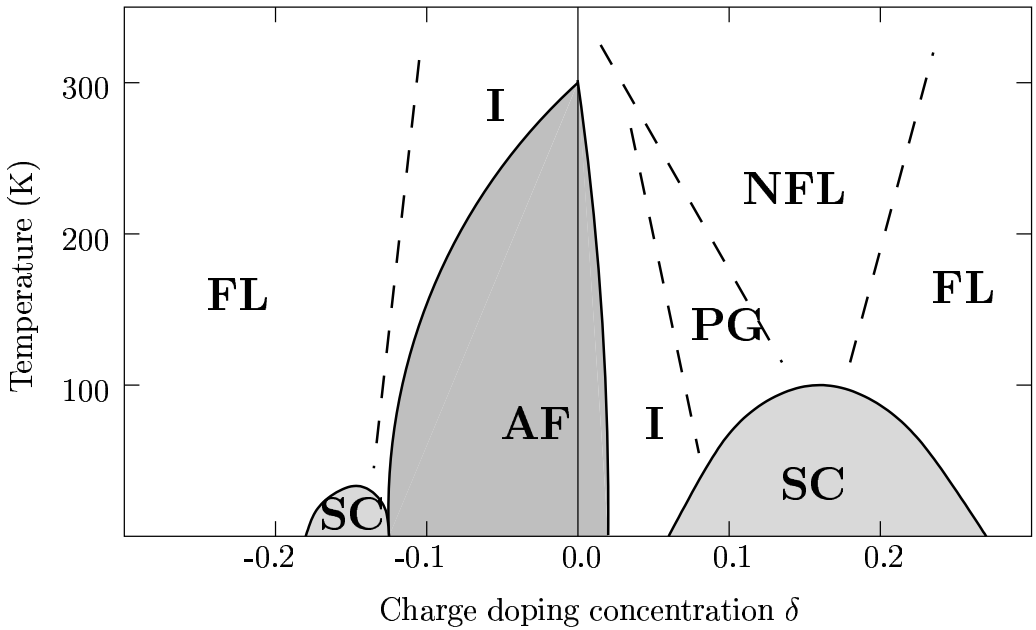
Helmut Eschrig and Klaus Koepernik
Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden
Leibniz-Institute for Solid State and Materials Research Dresden

DENSITY FUNCTIONAL APPROACH TO THE ELECTRONIC STRUCTURE OF DOPED CUPRATES

1. Introduction
2. The Model System
3. The Computational Scheme
4. Results
5. Conclusions

1. INTRODUCTION

Temperature vs. doping phase diagram of doped cuprates:



At $T = 0$:

sequence: AF insulator$\longrightarrow x \approx 0.05 \longrightarrow$ spin glass$\longrightarrow x \approx 0.16 \longrightarrow$Fermi liquid

Questions:

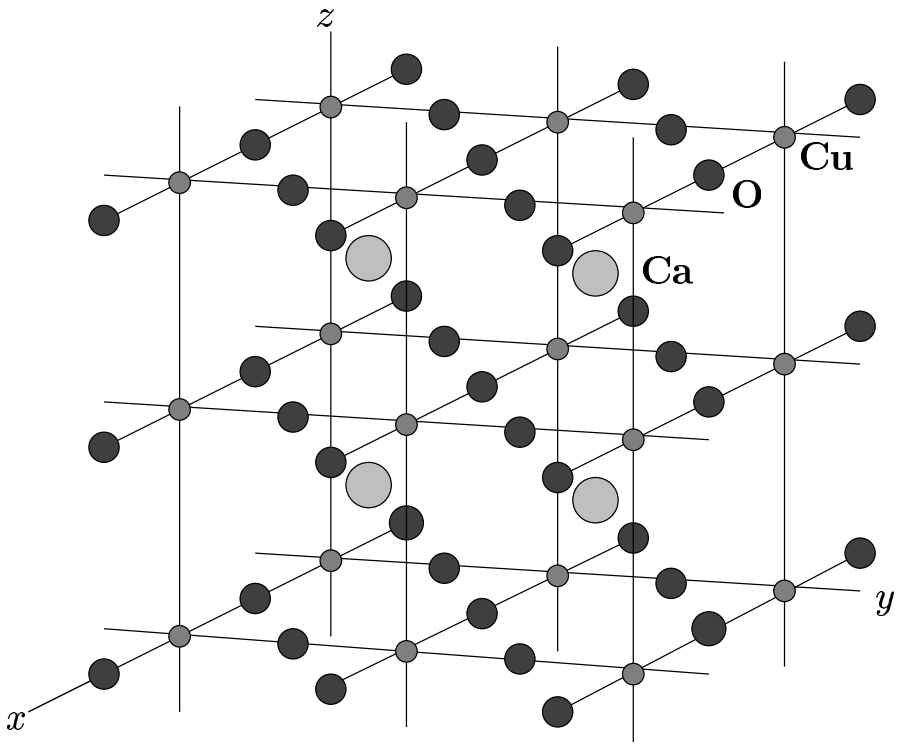
How well can a Hubbard U on copper sites describe the sequence of ground states?

How does U depend on doping?

How do the magnetic interactions behave?

2. THE MODEL SYSTEM

$Ca_{1-x}K_xCuO_2$ as the simplest model structure:



3. THE COMPUTATIONAL SCHEME

LSDA+U - CPA approach using our FPLO code

total energy calculations of constrained spin structures

CPA Bloch spectral densities (band structure)
understanding the Kohn-Sham potential as an approximation to the electron-electron self-energy

Spin structures:

AFM: antiferromagnetic structure with alternating copper spins in all directions

FM: ferromagnetic order of copper spins

DLM: disordered local moments on copper sites, treated in CPA

NSP: non-magnetic state (equal occupation of spin up and down Cu states)

Oxygen spin polarization:

AFM: for symmetry reasons no polarization

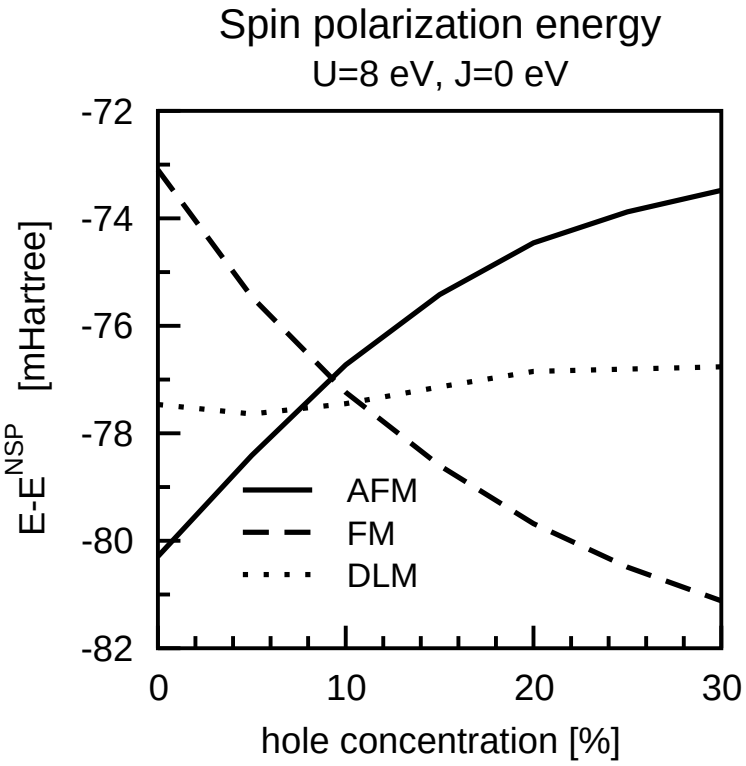
FM: always ferrimagnetic polarization obtained

