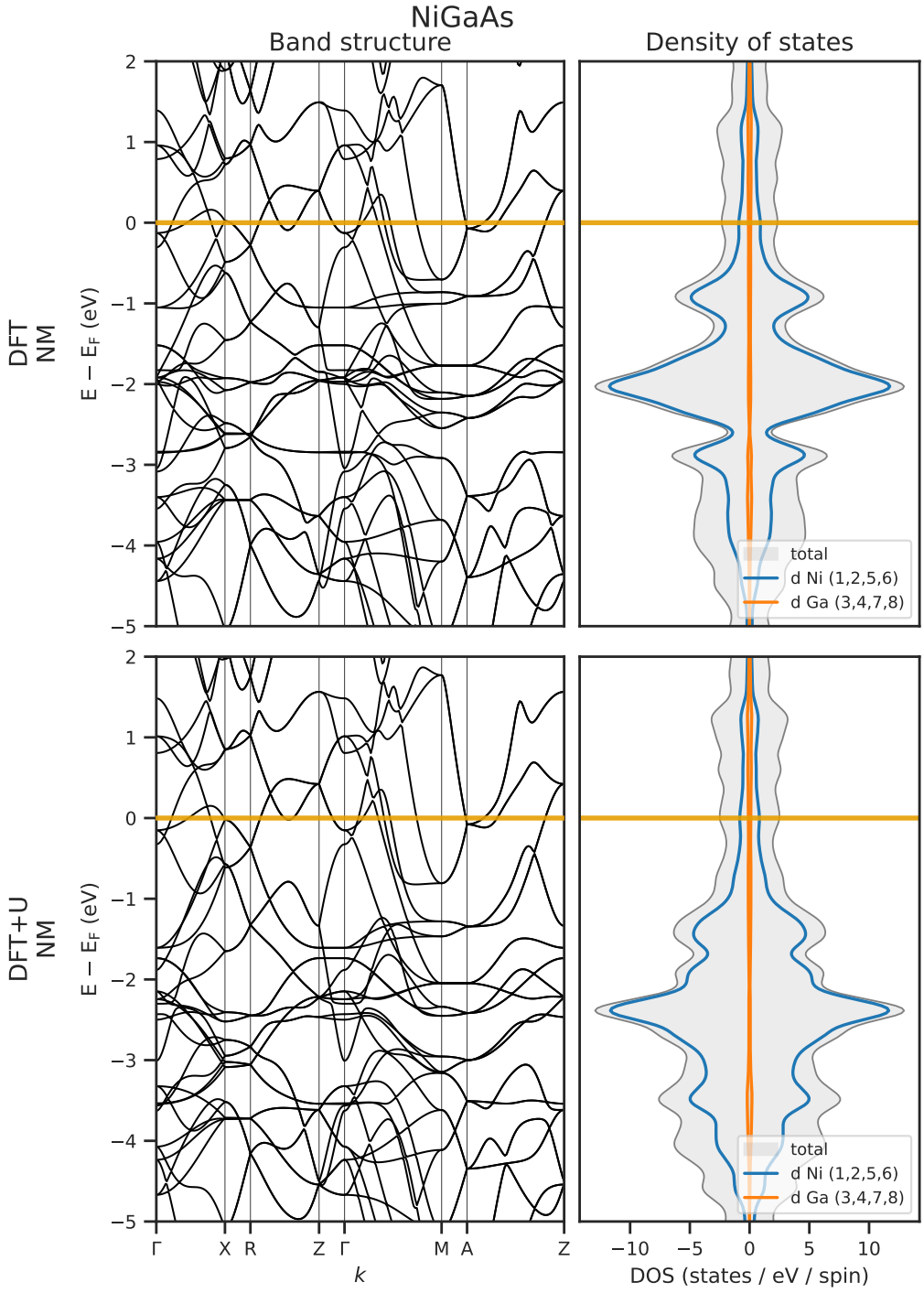


Figure 258: Band structure and Density of states of the lowest in energy calculations.

Configuration: GaNiAs ■ higher-energy

Structure

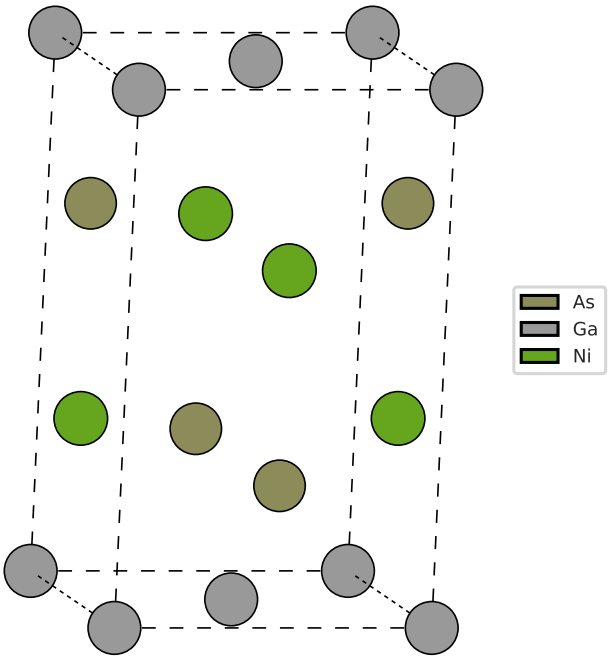


Figure 259: Structure of GaNiAs

a (Å)	c (Å)	z_1	z_2
3.7194	6.6365	0.2574	0.3743

Table 263: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-38165.162887	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 264: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

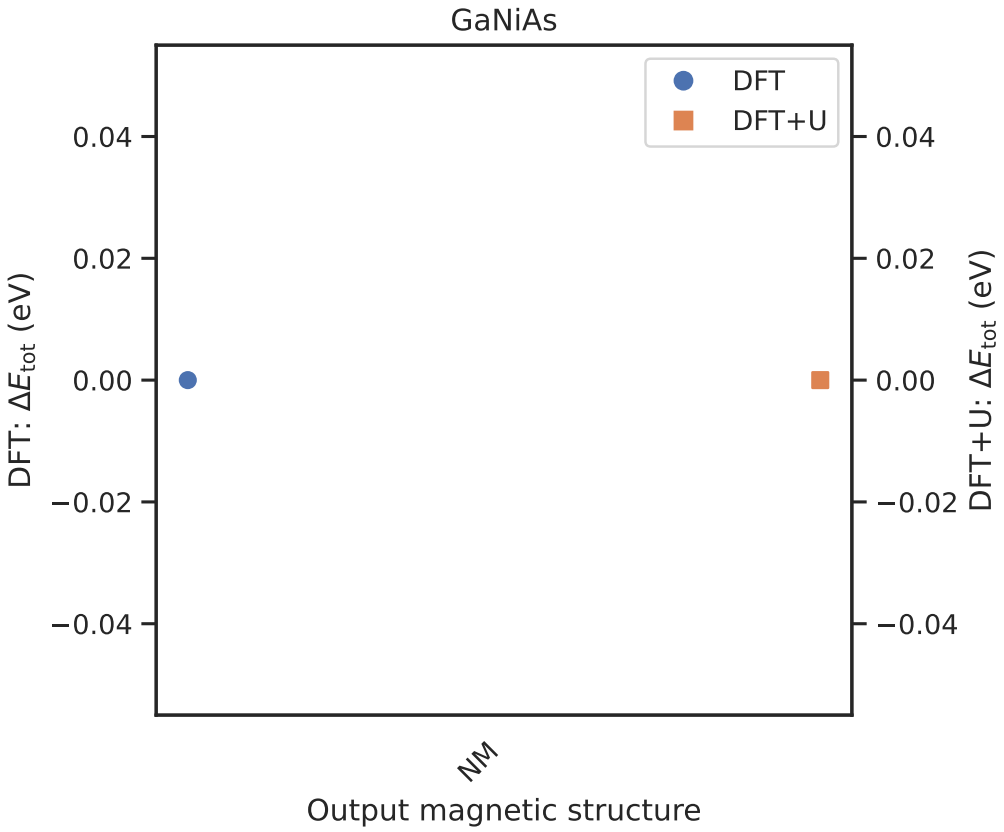


Figure 260: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-38157.972362	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-38157.972353	0.000008	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-38157.972337	0.000024	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-38157.972329	0.000033	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 265: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

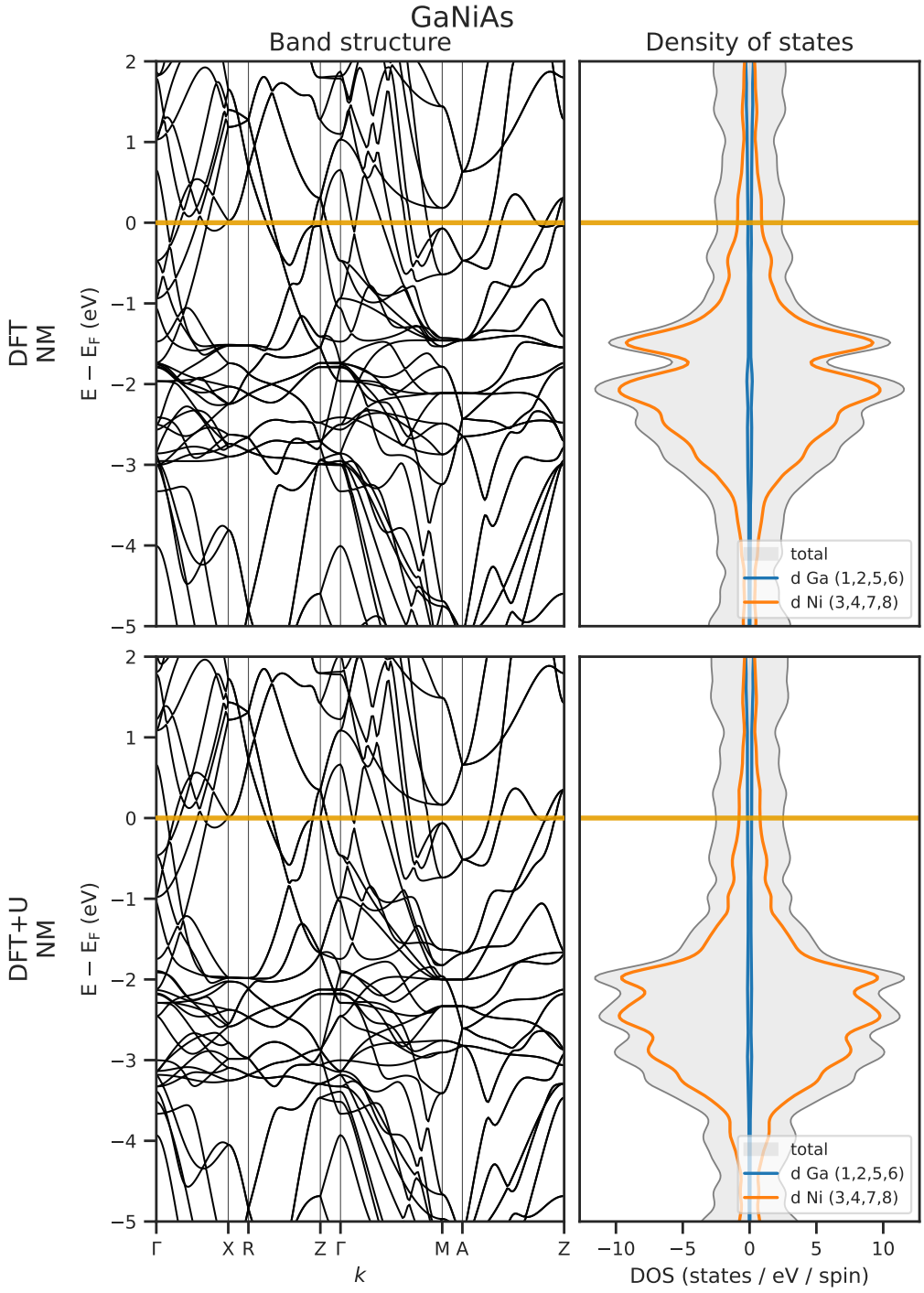


Figure 261: Band structure and Density of states of the lowest in energy calculations.

