

%%
I) W(bulk)
 %%%

Experimental lattice parameter of W: 3.165 \AA

%%
I.1) no spin-orbit:
 %%%
 $E_F = 0.14247 \text{ Ry}$

Occ.:

s-up 0.5662
 p-up 0.1943
 d-up 2.2395

 s-dw 0.5662
 p-dw 0.1943
 d-dw 2.2395

Cbar

Dbar1/2

s	-0.255781	0.422935	-0.078179	-0.471928
p	0.558431	0.250566	0.559499	-0.686670
d	0.145829	0.191739	0.116930	-0.205897
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%
I.2) with spin-orbit:
 %%%
 $E_F = 0.11903 \text{ Ry}$

Occ.:

s-up 0.5534
 p-up 0.2724
 d-up 2.1742

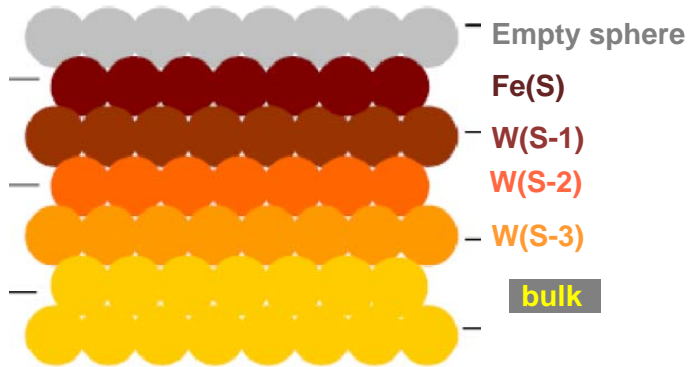
 s-dw 0.5534
 p-dw 0.2724
 d-dw 2.1742

Cbar

Dbar1/2

s	-0.267589	0.420719	-0.067520	-0.475752
p	0.545429	0.250631	0.559662	-0.685803
d	0.126913	0.190682	0.123989	-0.215405
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

II) Fe/W(110)



II.1) SOLUCAO FM

II.1.A) No relax. + no spin-orbit:

Experimental lattice parameter of W: 3.165 Å

Emp. Sphere

Occ.:

s-up	0.024
p-up	0.027
d-up	0.013
s-dw	0.022
p-dw	0.023
d-dw	0.010

Cbar

Dbar1/2

(UP)

s	0.415813	0.218288	0.400475	-1.036196
p	0.484469	0.114081	0.469682	-1.515913
d	0.252046	0.029286	0.207608	-4.482909
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	0.454670	0.227738	0.391514	-0.983308
p	0.557077	0.122305	0.488608	-1.410802
d	0.335375	0.034757	0.242919	-3.776614
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%
Fe(S):
 %%%%%%%%%

Occ.:

s-up 0.368
 p-up 0.309
 d-up 4.690

 s-dw 0.359
 p-dw 0.322
 d-dw 1.885

m_spin = 2.80 μ_B

Cbar

Dbar1/2

(UP)

s	-0.110456	0.361558	0.045069	-0.546558
p	0.453045	0.235877	0.500978	-0.691536
d	-0.024034	0.091673	0.004829	1.548121
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.069161	0.362729	0.063938	-0.550116
p	0.492409	0.238217	0.508063	-0.684234
d	0.165495	0.113325	0.106689	0.686767
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%
W(S-1)
 %%%%%%%%%

Occ.:

s-up 0.416
 p-up 0.420
 d-up 2.075
 s-dw 0.425
 p-dw 0.456
 d-dw 2.139

m_spin = -0.11 μ_B

Cbar

Dbar1/2

(UP)

s	-0.219897	0.390065	0.073910	-0.533973
p	0.503078	0.232029	0.579980	-0.746980
d	0.132498	0.181454	0.210028	-0.337477
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.225328	0.390621	0.071952	-0.532915
p	0.515364	0.235655	0.577021	-0.733831
d	0.128349	0.181546	0.212009	-0.339472
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%%

W(S-2)