DLM: single-site CPA treatment does not allow for polarization

NSP: no polarization as constraint

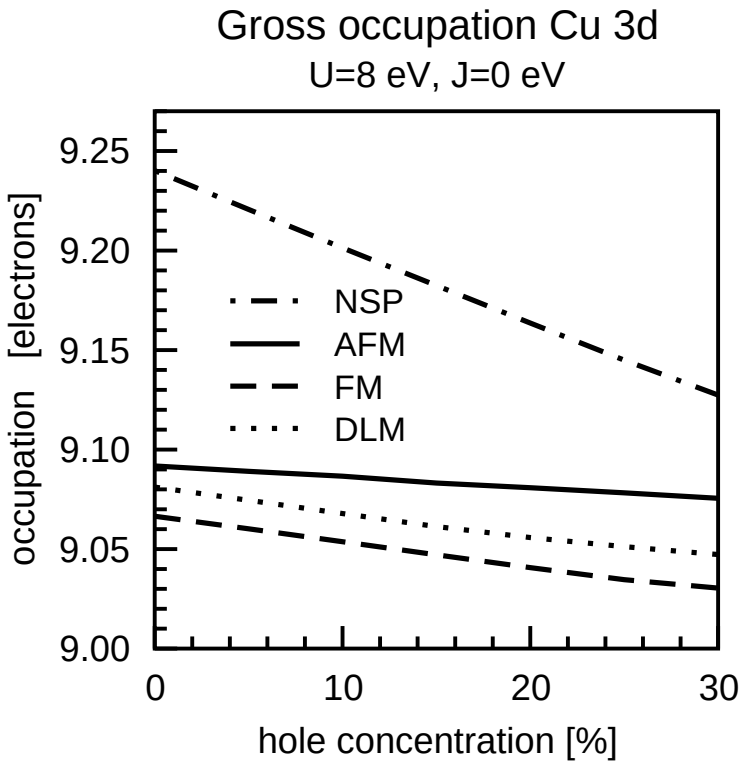
4. RESULTS

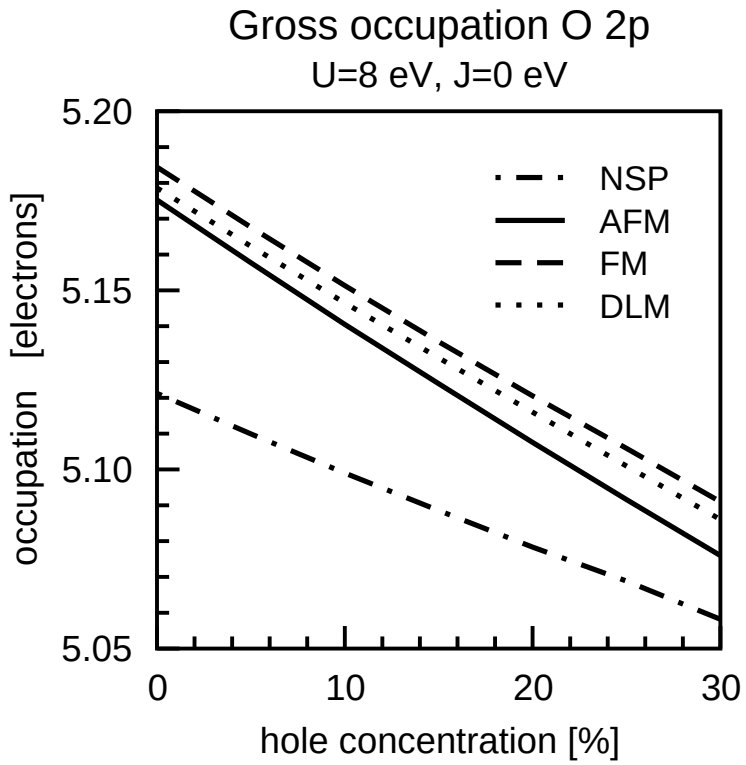
4.1 Total Energy Differences (per 2 Cu atoms):



For $x = 0$, the energy difference between the AFM and the FM states well corresponds to the experimental nearest neighbor Cu-Cu exchange constant: it yields $J \approx -100$ meV.

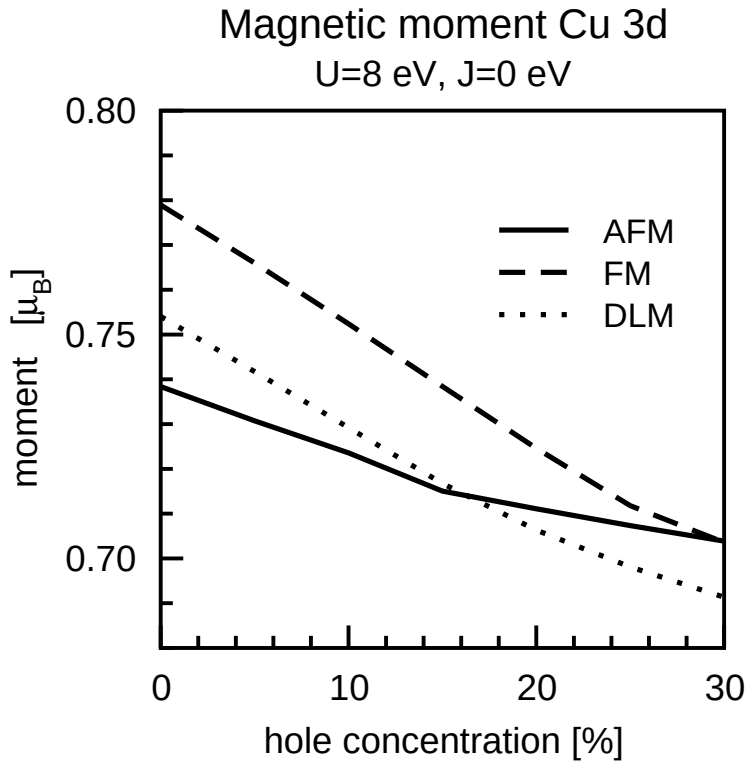
4.2 Site Occupation:

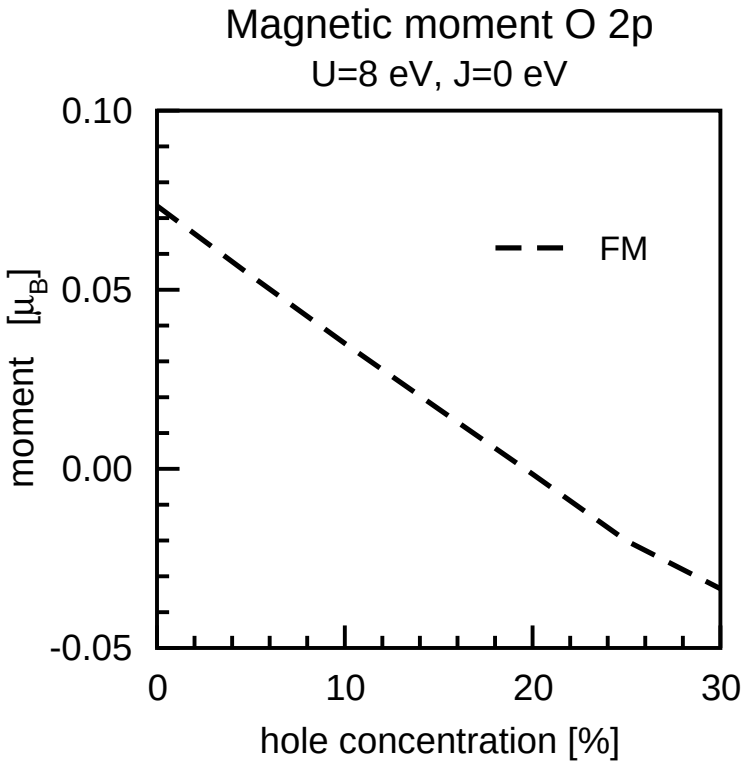




In the spin polarized cases, the doped holes nearly exclusively go to the oxygen sites.

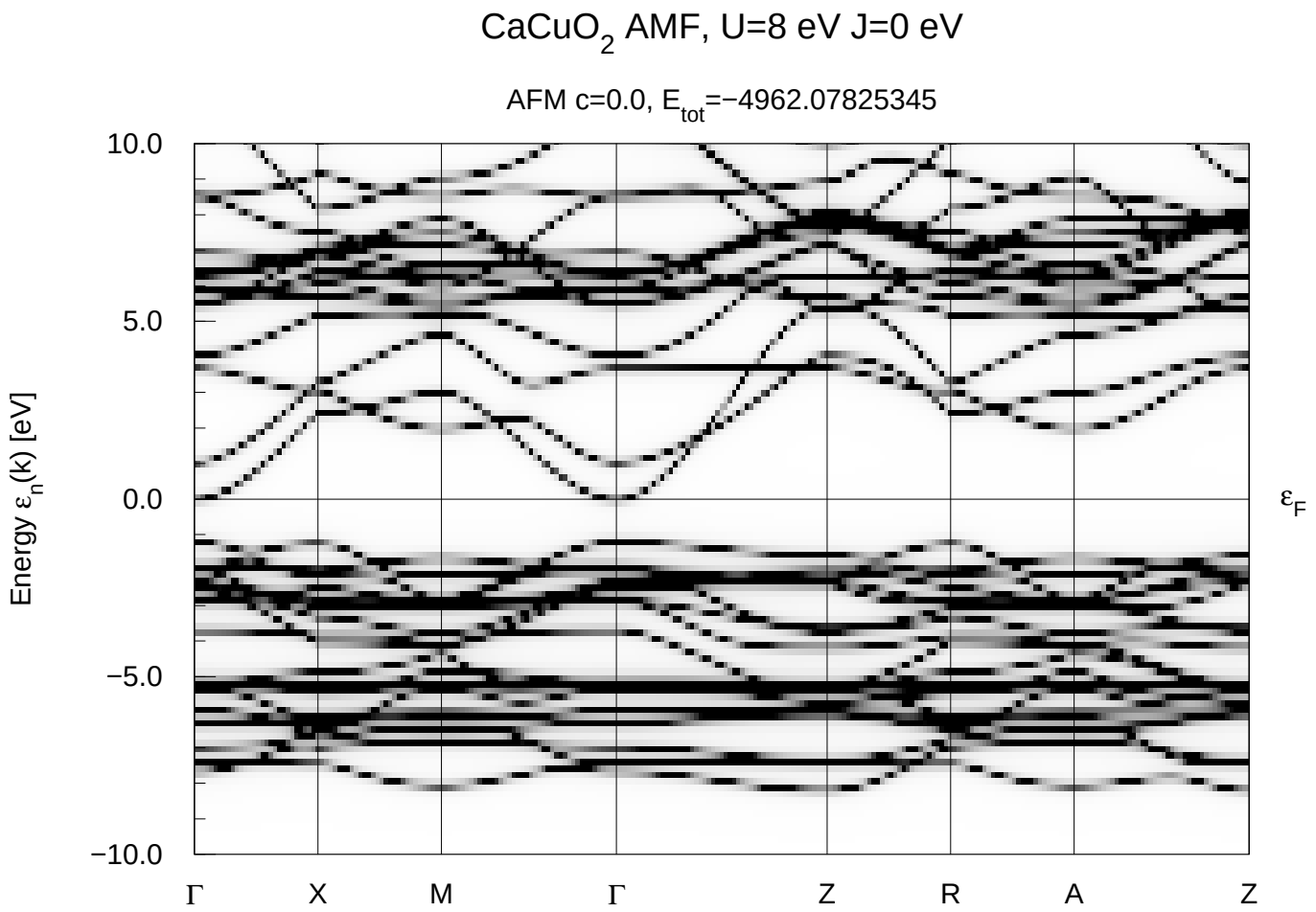
4.2 Site Spin Moment:

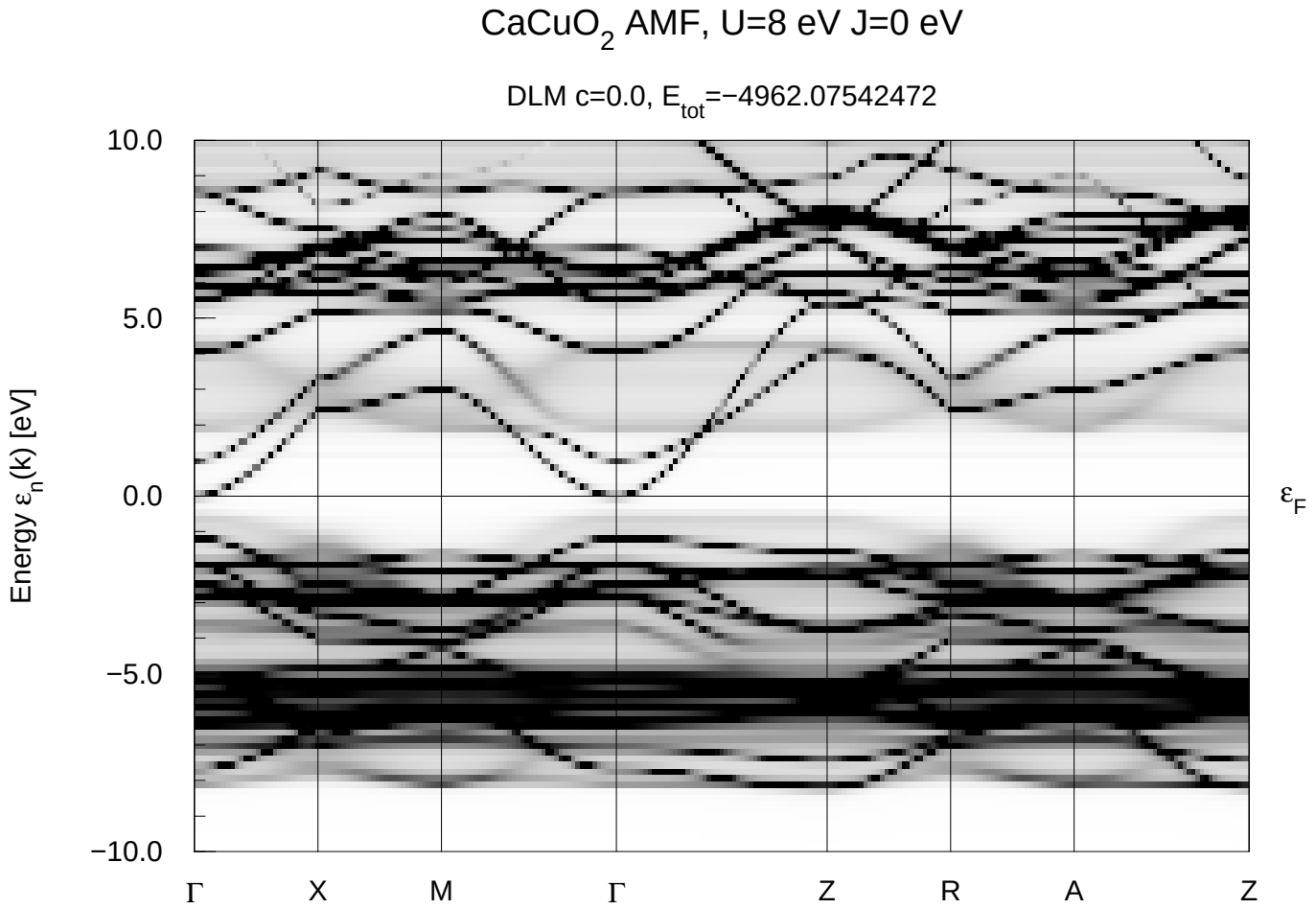


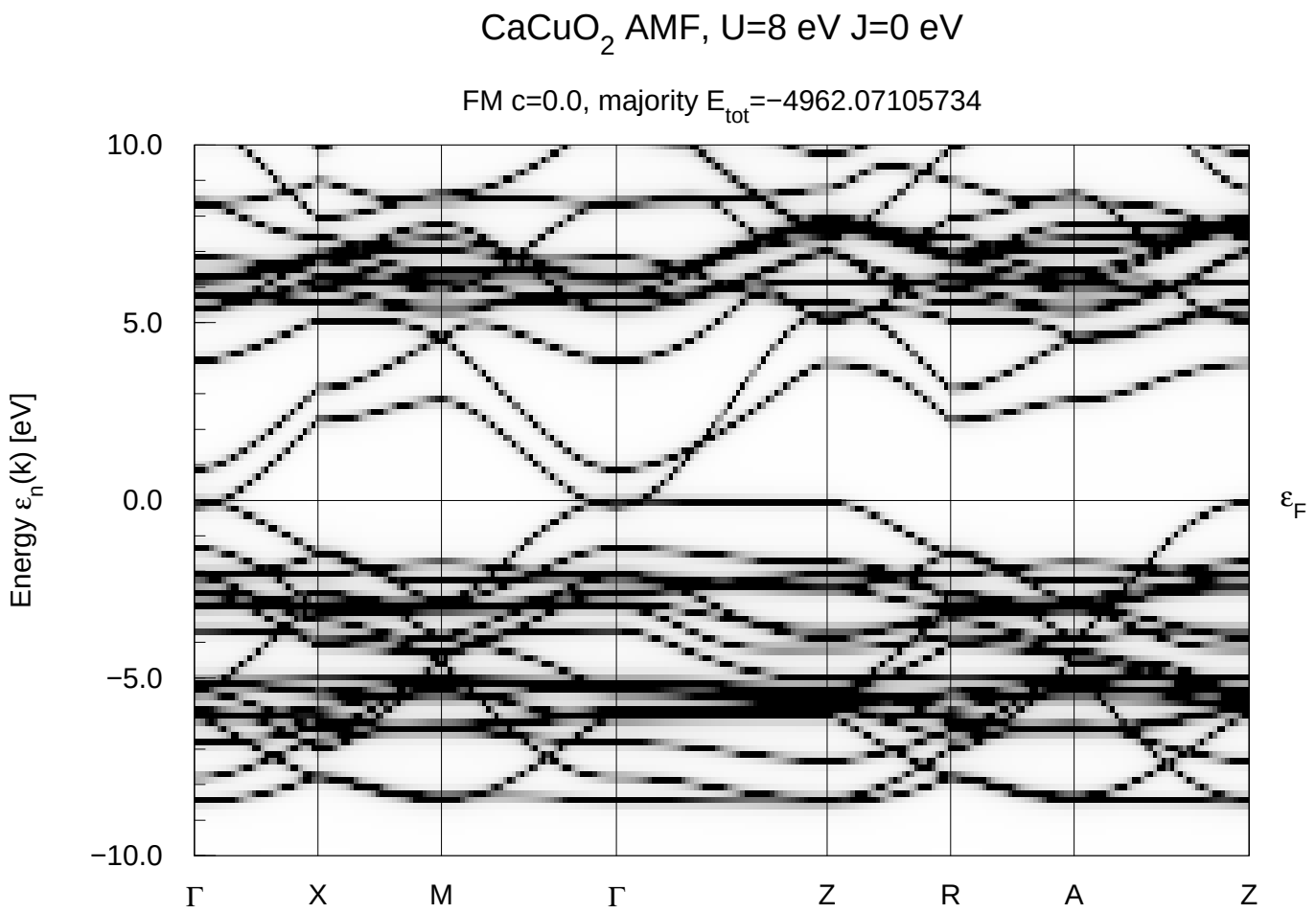


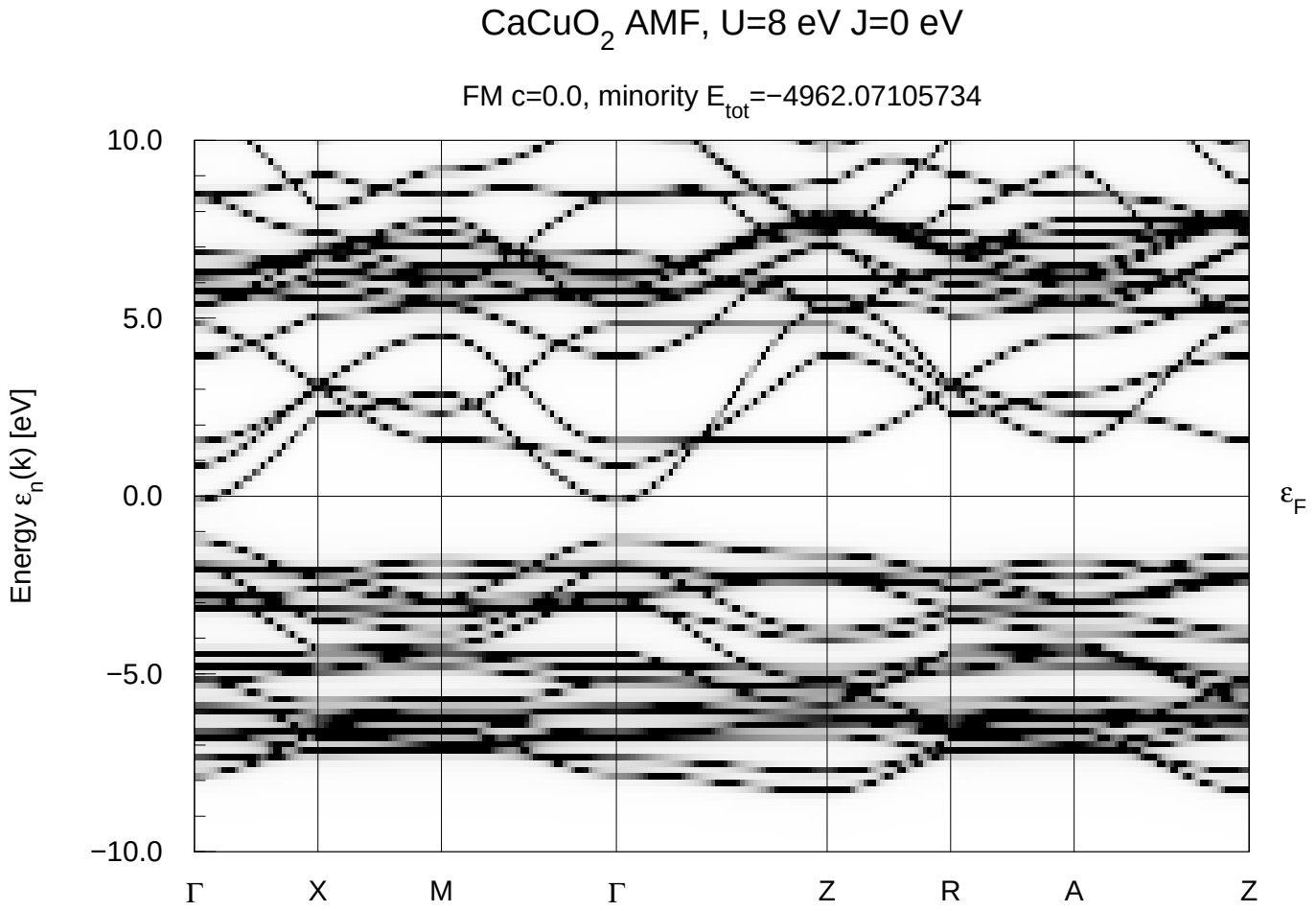
The anti-alignment of the oxygen spins with the copper spins speaks of a very strong