Material: GaNiSb

Configuration: GaNiSb ■ lower-energy

Structure

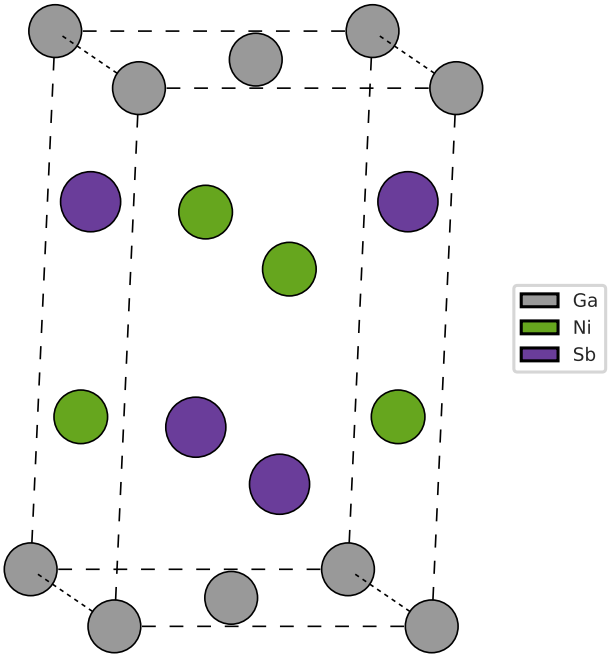


Figure 262: Structure of GaNiSb

a (Å)	c (Å)	z_1	z_2
3.8664	6.9965	0.2411	0.3671

Table 266: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ga atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-36052.875357	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36052.875199	0.000157	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 267: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

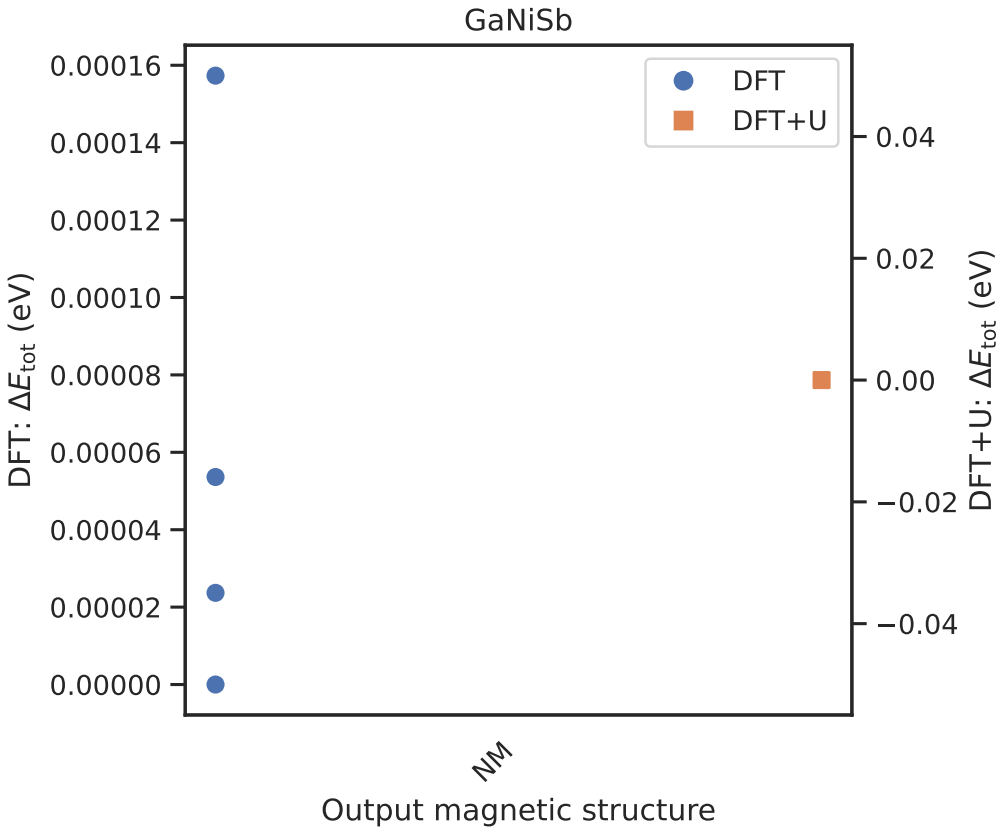


Figure 263: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-36045.872140	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36045.872132	0.000007	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36045.872128	0.000011	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36045.872091	0.000048	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 268: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

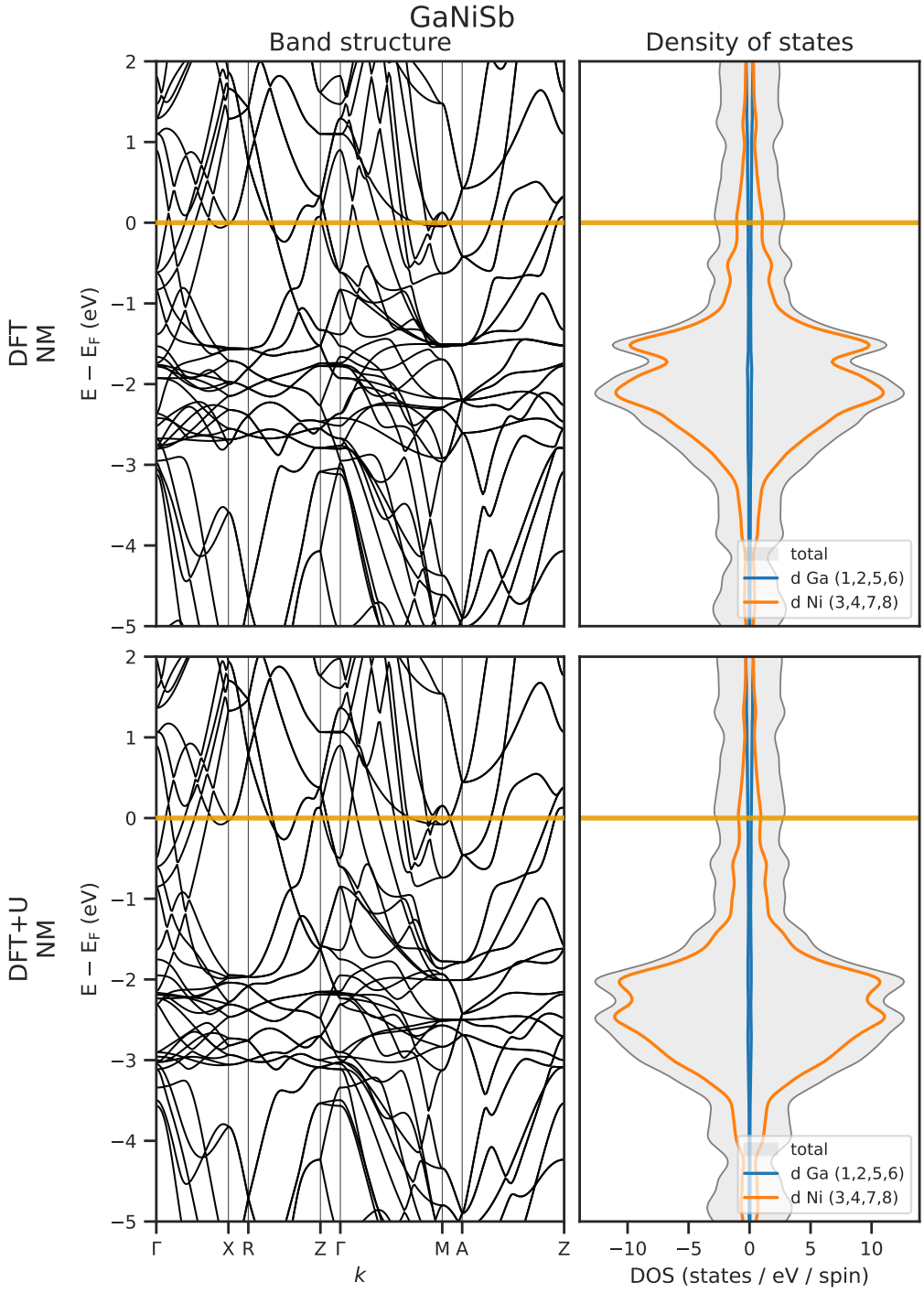


Figure 264: Band structure and Density of states of the lowest in energy calculations.

Configuration: NiGaSb ■ higher-energy

Structure

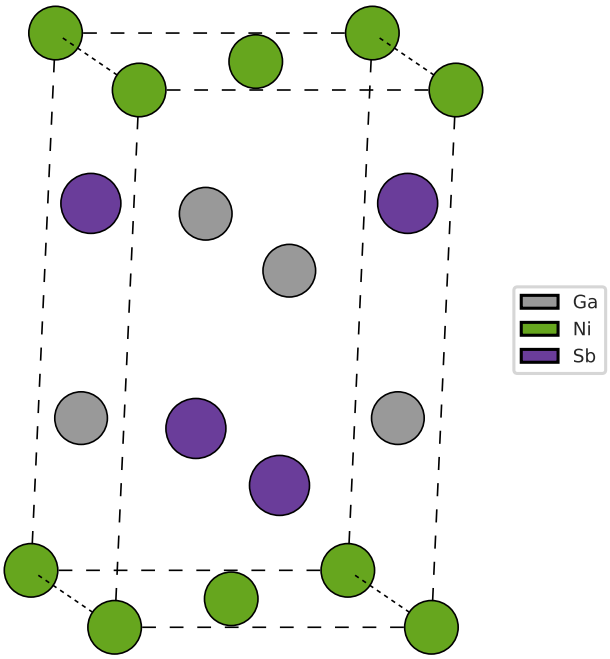


Figure 265: Structure of NiGaSb

a (Å)	c (Å)	z_1	z_2
4.3400	5.9663	0.2379	0.2789

Table 269: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of a Ga atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-36052.672572	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 270: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

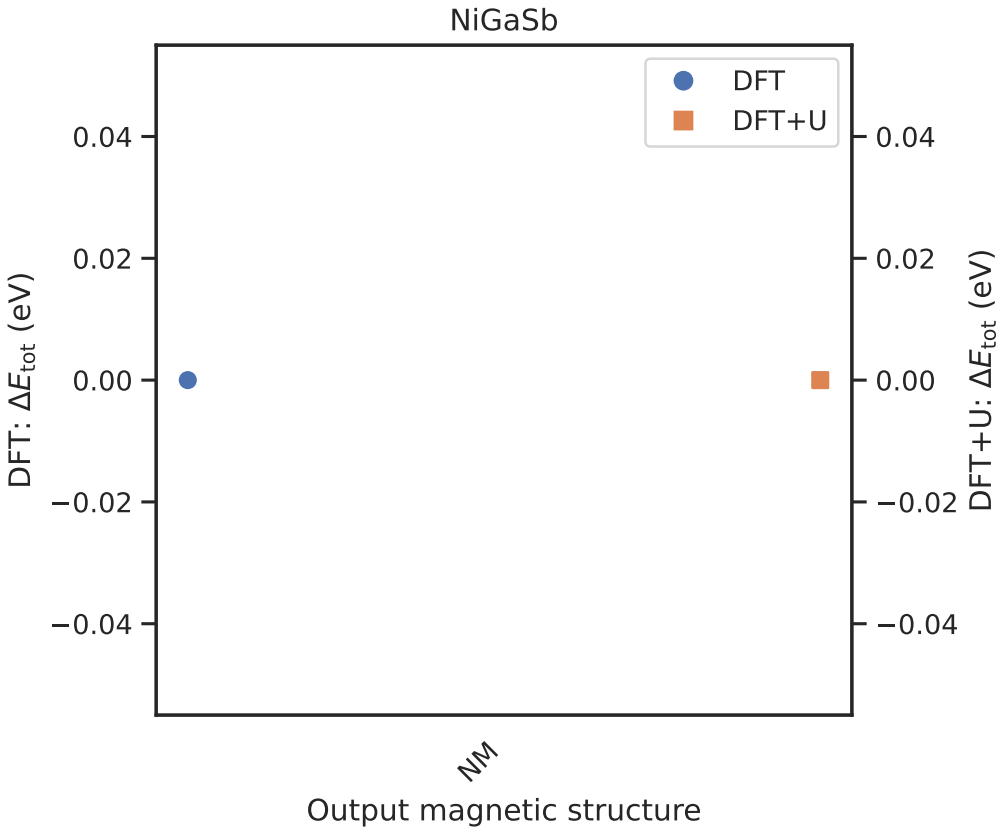


Figure 266: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-36045.789496	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36045.789496	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36045.789496	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-36045.789495	0.000001	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 271: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

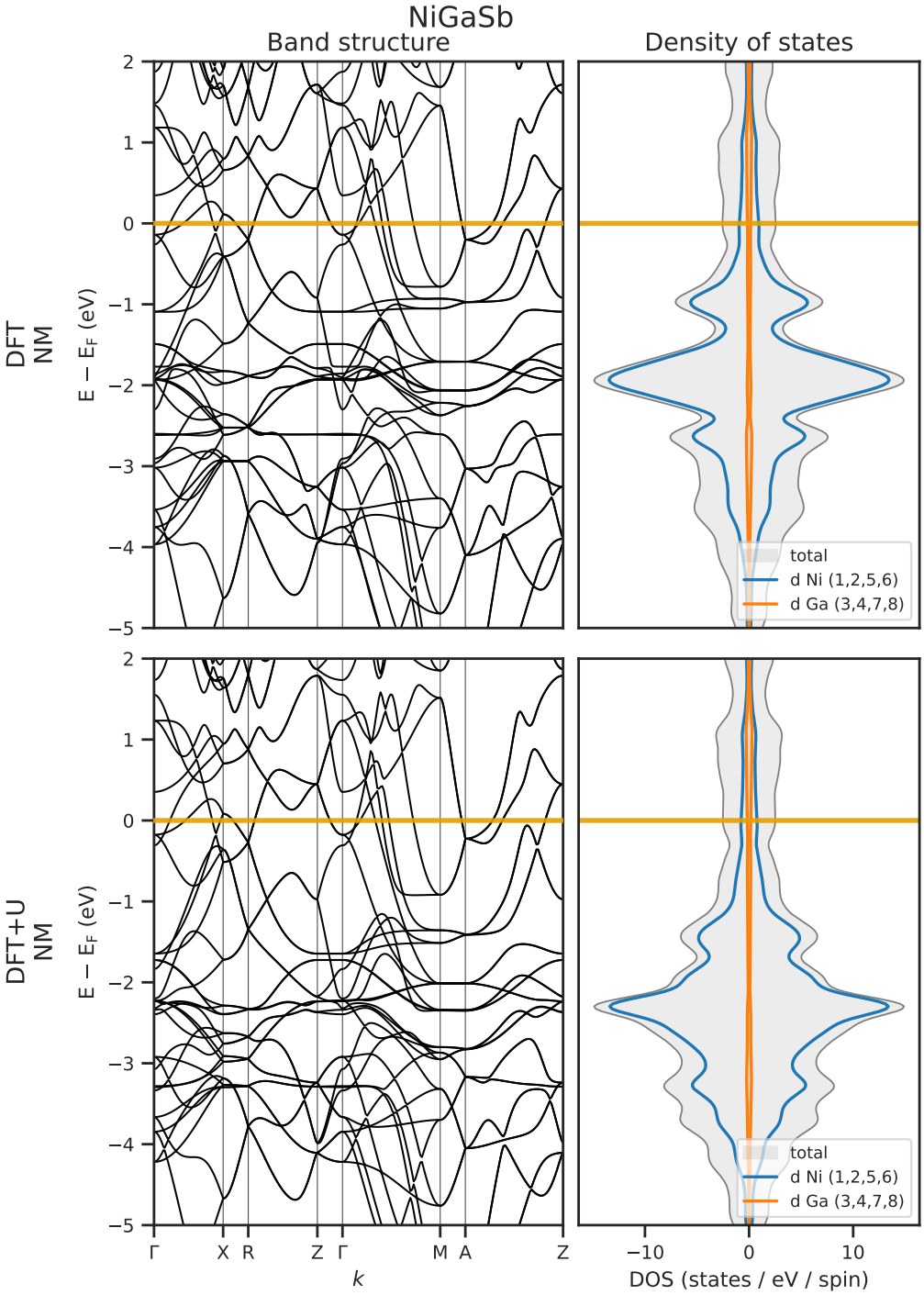


Figure 267: Band structure and Density of states of the lowest in energy calculations.

Material: Mn_2As

Configuration: Mn_2As

Structure

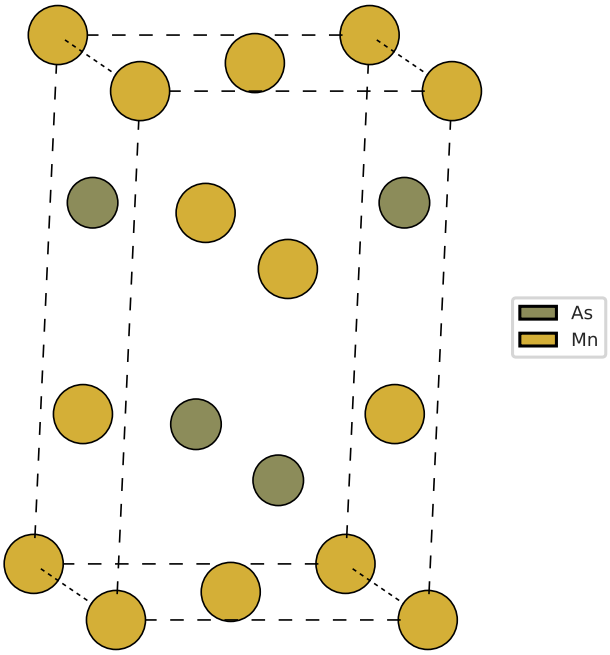


Figure 268: Structure of Mn_2As

a (Å)	c (Å)	z_1	z_2
3.7517	6.1438	0.3350	0.2645

Table 272: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

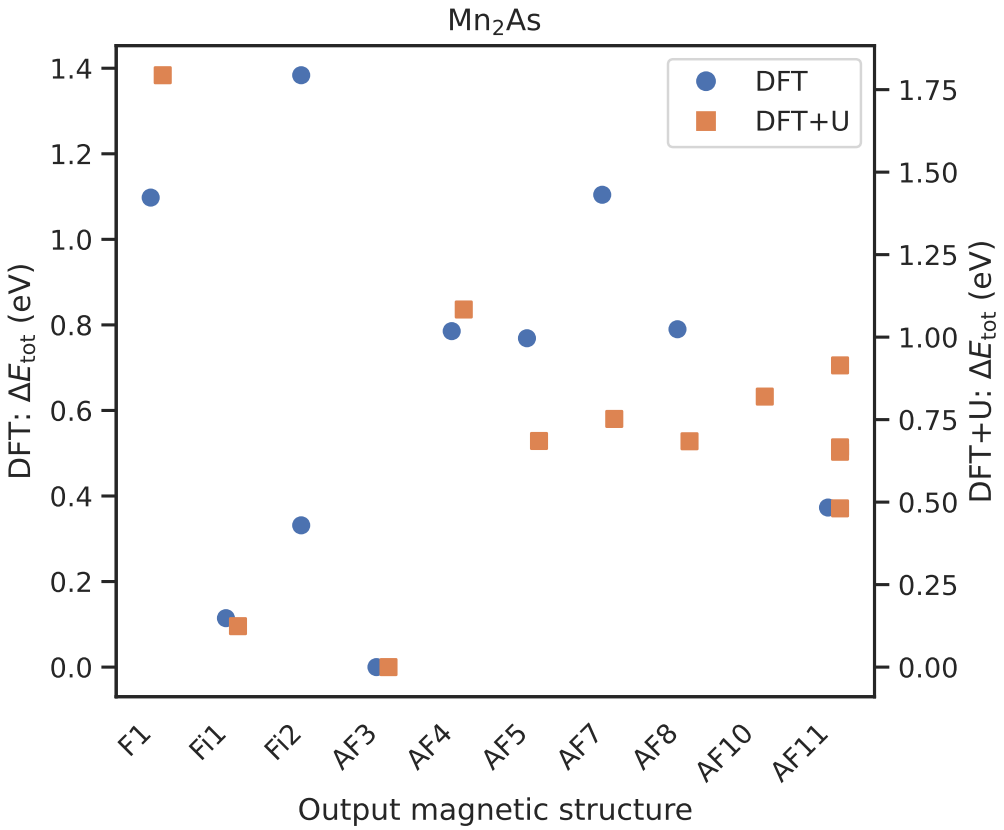


Figure 269: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-34397.563045	0.000000	2.18, 2.18, -3.85, 3.85, -2.18, -2.18, 3.85, -3.85
Fi1	-34397.448641	0.114404	2.49, 2.49, -3.83, -3.83, 2.49, 2.49, -3.83, -3.83
Fi2	-34397.231599	0.331446	-2.21, -2.21, -3.69, -3.83, 2.33, 2.33, -3.84, 3.87
AF11	-34397.190042	0.373003	2.23, 2.23, -3.86, 3.86, -2.23, -2.23, -3.74, 3.74
AF5	-34396.794235	0.768810	2.47, -2.47, -3.74, 3.74, 2.47, -2.47, -3.74, 3.74
AF4	-34396.777628	0.785417	2.13, 2.13, 3.60, -3.60, -2.13, -2.13, -3.60, 3.60
AF8	-34396.773194	0.789851	2.72, -2.72, -3.76, 3.76, -2.72, 2.72, -3.76, 3.76
F1	-34396.465430	1.097615	2.08, 2.08, 3.51, 3.51, 2.08, 2.08, 3.51, 3.51
AF7	-34396.458836	1.104209	2.77, -2.77, 3.79, 3.79, 2.77, -2.77, -3.79, -3.79
Fi2	-34396.179388	1.383657	-2.99, 0.52, 3.76, -3.89, 2.28, 2.26, -0.18, -3.64

Table 273: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-34382.608277	0.000000	3.98, 3.98, -4.74, 4.74, -3.98, -3.98, 4.74, -4.74
Fi1	-34382.484207	0.124070	3.95, 3.95, -4.73, -4.73, 3.95, 3.95, -4.73, -4.73
AF11	-34382.127194	0.481083	4.00, 4.00, -4.71, 4.71, -4.00, -4.00, -4.47, 4.47
AF11	-34381.955660	0.652617	4.35, -4.16, -4.58, 4.58, 4.16, -4.35, 4.58, -4.58
AF11	-34381.942257	0.666020	4.34, -4.14, -4.57, 4.57, -4.34, 4.14, 4.57, -4.57
AF8	-34381.923894	0.684382	4.21, -4.21, -4.57, 4.57, -4.21, 4.21, -4.57, 4.57
AF5	-34381.922996	0.685281	4.23, -4.23, -4.57, 4.57, 4.23, -4.23, -4.57, 4.57
AF7	-34381.856218	0.752058	4.23, -4.23, 4.55, 4.55, 4.23, -4.23, -4.55, -4.55
AF10	-34381.788453	0.819824	4.23, -4.23, 4.53, 4.53, -4.23, 4.23, -4.53, -4.53
AF11	-34381.693914	0.914363	4.01, 4.01, 4.48, 4.72, -4.01, -4.01, -4.48, -4.72
AF4	-34381.524558	1.083719	3.95, 3.95, 4.49, -4.49, -3.95, -3.95, -4.49, 4.49
F1	-34380.814600	1.793677	3.91, 3.91, 4.44, 4.44, 3.91, 3.91, 4.44, 4.44

Table 274: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

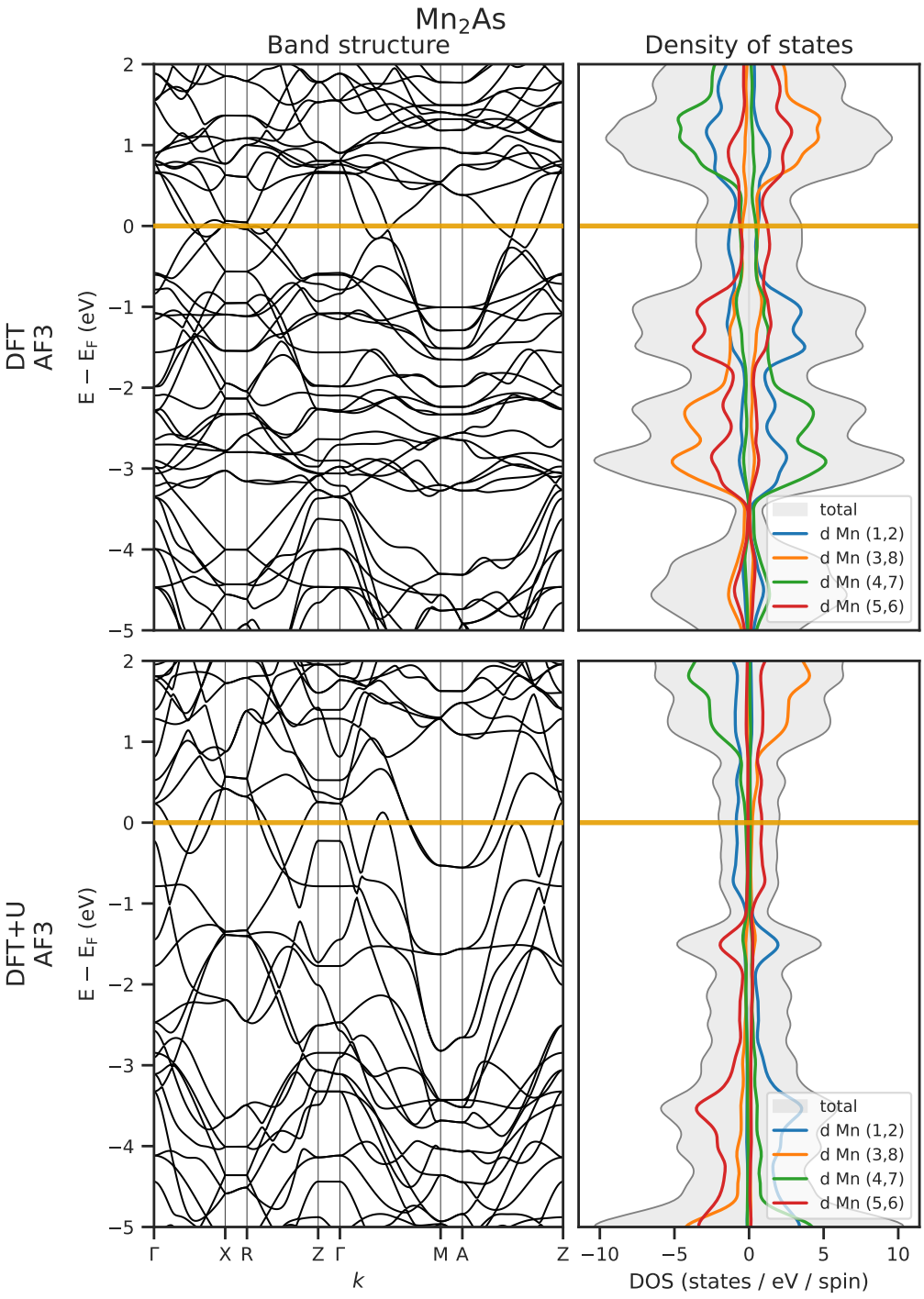


Figure 270: Band structure and Density of states of the lowest in energy calculations.

Material: Mn_2Sb

Configuration: Mn_2Sb

Structure

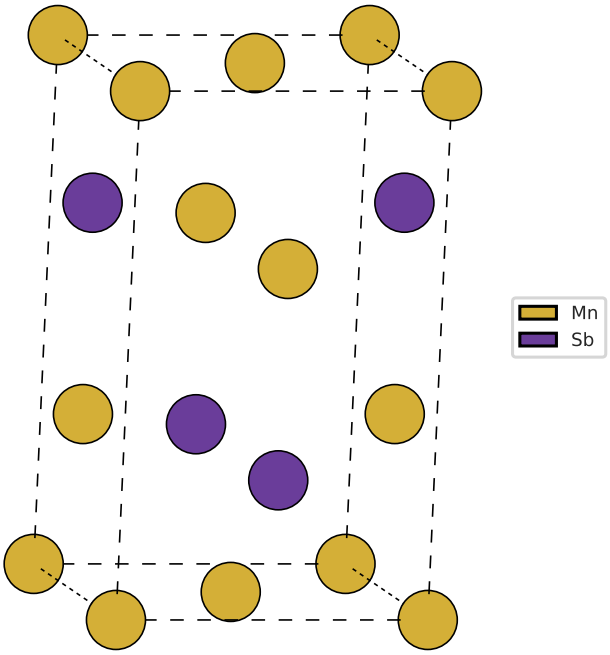


Figure 271: Structure of Mn_2Sb

a (Å)	c (Å)	z_1	z_2
4.0622	6.4373	0.2883	0.2807

Table 275: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of an Sb atom in the unit cell.