AFM Cu-O exchange constant J_x (by far larger than J) which provides an effective FM Cu-Cu exchange proportional to x.

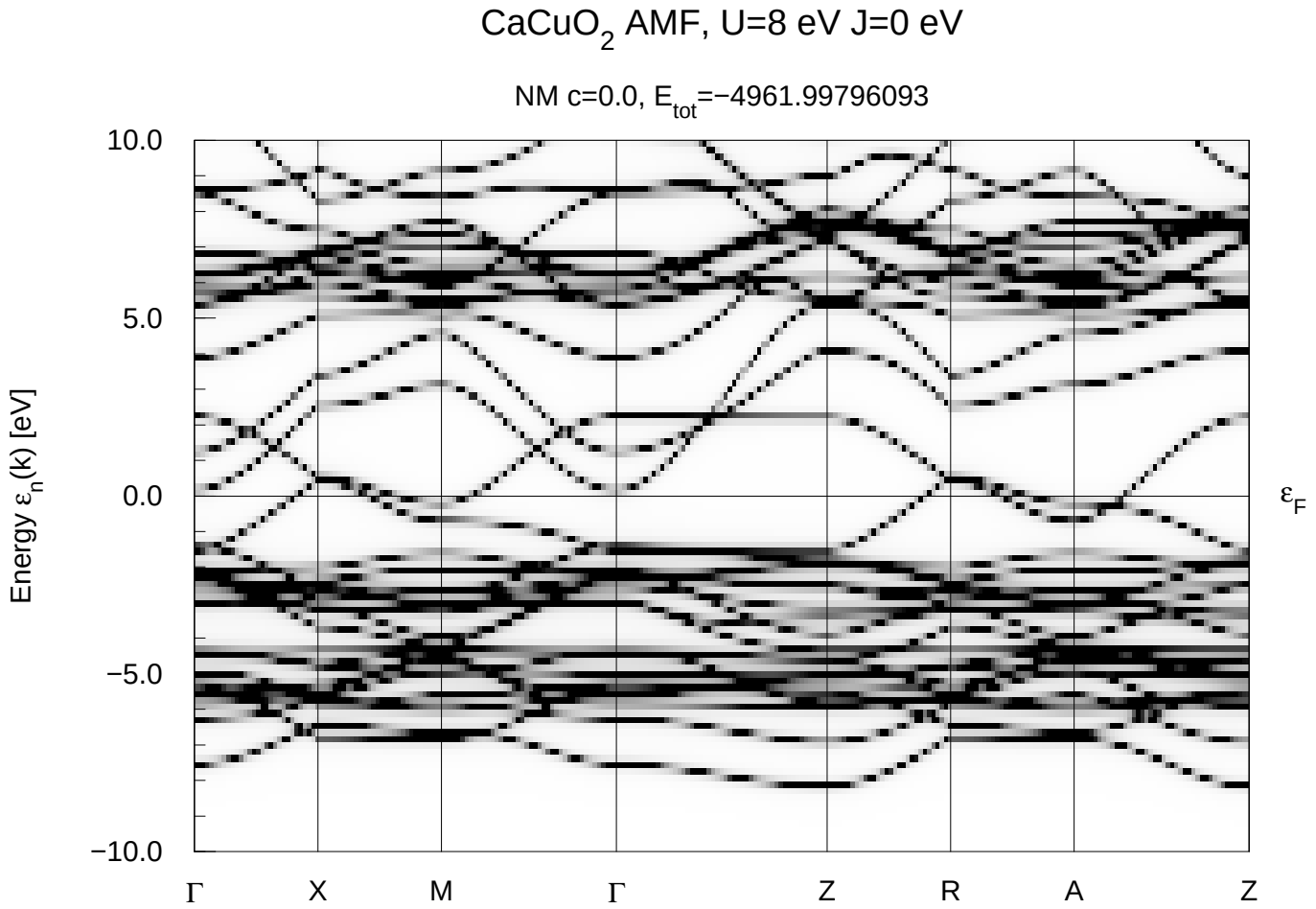
4.3 Bloch Spectral Functions for $x = 0$:



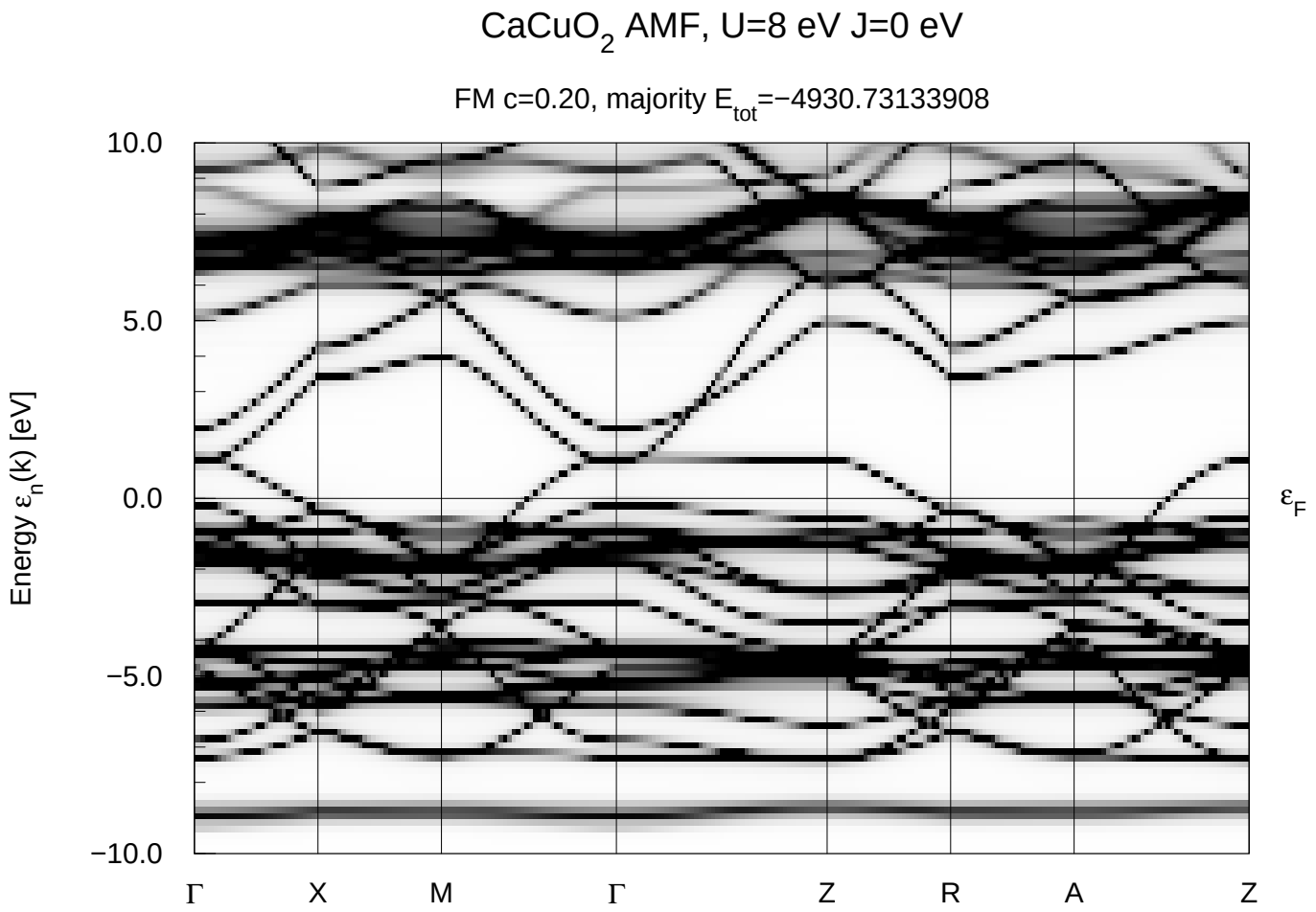

CaCuO2 AMF, U=8 eV J=0 eV
DLM c=0.0, Etot=−4962.07542472
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z

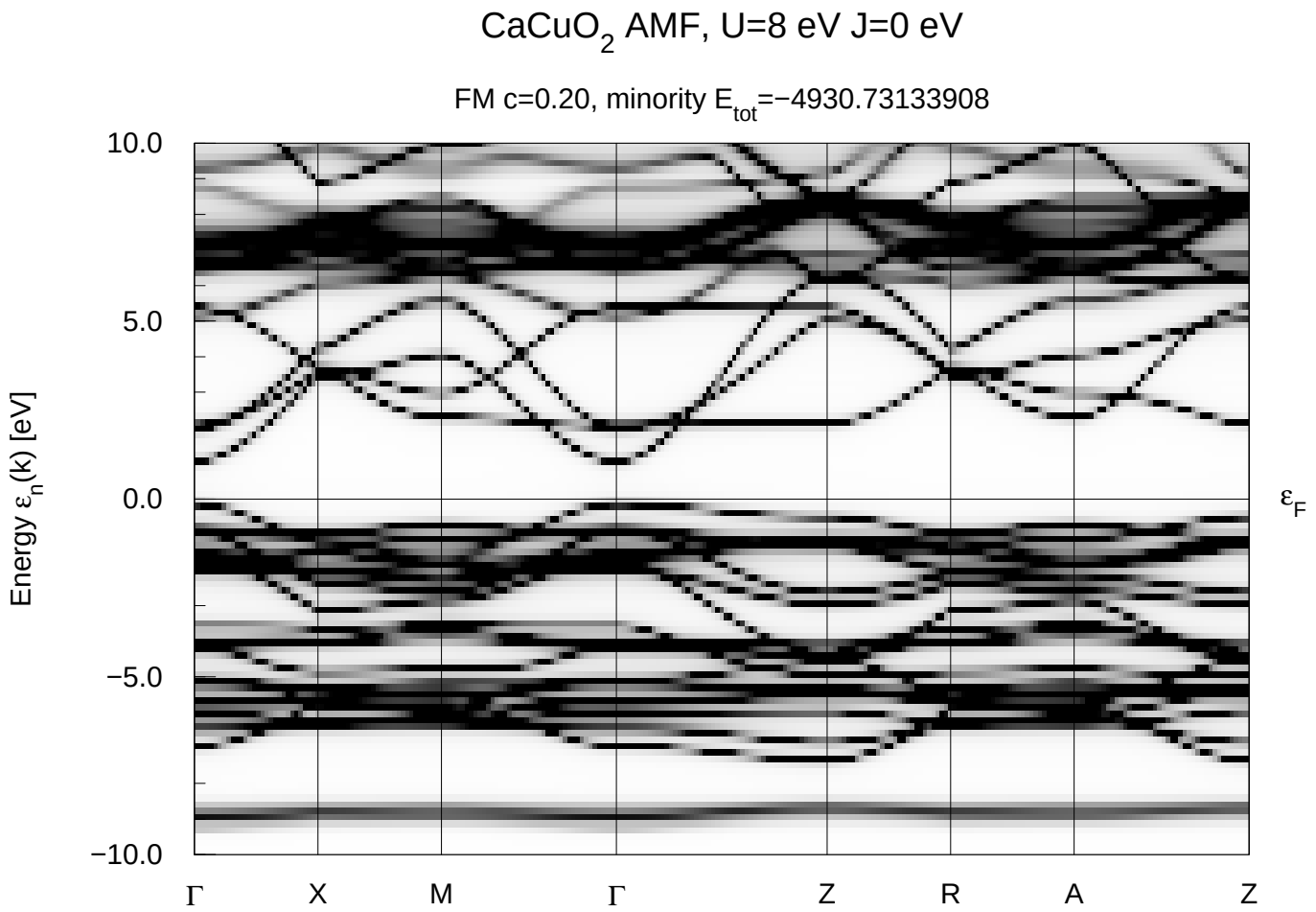

CaCuO2 AMF, U=8 eV J=0 eV
FM c=0.0, majority Etot=−4962.07105734
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z

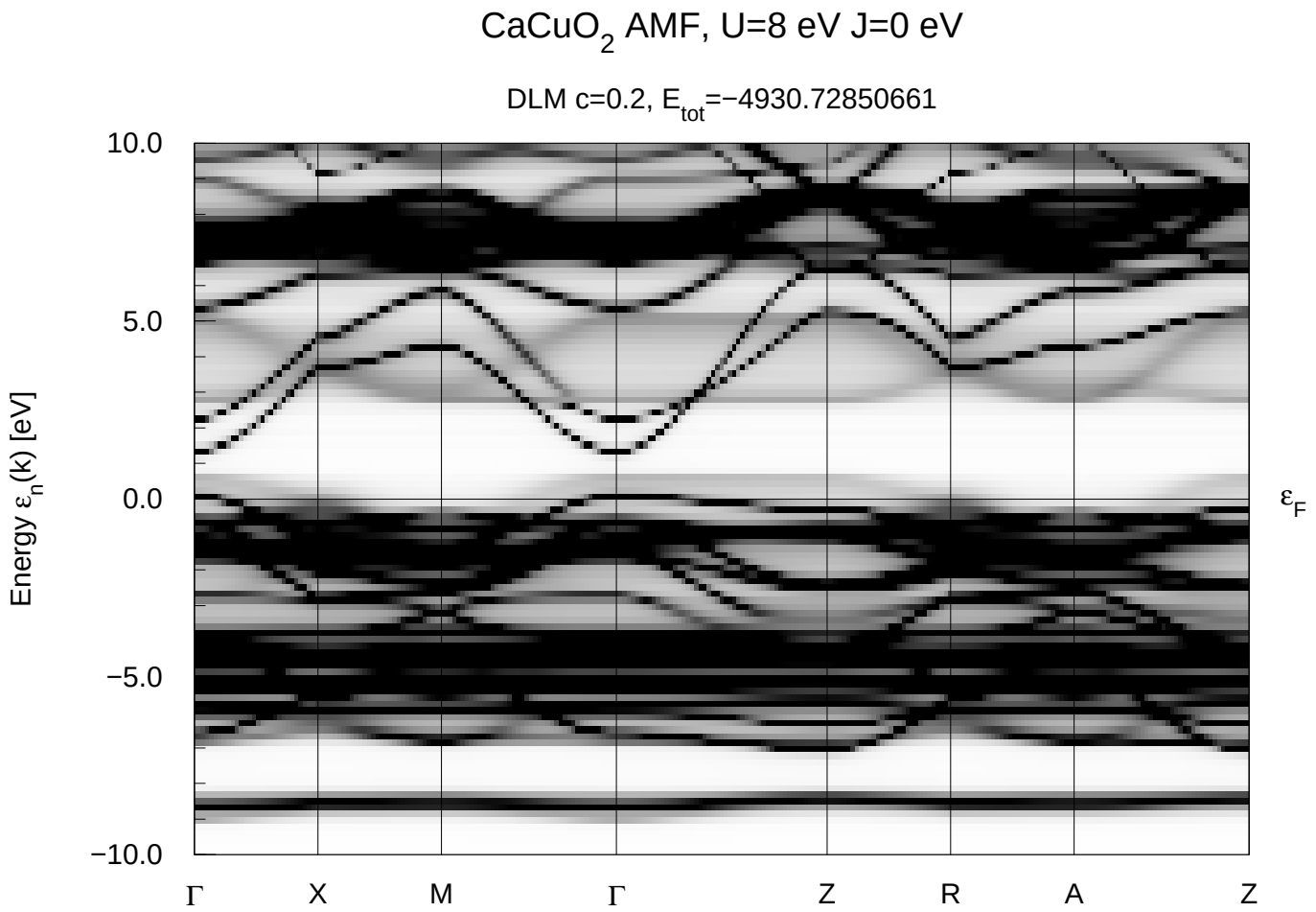

CaCuO2 AMF, U=8 eV J=0 eV
FM c=0.0, minority Etot=−4962.07105734
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z

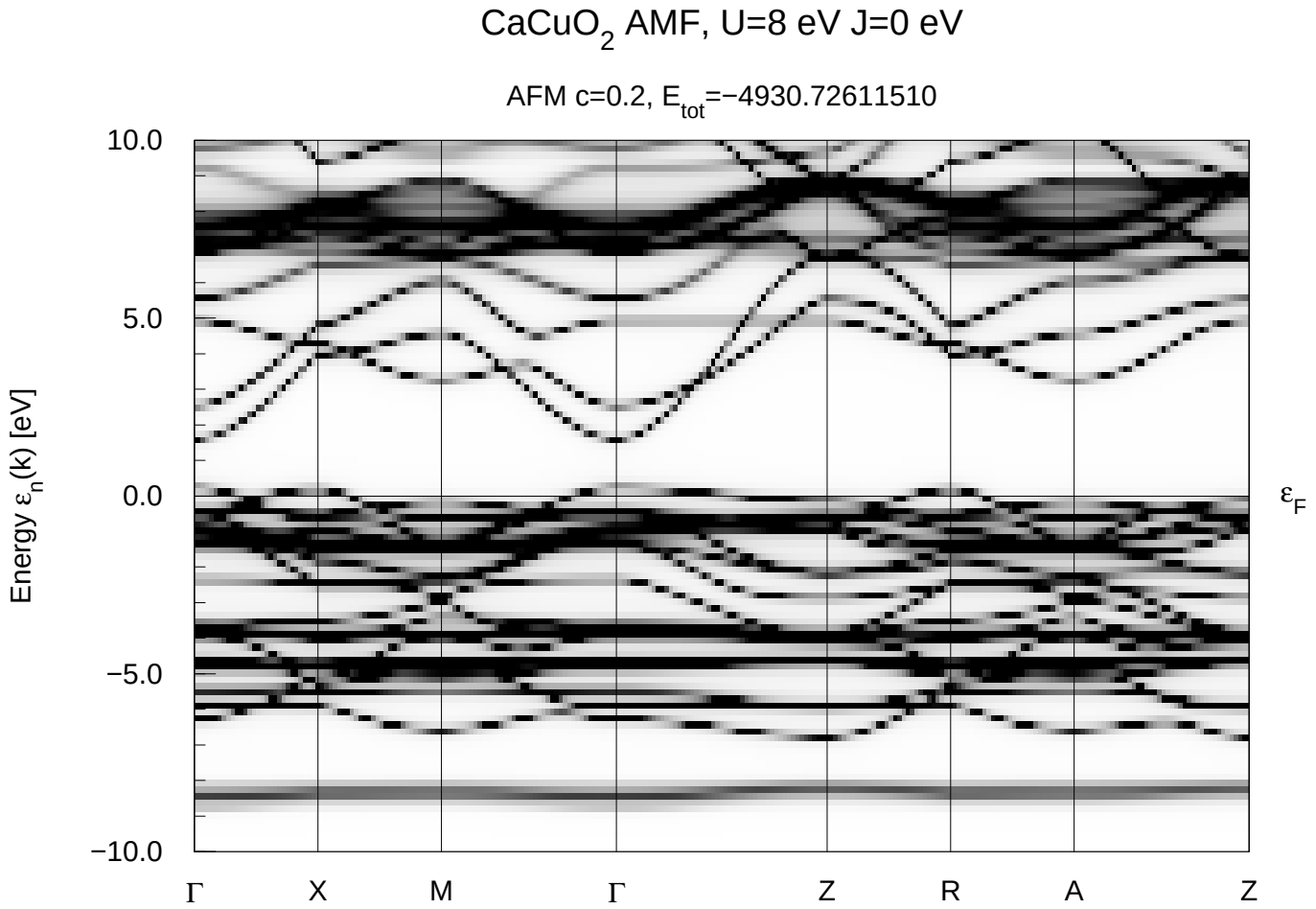

CaCuO2 AMF, U=8 eV J=0 eV
NM c=0.0, Etot=−4961.99796093
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z

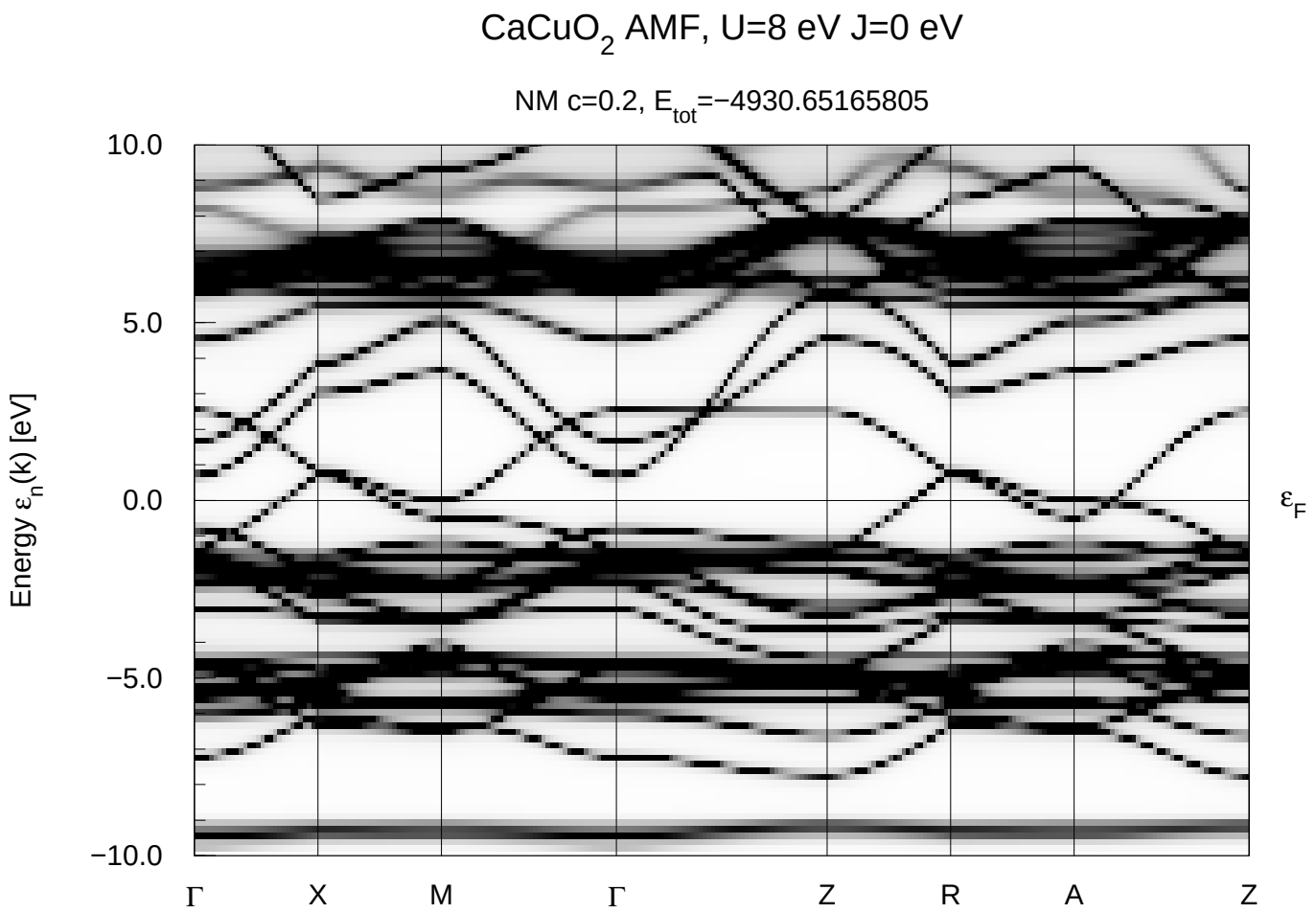
4.3 Bloch Spectral Functions for $x = 0.2$:



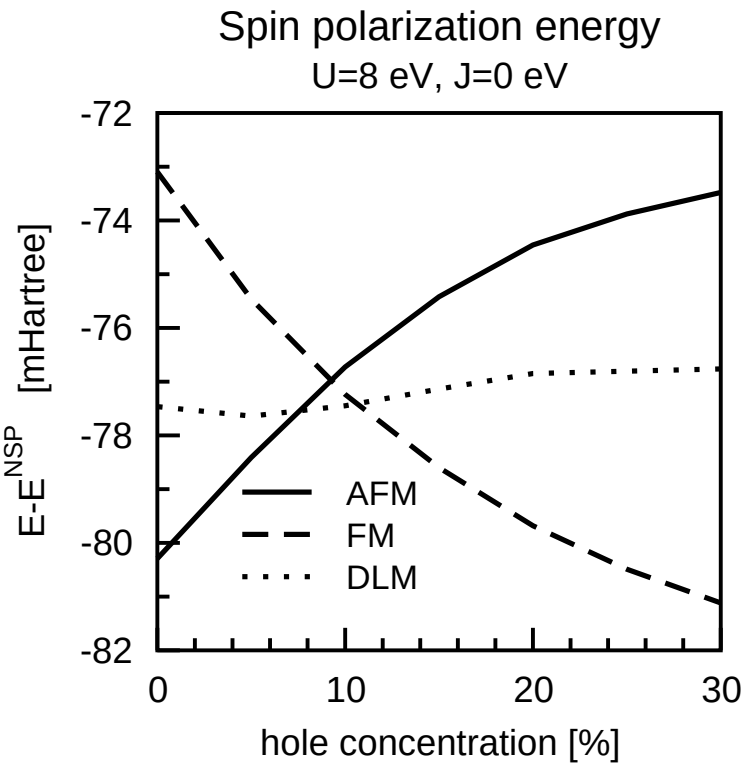

CaCuO2 AMF, U=8 eV J=0 eV
FM c=0.20, minority Etot=−4930.73133908
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z


CaCuO2 AMF, U=8 eV J=0 eV
DLM c=0.2, Etot=−4930.72850661
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z

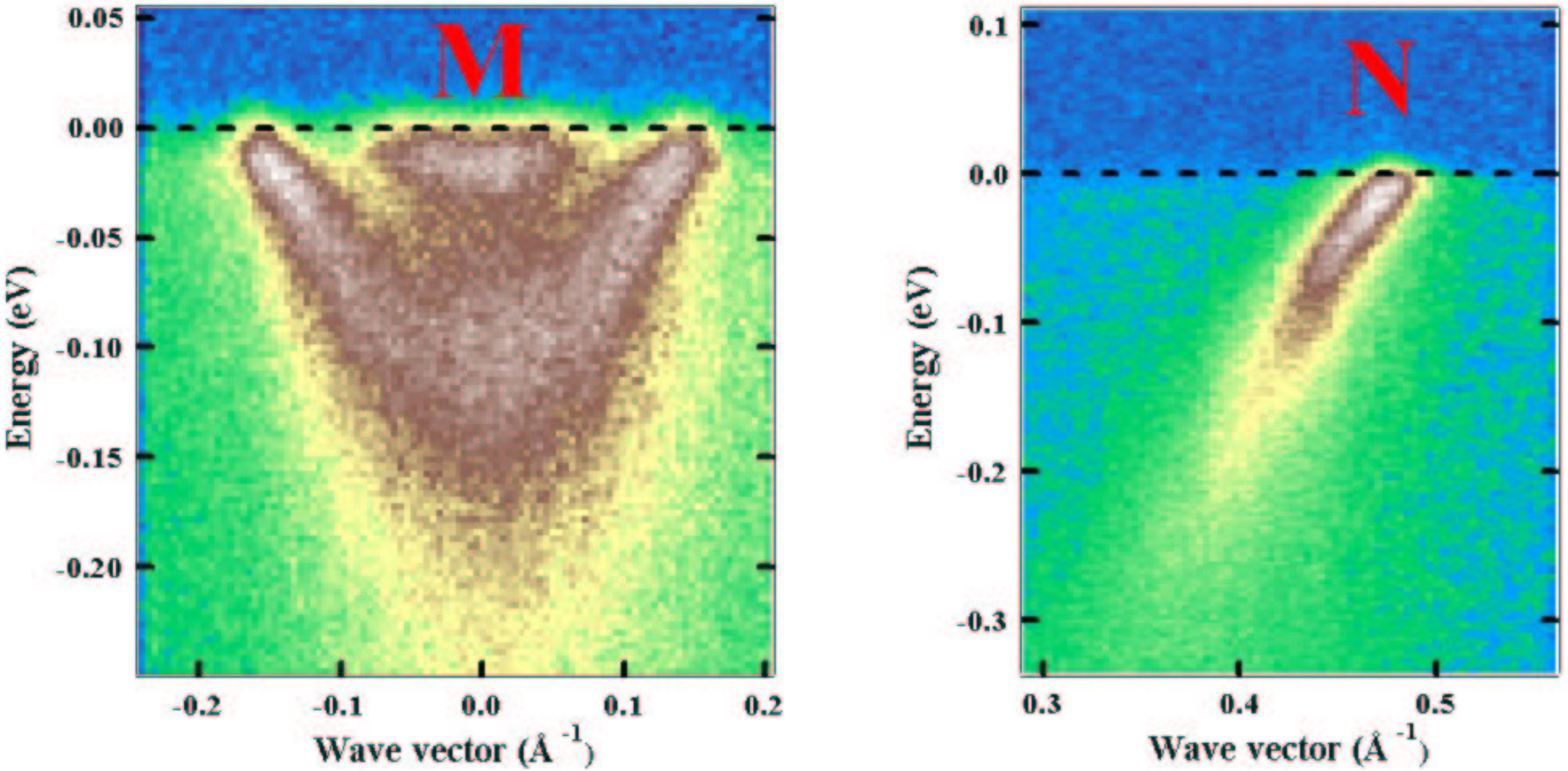

CaCuO2 AMF, U=8 eV J=0 eV
AFM c=0.2, Etot=−4930.72611510
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z