Magnetic structure and energy

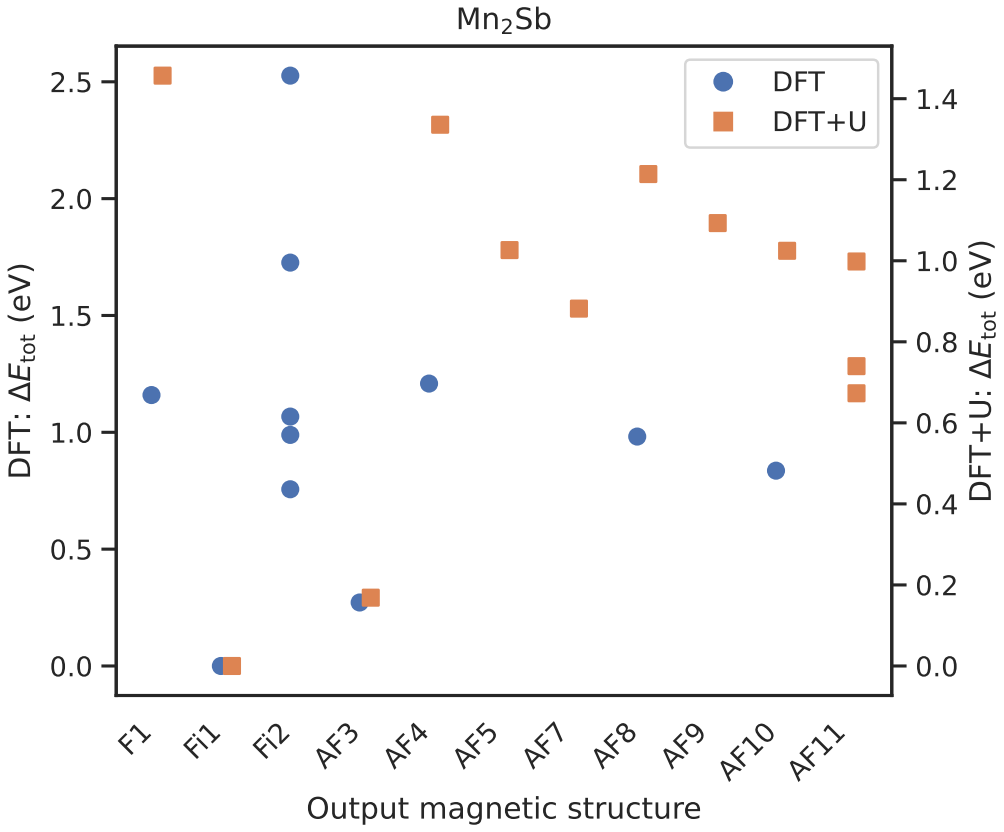


Figure 272: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-32281.915185	0.000000	3.11, 3.11, -4.16, -4.16, 3.11, 3.11, -4.16, -4.16
AF3	-32281.643502	0.271683	3.28, 3.28, -4.09, 4.09, -3.28, -3.28, 4.09, -4.09
Fi2	-32281.158935	0.756250	1.74, -3.48, 3.95, -3.89, -3.02, -2.92, 4.18, 3.97
AF10	-32281.079330	0.835855	3.07, -3.07, 3.94, 3.94, -3.07, 3.07, -3.94, -3.94
AF8	-32280.933376	0.981809	2.94, -2.94, -3.93, 3.93, -2.94, 2.94, -3.93, 3.93
Fi2	-32280.926279	0.988906	3.45, -2.07, -3.94, 4.01, 2.90, -3.33, 4.01, -3.94
Fi2	-32280.847869	1.067316	3.31, -2.87, -3.98, 3.93, -3.42, 2.07, 3.93, -3.98
F1	-32280.755744	1.159442	3.03, 3.03, 3.92, 3.92, 3.03, 3.03, 3.92, 3.92
AF4	-32280.706650	1.208535	3.09, 3.09, 3.86, -3.86, -3.09, -3.09, -3.86, 3.86
Fi2	-32280.188942	1.726243	3.44, -0.47, 4.01, -0.60, -3.15, -3.17, 4.20, -4.00
Fi2	-32279.388780	2.526406	-3.17, -3.07, 4.20, 3.97, 2.73, -3.50, 0.05, -0.13

Table 276: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
Fi1	-32269.398069	0.000000	4.36, 4.36, -4.93, -4.93, 4.36, 4.36, -4.93, -4.93
AF3	-32269.229470	0.168599	4.22, 4.22, -4.88, 4.88, -4.22, -4.22, 4.88, -4.88
AF11	-32268.725049	0.673021	4.29, 4.29, 4.53, 4.88, -4.29, -4.29, -4.53, -4.88
AF11	-32268.658126	0.739943	4.25, 4.25, -4.84, 4.84, -4.25, -4.25, -4.49, 4.49
AF7	-32268.516114	0.881955	4.40, -4.40, 4.70, 4.70, 4.40, -4.40, -4.70, -4.70
AF11	-32268.399825	0.998244	4.47, -4.37, -4.68, 4.68, 4.37, -4.47, 4.68, -4.68
AF10	-32268.373422	1.024647	4.41, -4.41, 4.69, 4.69, -4.41, 4.41, -4.69, -4.69
AF5	-32268.371701	1.026368	4.41, -4.41, -4.68, 4.68, 4.41, -4.41, -4.68, 4.68
AF9	-32268.305082	1.092988	4.47, -4.37, -4.69, 4.69, -4.47, 4.38, 4.69, -4.69
AF8	-32268.184085	1.213984	4.38, -4.38, -4.67, 4.67, -4.38, 4.38, -4.67, 4.67
AF4	-32268.062344	1.335726	4.18, 4.18, 4.52, -4.52, -4.18, -4.18, -4.52, 4.52
F1	-32267.941163	1.456906	4.17, 4.17, 4.51, 4.51, 4.17, 4.17, 4.51, 4.51

Table 277: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

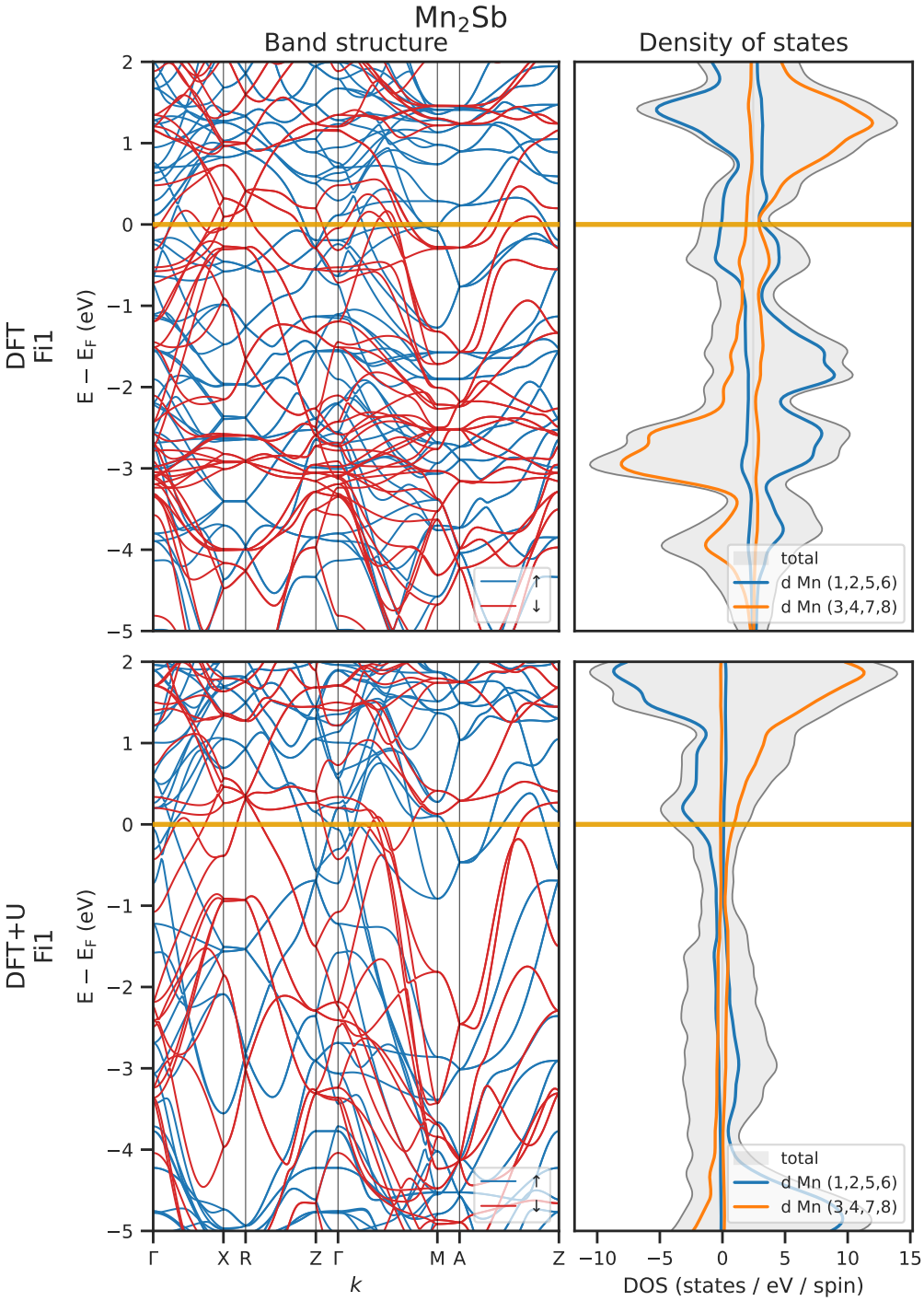


Figure 273: Band structure and Density of states of the lowest in energy calculations.

Material: NiMnAs

Configuration: NiMnAs ■ lower-energy

Structure

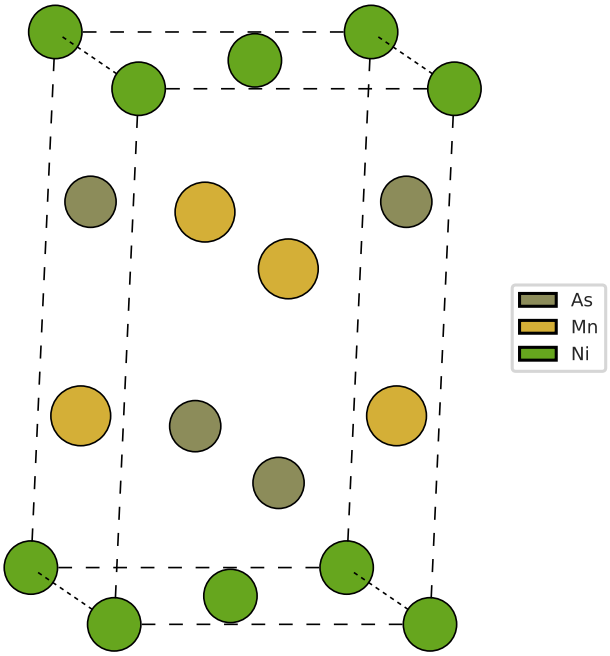


Figure 274: Structure of NiMnAs

a (Å)	c (Å)	z_1	z_2
3.7049	6.1093	0.3381	0.2586

Table 278: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3′	-41230.337485	0.000000	0.04, 0.04, -3.82, 3.82, -0.04, -0.04, 3.82, -3.82
AF2′	-41230.121480	0.216005	0.00, 0.00, -3.86, 3.86, 0.00, 0.00, -3.86, 3.86
F1′	-41229.893505	0.443979	-0.05, -0.05, -3.90, -3.90, -0.05, -0.05, -3.90, -3.90
AF1′	-41229.758060	0.579425	0.00, 0.00, 3.83, 3.83, 0.00, 0.00, -3.83, -3.83
Fi2′	-41229.040692	1.296793	0.01, 0.01, 3.78, -0.54, 0.04, 0.04, 3.91, -3.86

Table 279: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

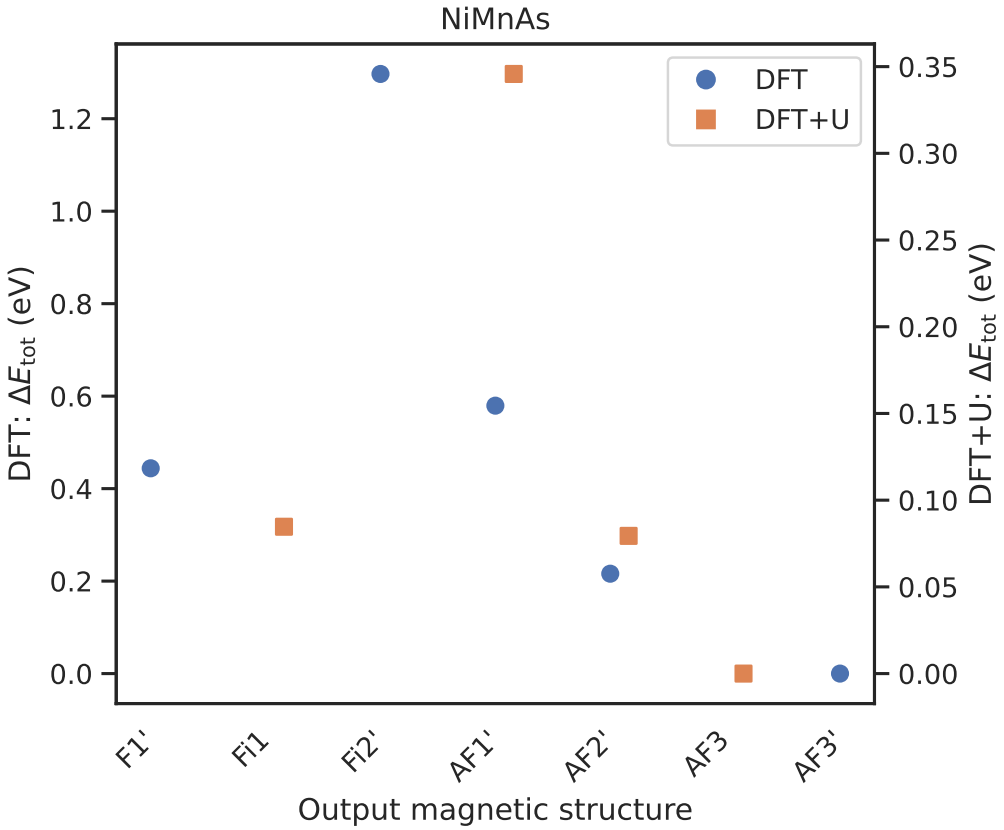


Figure 275: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF3	-41217.415218	0.000000	0.18, 0.18, -4.61, 4.61, -0.18, -0.18, 4.61, -4.61
AF3	-41217.415218	0.000000	0.18, 0.18, -4.61, 4.61, -0.18, -0.18, 4.61, -4.61
AF3	-41217.415218	0.000000	0.18, 0.18, -4.61, 4.61, -0.18, -0.18, 4.61, -4.61
AF3	-41217.415218	0.000000	-0.18, -0.18, 4.61, -4.61, 0.18, 0.18, -4.61, 4.61
AF2′	-41217.335808	0.079411	0.00, 0.00, -4.62, 4.62, 0.00, 0.00, -4.62, 4.62
AF2′	-41217.335808	0.079411	0.00, 0.00, -4.62, 4.62, 0.00, 0.00, -4.62, 4.62
AF2′	-41217.335808	0.079411	0.00, 0.00, -4.62, 4.62, 0.00, 0.00, -4.62, 4.62
Fi1	-41217.330542	0.084677	0.18, 0.18, -4.62, -4.62, 0.18, 0.18, -4.62, -4.62
Fi1	-41217.330542	0.084677	-0.18, -0.18, 4.62, 4.62, -0.18, -0.18, 4.62, 4.62
AF1′	-41217.069444	0.345774	0.00, 0.00, 4.61, 4.61, 0.00, 0.00, -4.61, -4.61
AF1′	-41217.069444	0.345774	0.00, 0.00, 4.61, 4.61, 0.00, 0.00, -4.61, -4.61
AF1′	-41217.069444	0.345774	0.00, 0.00, 4.61, 4.61, 0.00, 0.00, -4.61, -4.61

Table 280: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

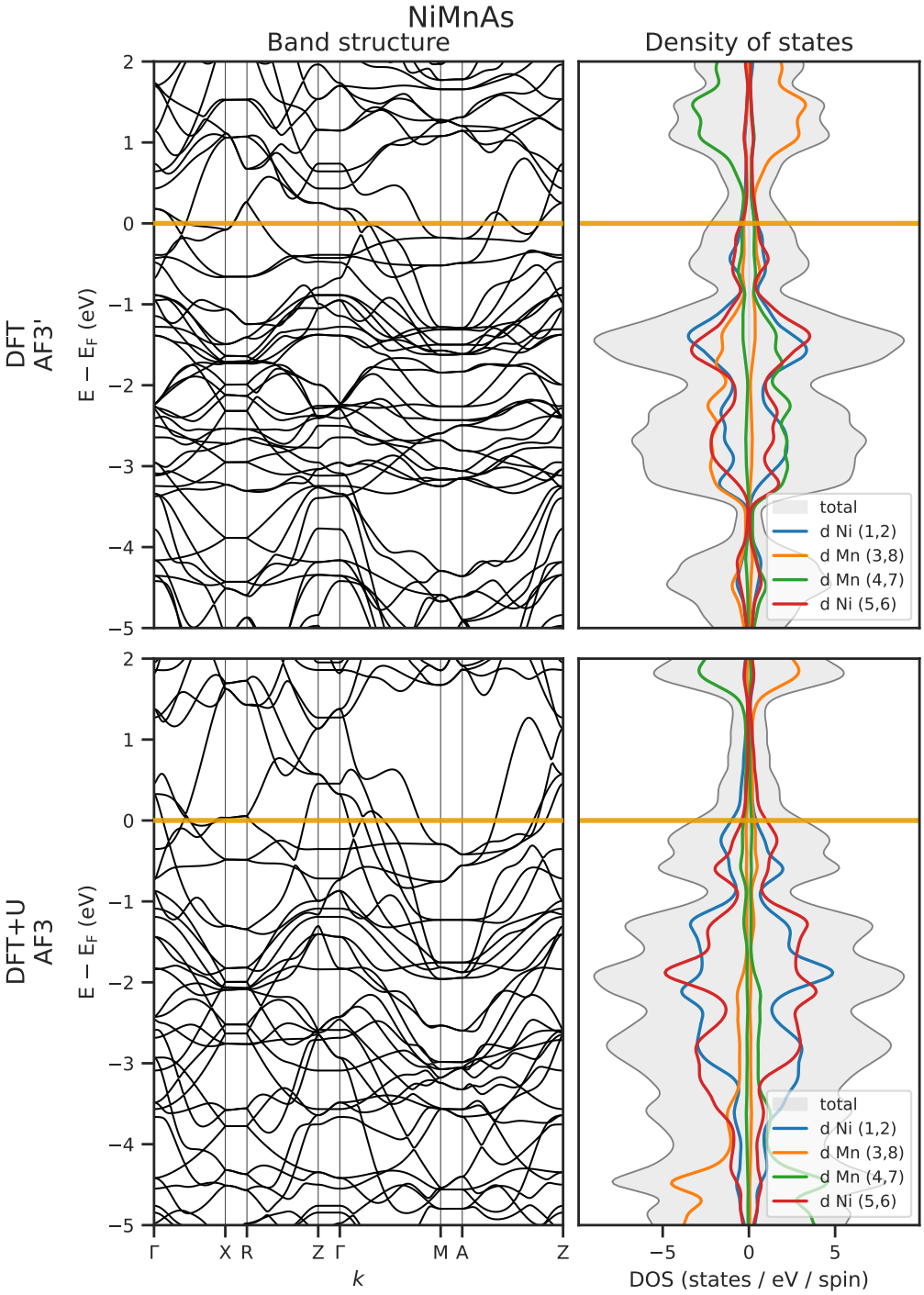


Figure 276: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnNiAs ■ higher-energy

Structure

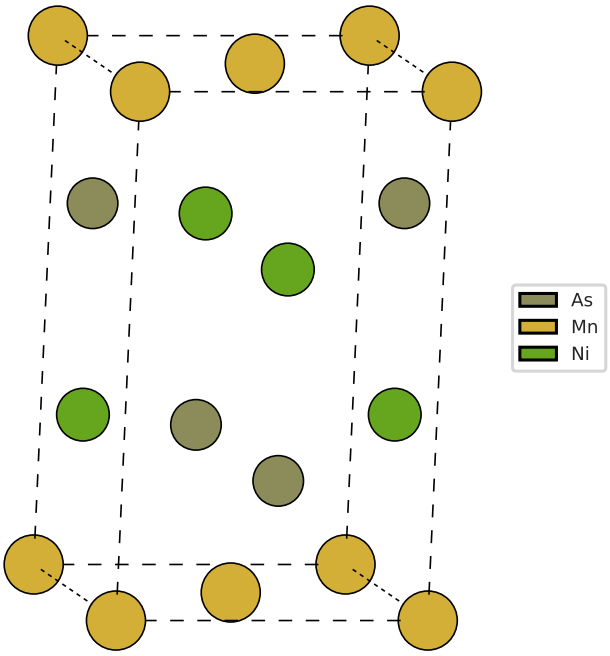


Figure 277: Structure of MnNiAs

a (Å)	c (Å)	z_1	z_2
3.6848	6.0610	0.3036	0.2964

Table 281: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

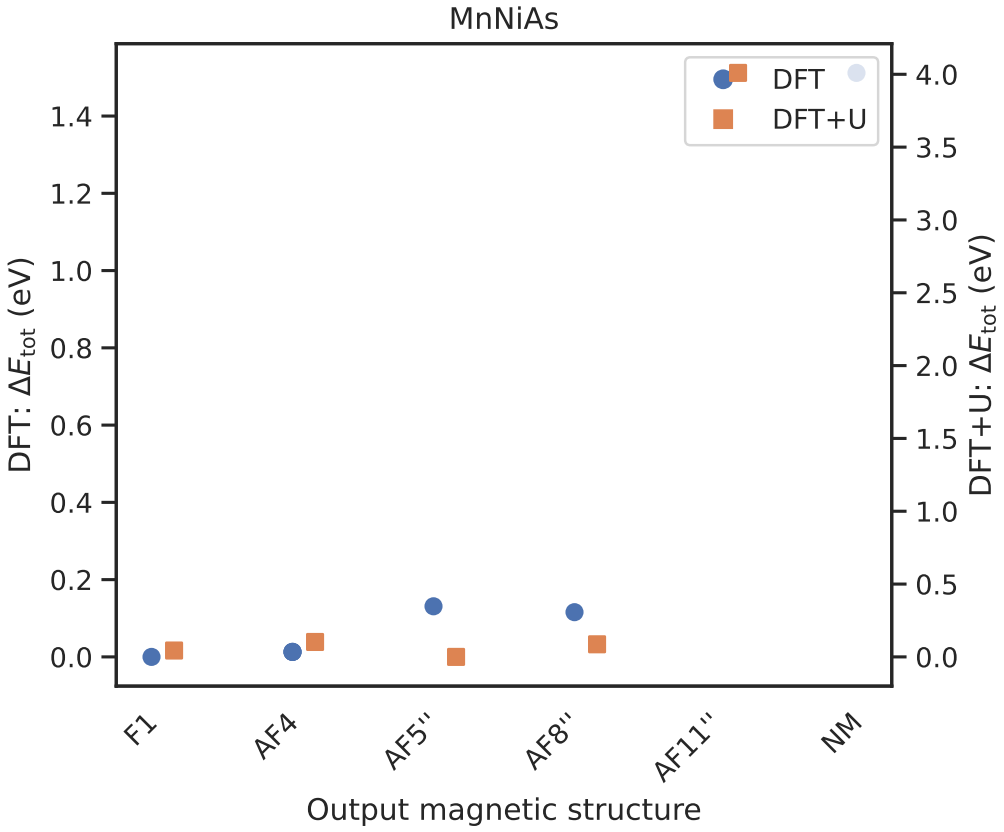


Figure 278: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-41228.421094	0.000000	2.58, 2.58, 0.14, 0.14, 2.58, 2.58, 0.14, 0.14
AF4	-41228.408255	0.012840	2.62, 2.62, 0.19, -0.19, -2.62, -2.62, -0.19, 0.19
AF4	-41228.408041	0.013053	2.62, 2.62, 0.19, -0.19, -2.62, -2.62, -0.19, 0.19
AF8″	-41228.305338	0.115756	3.04, -3.04, 0.00, 0.00, -3.04, 3.04, 0.00, 0.00
AF5″	-41228.290106	0.130988	3.10, -3.10, 0.00, 0.00, 3.10, -3.10, 0.00, 0.00
NM	-41226.909367	1.511727	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 282: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-41213.510407	0.000000	4.49, -4.49, 0.00, 0.00, 4.49, -4.49, 0.00, 0.00
AF5″	-41213.510407	0.000000	4.49, -4.49, 0.00, 0.00, 4.49, -4.49, 0.00, 0.00
AF5″	-41213.510406	0.000000	4.49, -4.49, 0.00, 0.00, 4.49, -4.49, 0.00, 0.00
F1	-41213.466642	0.043765	4.33, 4.33, 0.26, 0.26, 4.33, 4.33, 0.26, 0.26
F1	-41213.466642	0.043765	4.33, 4.33, 0.26, 0.26, 4.33, 4.33, 0.26, 0.26
AF8″	-41213.423914	0.086493	4.49, -4.49, 0.00, 0.00, -4.49, 4.49, 0.00, 0.00
AF8″	-41213.423913	0.086493	4.49, -4.49, 0.00, 0.00, -4.49, 4.49, 0.00, 0.00
AF4	-41213.407867	0.102540	4.33, 4.33, 0.32, -0.32, -4.33, -4.33, -0.32, 0.32
AF4	-41213.407867	0.102540	4.33, 4.33, 0.32, -0.32, -4.33, -4.33, -0.32, 0.32
AF4	-41213.407867	0.102540	4.33, 4.33, 0.32, -0.32, -4.33, -4.33, -0.32, 0.32
AF4	-41213.407866	0.102541	4.33, 4.33, 0.32, -0.32, -4.33, -4.33, -0.32, 0.32
AF11″	-41209.500762	4.009644	0.46, -0.46, 0.06, -0.06, -4.50, 4.48, -0.01, -0.00