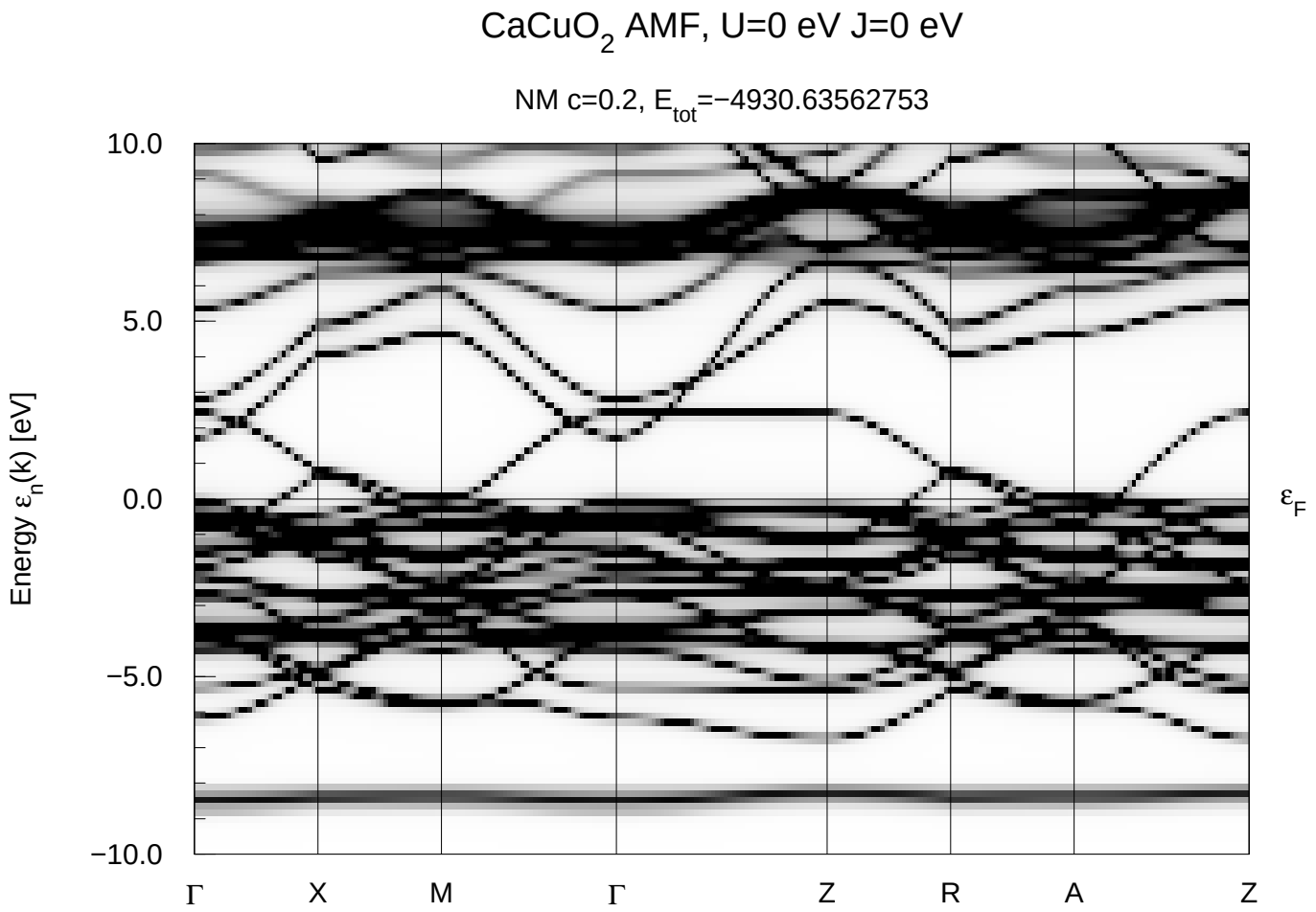

CaCuO2 AMF, U=8 eV J=0 eV
NM c=0.2, Etot=−4930.65165805
10.0
5.0
0.0
−5.0
−10.0
Energy εn(k) [eV]
εF
Γ
X
M
Γ
Z
R
A
Z

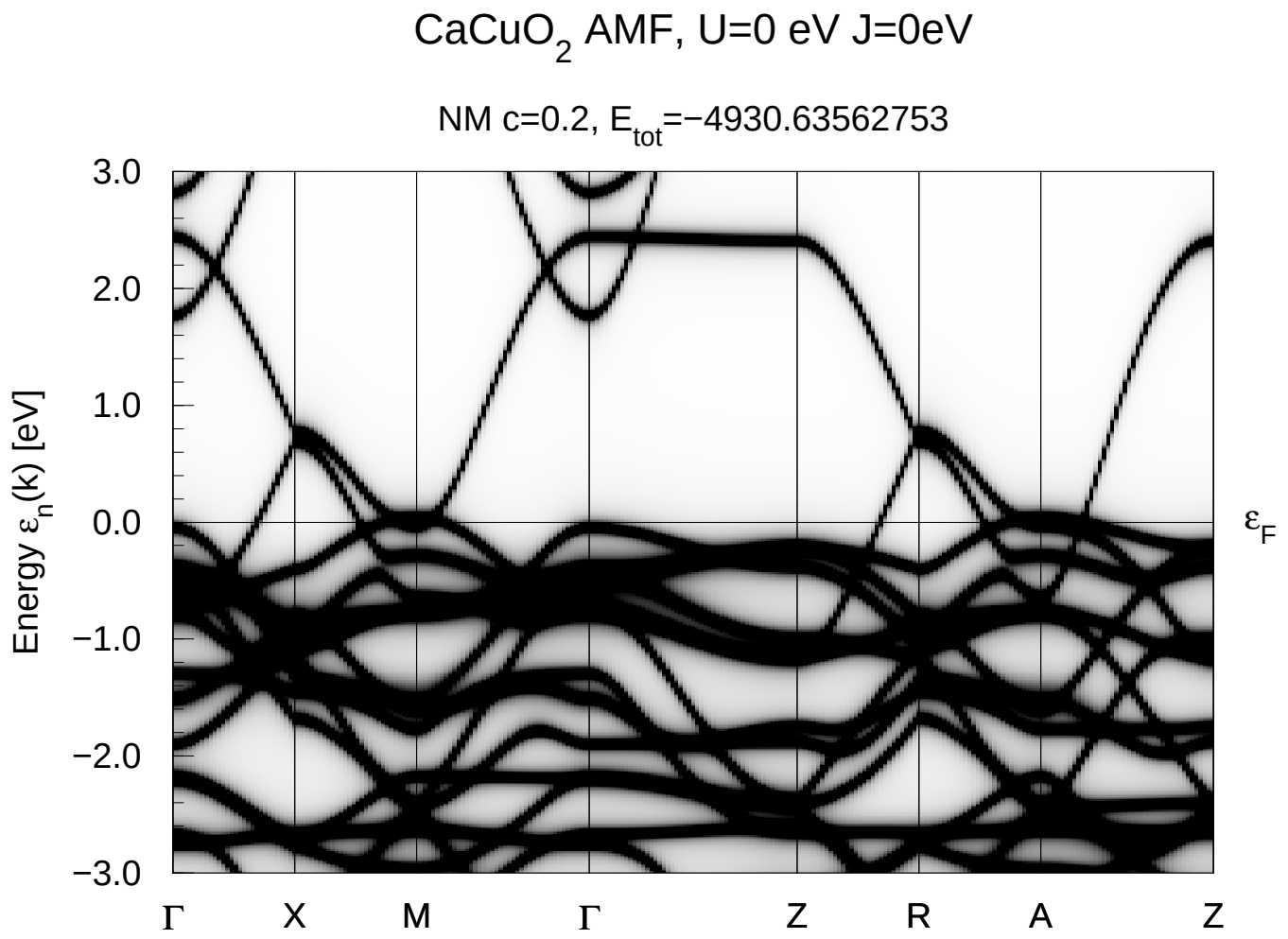
Total Energy Differences (per 2 Cu atoms):



ARPES band structure of optimally doped $Bi_2SrCa_2Cu_2O_{7+\delta}$:




CaCuO2 AMF, U=0 eV J=0 eV
NM c=0.2, Etot=−4930.63562753
Energy εn(k) [eV]
10.0
5.0
0.0
−5.0
−10.0
εF
Γ
X
M
Γ
Z
R
A
Z


CaCuO2 AMF, U=0 eV J=0eV
NM c=0.2, Etot=−4930.63562753
Energy εn(k) [eV]
3.0
2.0
1.0
0.0
−1.0
−2.0
−3.0
εF
Γ
X
M
Γ
Z
R
A
Z

5. CONCLUSIONS

- The AFM ground state of undoped cuprates and its magnetic nearest neighbor Cu-Cu spin coupling with an exchange constant $J \approx -100$ meV are well described by the LSDA+U approach of density functional theory with $U = 8$ eV and $J = 0$ which keeps the exchange energy in the LSDA functional.

- The Bloch spectral function well resembles ARPES results for $Sr_2CuO_2Cl_2$ in this case.

- Doped additional holes go predominantly to oxygen sites and develop a strong antiparallel coupling of their spin to the Cu spin with a Cu-O exchange coupling constant J_x much larger than J in magnitude.

- At a hole doping concentration of $x \approx 0.07$, the transition into a spin glass ground state is obtained, mainly caused by a strong effective FM Cu-Cu exchange coupling introduced by the O-holes.

- For $U = 8$ eV, a transition into a FM ground state is obtained at a hole concentration $x \approx 0.11$. The treatment of a superconducting ground state is beyond the applied density functional approach.

- For $U = 8$ eV and $x = 0.2$, a FM ground state is obtained, which together with its Bloch spectral function is in stark contradiction with experimental findings.

- For $U = 0$ and $x = 0.2$, the non spin polarized ground state is obtained with a Bloch spectral function in close resemblance of the ARPES results for $Bi_2SrCa_2Cu_2O_{7+\delta}$.

- In this case, the states at the Fermi level are very weakly scattered by the disorder potential in the spacer layer.

- Rather a switching behavior of U from about 8 eV to zero at a localization-delocalization transition of the nominal Cu holes between $x = 0.1$ and $x = 0.2$ is indicated instead of a gradual decrease of U.

- Unfortunately, total energies for different U-values seem not to be comparable.

Acknowledgement

Helpful discussions with:

Amnon Aharony
Ora Entin-Wohlman
Erwin Müller-Hartmann
Manuel Richter
Igor Chaplygin
Helge Rosner

Financial support by GIF Grant I-614-13.14/99