Table 283: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

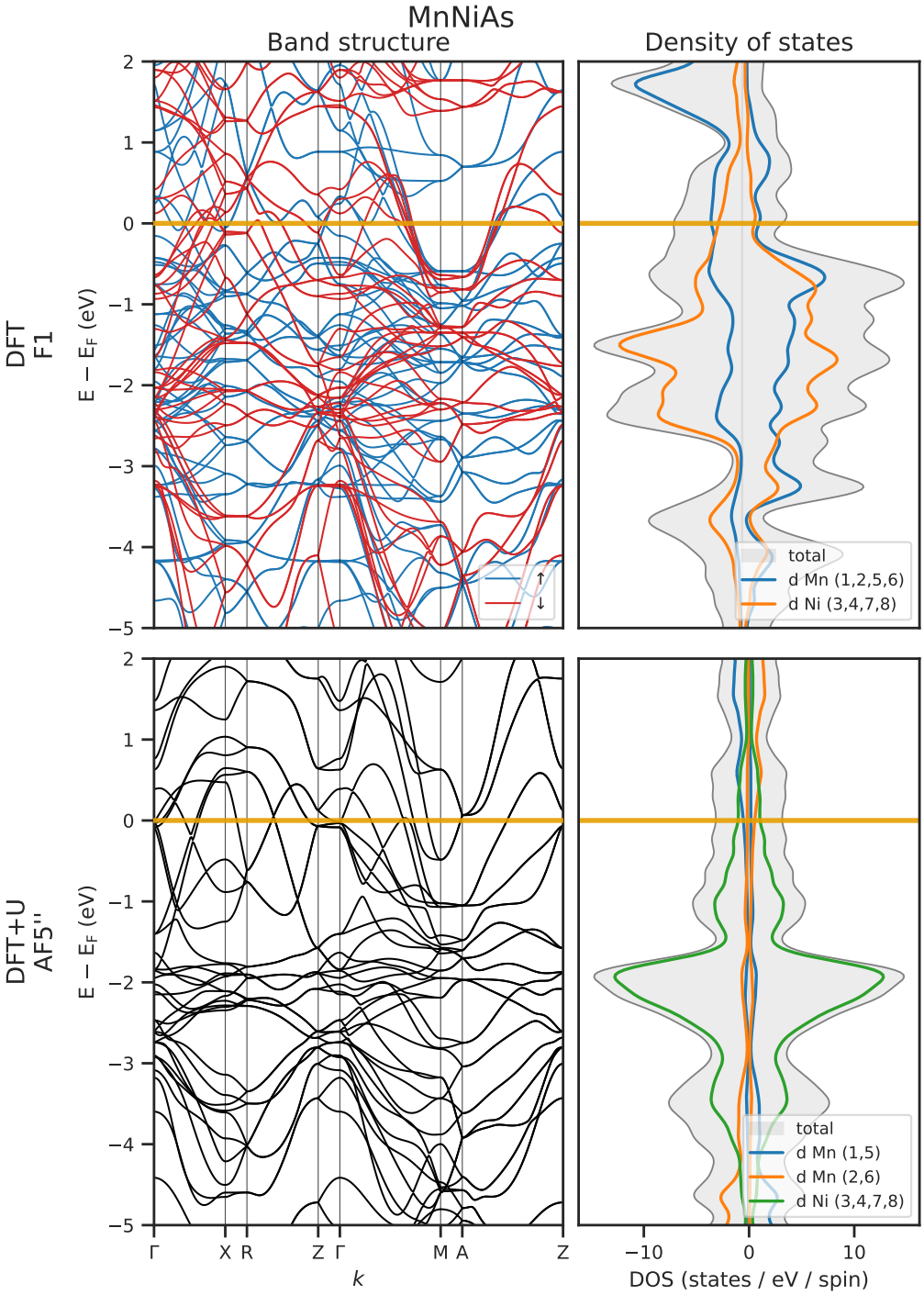


Figure 279: Band structure and Density of states of the lowest in energy calculations.

Material: NiMnSb

Configuration: NiMnSb ■ lower-energy

Structure

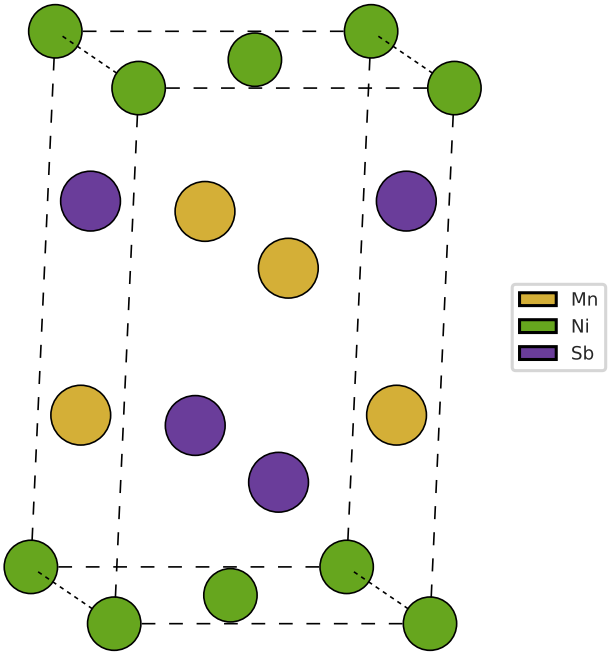


Figure 280: Structure of NiMnSb

a (Å)	c (Å)	z_1	z_2
4.1224	6.1231	0.2734	0.2711

Table 284: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of an Mn atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1′	-39115.871406	0.000000	-0.08, -0.08, -4.23, -4.23, -0.08, -0.08, -4.23, -4.23
AF3′	-39115.730678	0.140728	0.07, 0.07, 4.18, -4.18, -0.07, -0.07, -4.18, 4.18
AF2′	-39115.598688	0.272718	0.00, 0.00, -4.20, 4.20, 0.00, 0.00, -4.20, 4.20
AF1′	-39115.480241	0.391165	0.00, 0.00, 4.28, 4.28, 0.00, 0.00, -4.28, -4.28

Table 285: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

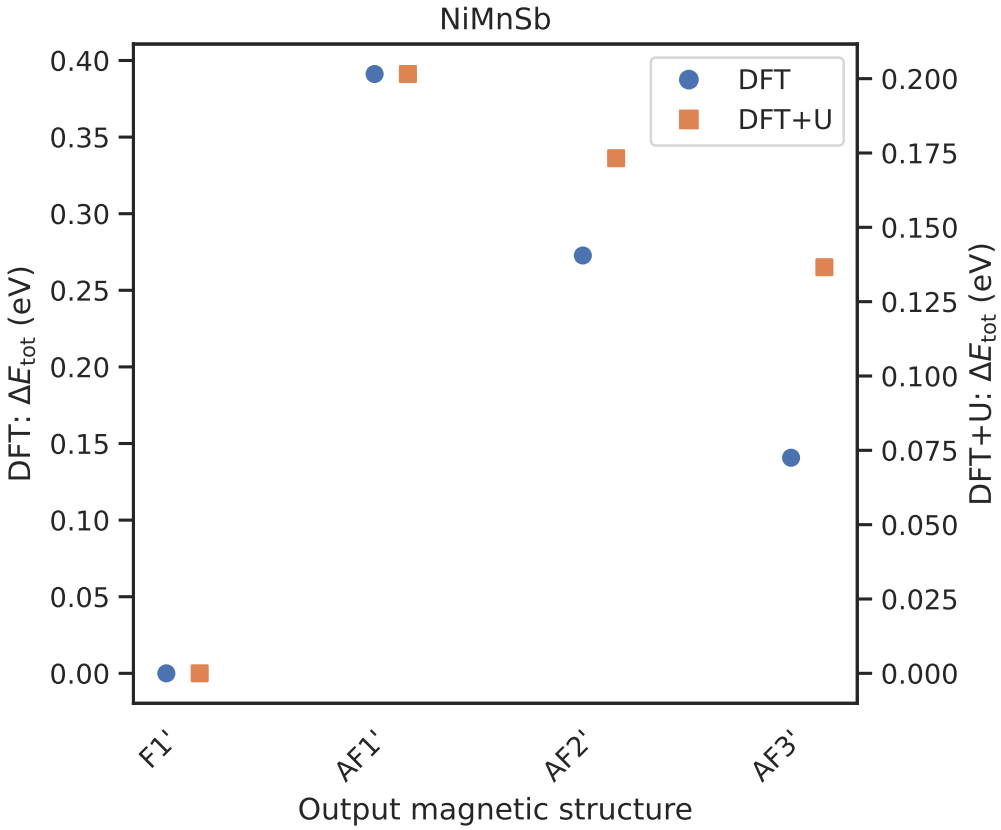


Figure 281: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
F1′	-39104.526696	0.000000	0.03, 0.03, -4.81, -4.81, 0.03, 0.03, -4.81, -4.81
F1′	-39104.526696	0.000000	-0.03, -0.03, 4.81, 4.81, -0.03, -0.03, 4.81, 4.81
AF3′	-39104.390120	0.136576	0.02, 0.02, -4.77, 4.77, -0.02, -0.02, 4.77, -4.77
AF3′	-39104.390120	0.136576	0.02, 0.02, -4.77, 4.77, -0.02, -0.02, 4.77, -4.77
AF3′	-39104.390120	0.136576	-0.02, -0.02, 4.77, -4.77, 0.02, 0.02, -4.77, 4.77
AF3′	-39104.390120	0.136576	0.02, 0.02, -4.77, 4.77, -0.02, -0.02, 4.77, -4.77
AF2′	-39104.353453	0.173243	0.00, 0.00, -4.78, 4.78, 0.00, 0.00, -4.78, 4.78
AF2′	-39104.353432	0.173264	0.00, 0.00, -4.78, 4.78, 0.00, 0.00, -4.78, 4.78
AF2′	-39104.353424	0.173272	0.00, 0.00, -4.78, 4.78, 0.00, 0.00, -4.78, 4.78
AF1′	-39104.325137	0.201559	0.00, 0.00, 4.84, 4.84, 0.00, 0.00, -4.84, -4.84
AF1′	-39104.325137	0.201559	0.00, 0.00, 4.84, 4.84, 0.00, 0.00, -4.84, -4.84
AF1′	-39104.325137	0.201559	0.00, 0.00, 4.84, 4.84, 0.00, 0.00, -4.84, -4.84

Table 286: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

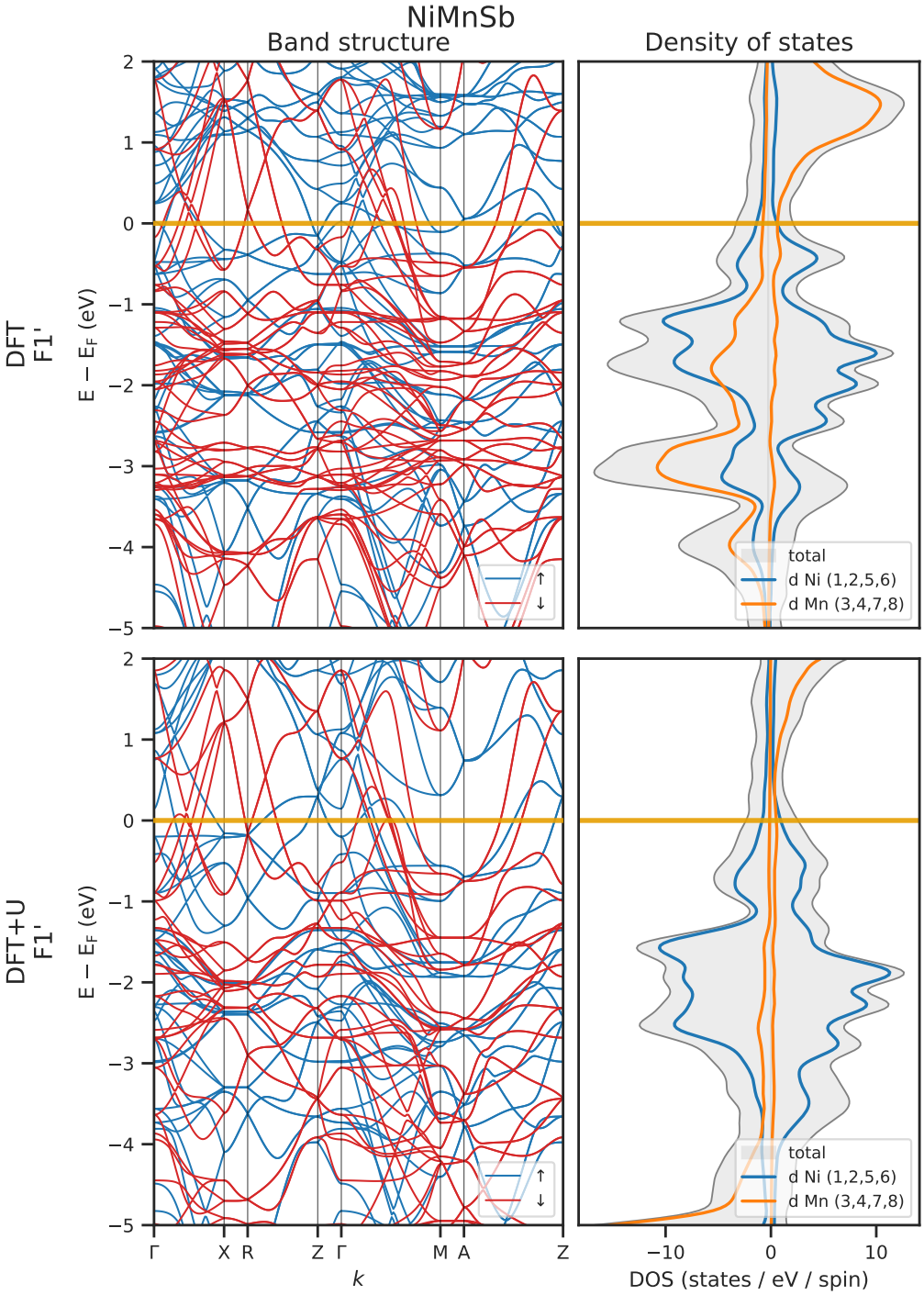


Figure 282: Band structure and Density of states of the lowest in energy calculations.

Configuration: MnNiSb ■ higher-energy

Structure

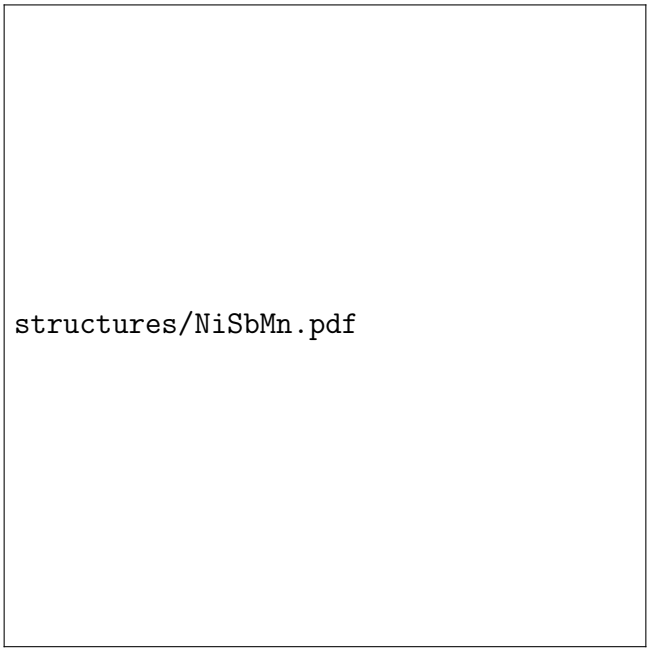


Figure 283: Structure of MnNiSb

a (Å)	c (Å)	z_1	z_2
3.8513	6.5510	0.2651	0.3229

Table 287: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of an Mn atom and z_2 is the independent z-coordinate of a Ni atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
AF5″	-39115.100351	0.000000	3.68, -3.68, 0.00, 0.00, 3.69, -3.69, 0.00, 0.00
AF8″	-39114.952893	0.147458	3.68, -3.68, 0.00, 0.00, -3.68, 3.68, 0.00, 0.00
F1	-39114.808545	0.291806	3.67, 3.67, 0.27, 0.27, 3.68, 3.68, 0.27, 0.27
AF4	-39114.751821	0.348530	3.34, 3.34, 0.21, -0.21, -3.30, -3.30, -0.21, 0.21
AF4	-39114.751025	0.349325	3.33, 3.33, 0.21, -0.21, -3.33, -3.33, -0.21, 0.21

Table 288: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

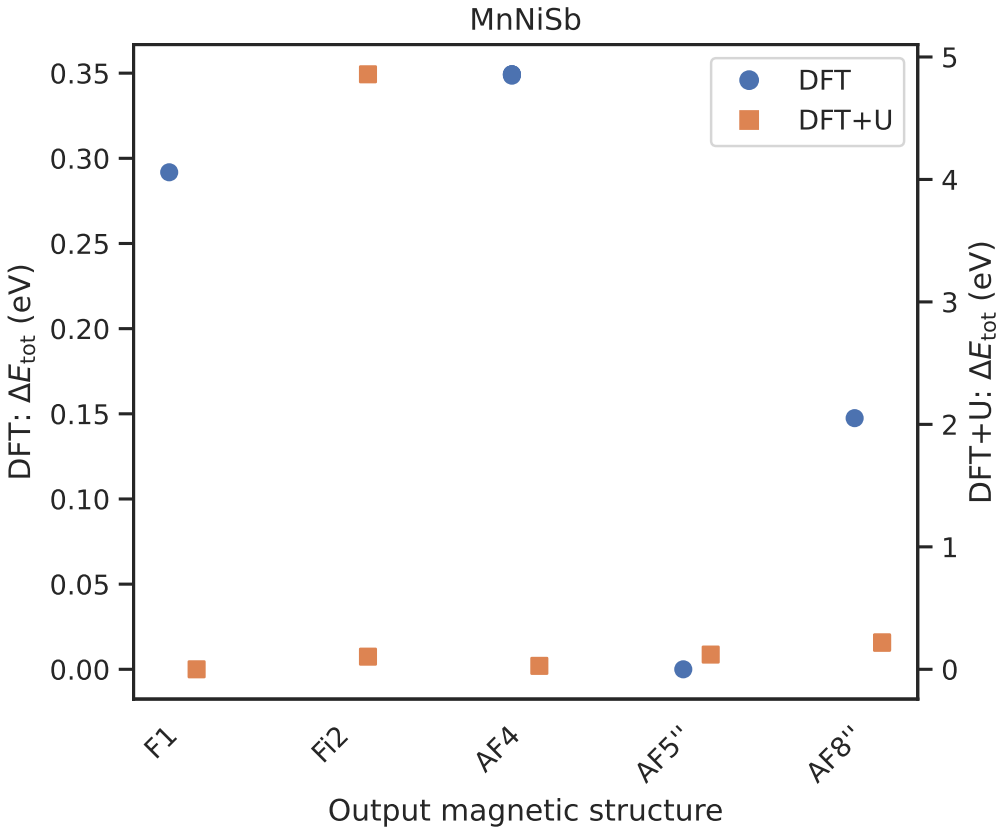


Figure 284: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
F1	-39102.034781	0.000000	4.45, 4.45, 0.22, 0.22, 4.45, 4.45, 0.22, 0.22
AF4	-39102.006644	0.028137	4.46, 4.46, 0.22, -0.22, -4.46, -4.46, -0.22, 0.22
AF4	-39102.006644	0.028137	4.46, 4.46, 0.22, -0.22, -4.46, -4.46, -0.22, 0.22
AF4	-39102.006644	0.028137	4.46, 4.46, 0.22, -0.22, -4.46, -4.46, -0.22, 0.22
AF4	-39102.006643	0.028138	4.46, 4.46, 0.22, -0.22, -4.46, -4.46, -0.22, 0.22
Fi2	-39101.931422	0.103360	4.46, 4.46, 0.21, 0.03, 4.71, -4.68, 0.03, 0.21
AF5″	-39101.914409	0.120372	4.69, -4.69, 0.00, 0.00, 4.69, -4.69, 0.00, 0.00
AF5″	-39101.914408	0.120373	4.69, -4.69, 0.00, 0.00, 4.69, -4.69, 0.00, 0.00
AF8″	-39101.816542	0.218239	4.70, -4.70, 0.00, 0.00, -4.70, 4.70, 0.00, 0.00
AF8″	-39101.816289	0.218492	4.70, -4.70, 0.00, 0.00, -4.70, 4.70, 0.00, 0.00
Fi2	-39097.176241	4.858540	-4.68, 4.71, 0.00, -0.05, 0.18, 0.66, -0.11, 0.01

Table 289: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

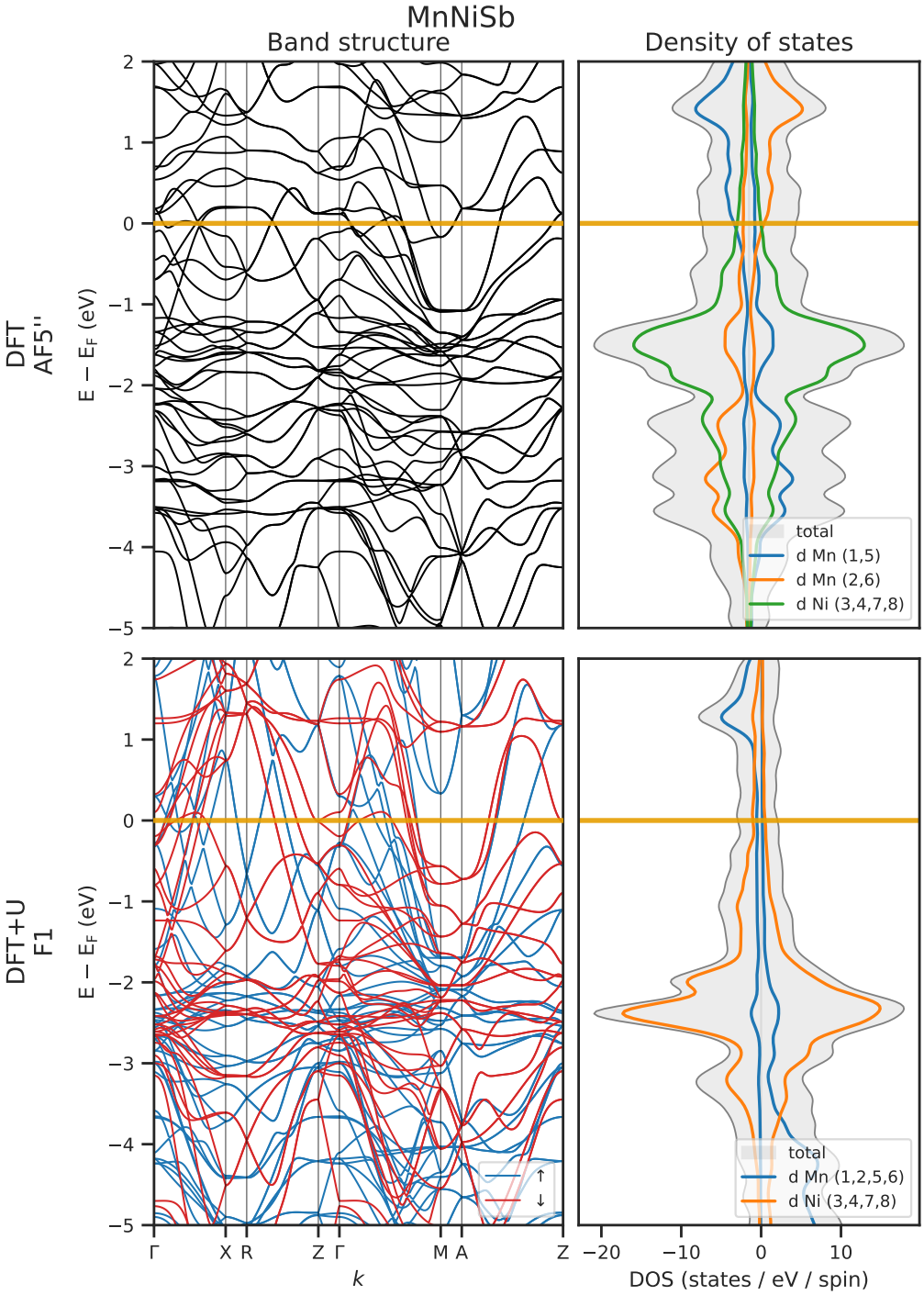


Figure 285: Band structure and Density of states of the lowest in energy calculations.

Material: Ni_2As

Configuration: Ni_2As

Structure

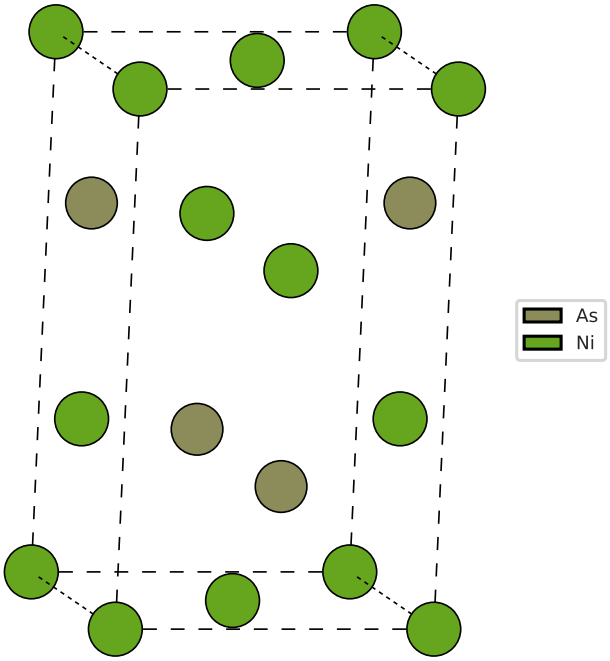


Figure 286: Structure of Ni_2As

a (Å)	c (Å)	z_1	z_2
3.6224	5.9331	0.3338	0.2713

Table 290: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of an As atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-48061.036386	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 291: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

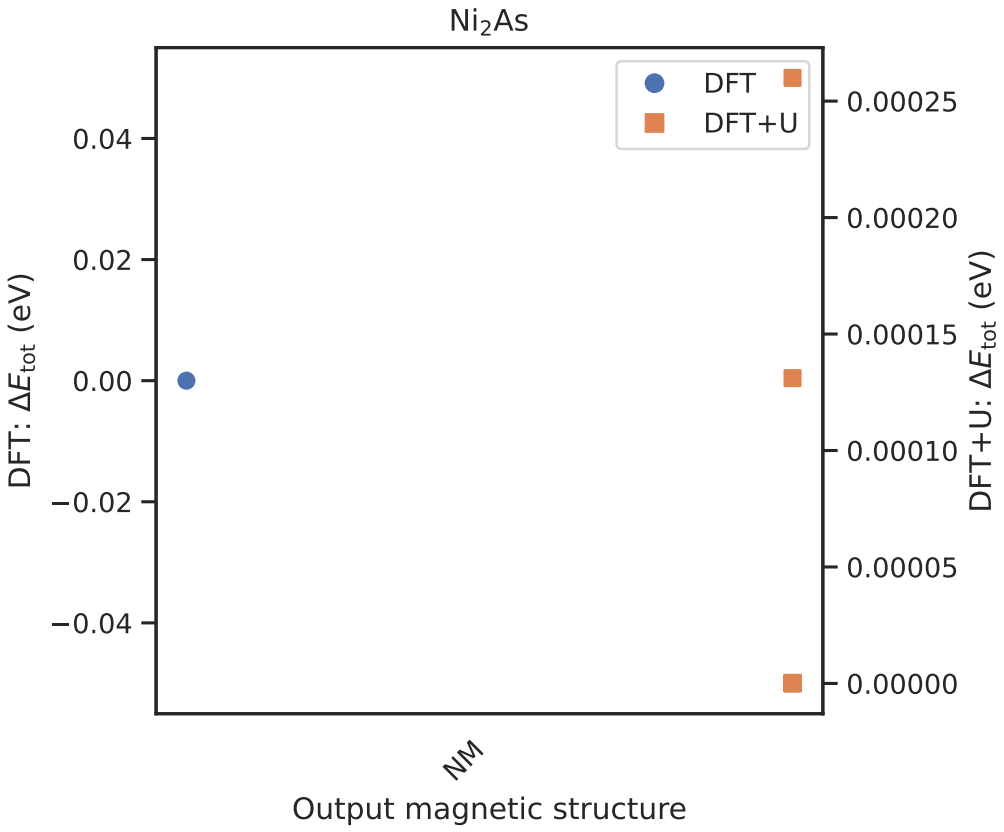


Figure 287: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-48046.348683	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348682	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348682	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348682	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348682	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348682	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348682	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348552	0.000131	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-48046.348423	0.000260	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 292: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

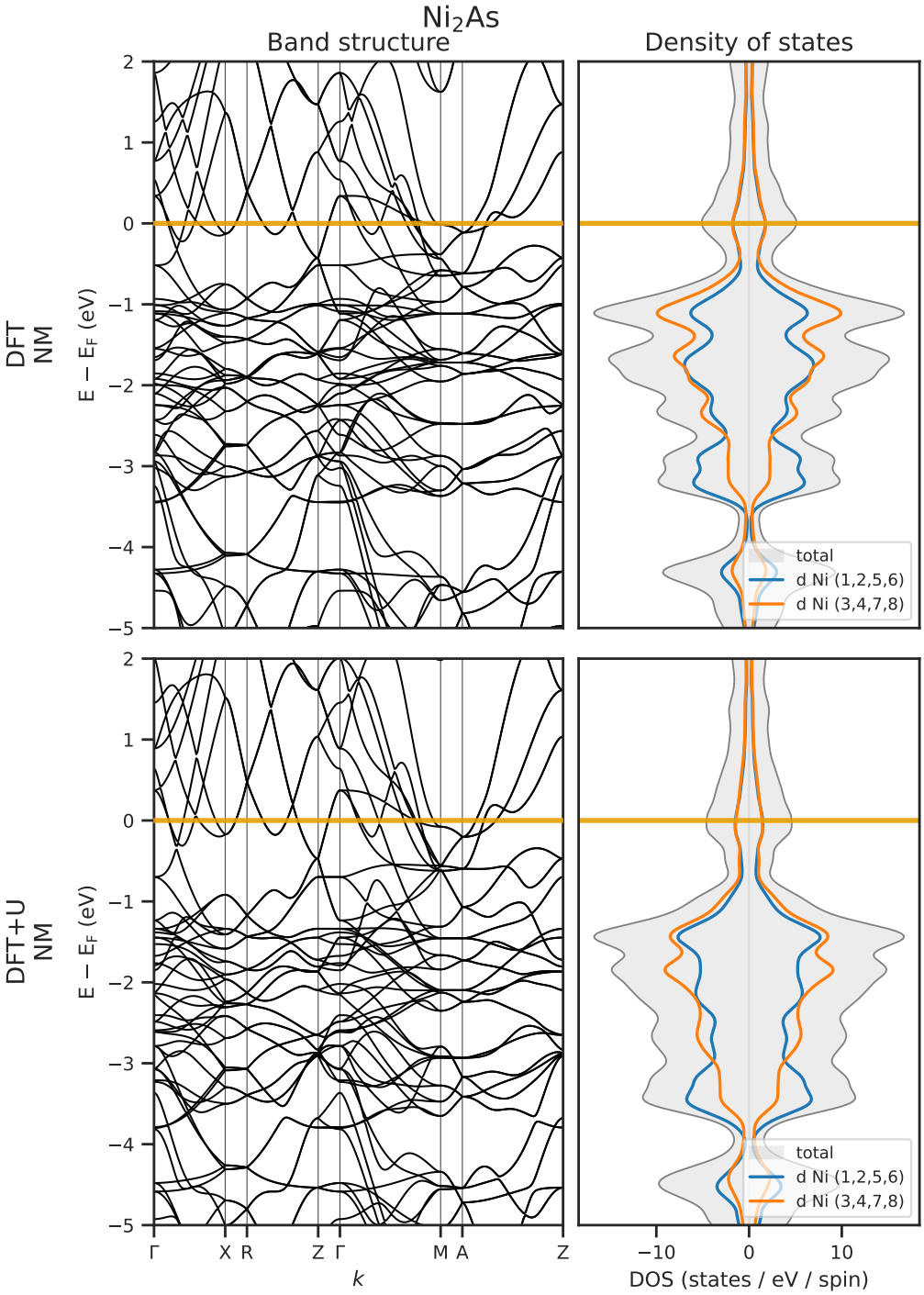


Figure 288: Band structure and Density of states of the lowest in energy calculations.

Material: Ni_2Sb

Configuration: Ni_2Sb

Structure

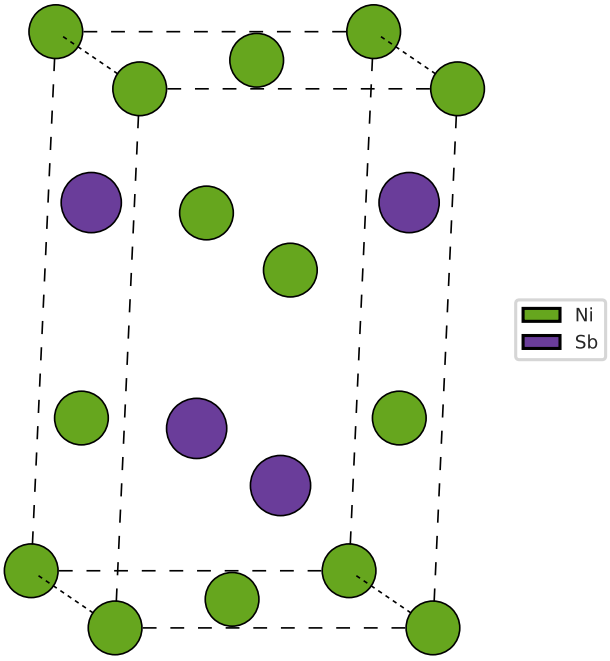


Figure 289: Structure of Ni_2Sb

a (Å)	c (Å)	z_1	z_2
3.8308	6.1571	0.2747	0.3007

Table 293: a and c are the lattice parameters of the unit cell. z_1 is the independent z-coordinate of a Ni atom and z_2 is the independent z-coordinate of an Sb atom in the unit cell.

Magnetic structure and energy

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_B)
NM	-45947.598705	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 294: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT calculation.

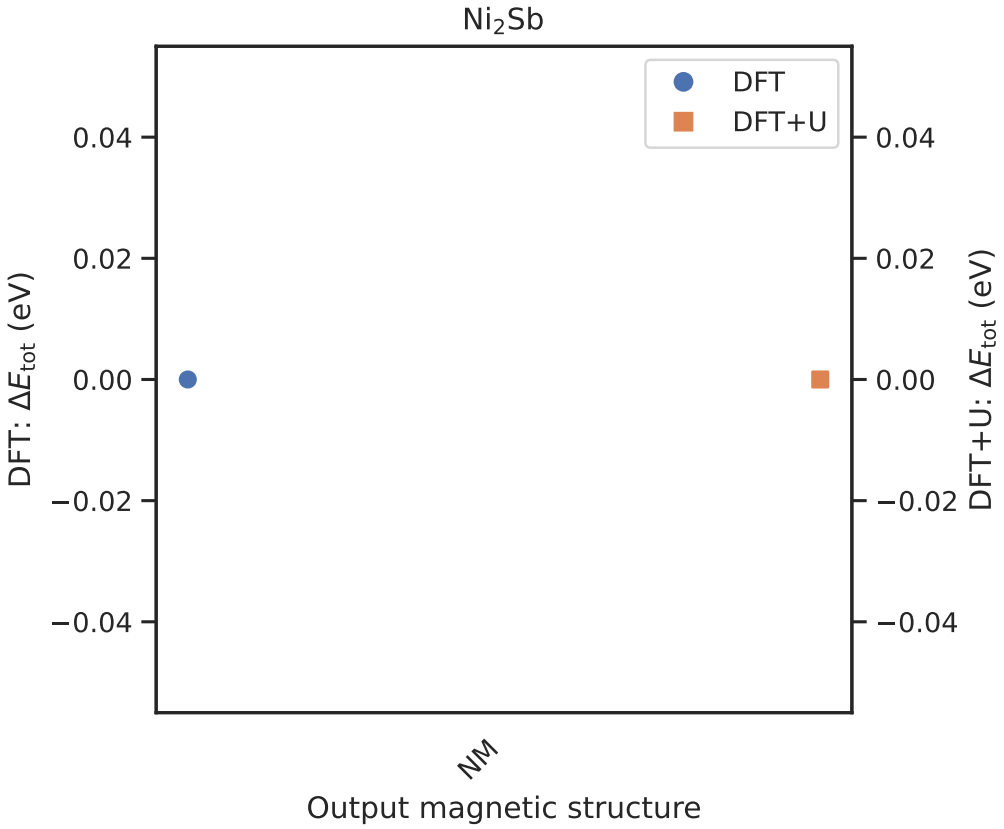


Figure 290: Relative energies of magnetic structures calculated with DFT and DFT+U. For each method, energies are given relative to the lowest-energy configuration within that group.

Magnetic structure	E_{tot} (eV)	ΔE (eV)	Magnetic moments (μ_{B})
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	-0.00, -0.00, 0.00, 0.00, -0.00, -0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188490	0.000000	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
NM	-45933.188489	0.000001	0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00

Table 295: Output magnetic structure, total energy, and energy difference relative to the lowest-energy DFT+U calculation.

Band structure and DOS

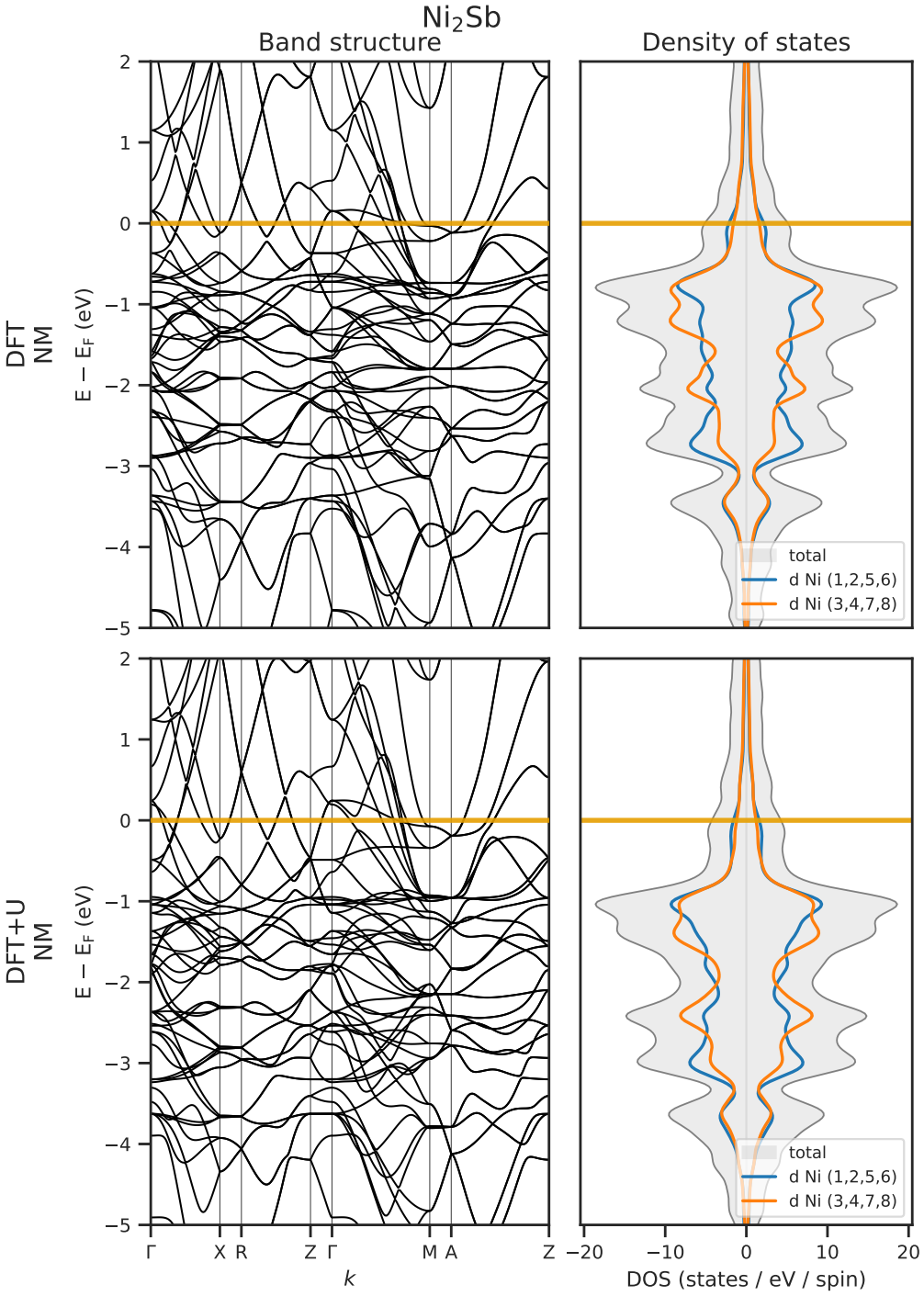


Figure 291: Band structure and Density of states of the lowest in energy calculations.