%%%%%%%%%

Occ.:

s-up	0.423
p-up	0.479
d-up	2.102

s-dw	0.423
p-dw	0.484
d-dw	2.094

m_spin = 0.003 μ_B

Cbar

Dbar1/2

(UP)

s	-0.221302	0.385286	0.095852	-0.543669
p	0.504557	0.232490	0.580316	-0.745005
d	0.130258	0.180192	0.227906	-0.360772
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.221318	0.385395	0.095487	-0.543449
p	0.506032	0.232817	0.580092	-0.743805
d	0.130306	0.180160	0.228755	-0.361784
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%%

W(S-3)

%%%%%%%%%

Occ.:

s-up	0.429
p-up	0.510
d-up	2.086

s-dw	0.430
p-dw	0.514
d-dw	2.084

m_spin = -0.001 μ_B

Cbar
Dbar1/2
(UP)

s	-0.216884	0.379467	0.120798	-0.555658
p	0.498584	0.229985	0.582653	-0.754101
d	0.134793	0.179195	0.239436	-0.376334
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.216924	0.379629	0.120179	-0.555323
p	0.500427	0.230382	0.582382	-0.752610
d	0.134722	0.179183	0.239790	-0.376756
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

II.1.B) No relax. + with spin-orbit:

Experimental lattice parameter of W: 3.165 \AA

\lambda_Fe
\lambda_W

Emp. Sphere

Occ.:

s-up	0.024
p-up	0.027
d-up	0.013
s-dw	0.023
p-dw	0.023
d-dw	0.010

Cbar
Dbar1/2
(UP)

s	0.387636	0.219121	0.399792	-1.031404
p	0.459758	0.114867	0.471584	-1.505237
d	0.232270	0.030088	0.212856	-4.363279
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	0.428334	0.229306	0.389812	-0.974844
p	0.535799	0.123605	0.491414	-1.395422
d	0.318145	0.035787	0.249441	-3.667813
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%%%
Fe(S):
 %%%%%%%%%%

Occ.:

s-up 0.365
 p-up 0.309
 d-up 4.697

s-dw 0.357
 p-dw 0.321
 d-dw 1.872

m_spin = 2.82 μ_B

Cbar

Dbar1/2

(UP)

-0.133308	0.361251	0.046035	-0.547301
0.430929	0.235966	0.500555	-0.691200
-0.048521	0.091514	0.004538	1.549685
\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

-0.091652	0.362596	0.064233	-0.550419
0.470575	0.238315	0.507703	-0.683882
0.142345	0.113275	0.106999	0.683515
\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%%%
W(S-1)
 %%%%%%%%%%

Occ.:

s-up 0.407
 p-up 0.489
 d-up 2.023
 s-dw 0.417
 p-dw 0.516
 d-dw 2.091

m_spin = -0.10 μ_B

Cbar

Dbar1/2

(UP)

s	-0.229043	0.388167	0.081890	-0.537684
p	0.484992	0.230243	0.581567	-0.753236
d	0.119439	0.180603	0.215766	-0.346224
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.233833	0.388929	0.078874	-0.536183
p	0.490802	0.232399	0.579948	-0.745317
d	0.115481	0.180696	0.216896	-0.347312
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%%

W(S-2)

%%%%%%%%%

Occ.:

s-up	0.414
p-up	0.537
d-up	2.052

s-dw	0.414
p-dw	0.540
d-dw	2.043

m_spin = 0.006 μ_B

Cbar

Dbar1/2

(UP)

s	-0.227777	0.383446	0.102796	-0.547295
p	0.481628	0.229128	0.582871	-0.757139
d	0.118727	0.179217	0.232527	-0.369081
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.227649	0.383461	0.102813	-0.547267
p	0.482267	0.229244	0.582820	-0.756698
d	0.118861	0.179166	0.233453	-0.370256
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%%

W(S-3)

%%%%%%%%%

Occ.:

s-up	0.420
p-up	0.573
d-up	2.035

s-dw	0.421
p-dw	0.575
d-dw	2.032

m_spin = 0.002 μ_B

Cbar
Dbar1/2
(UP)

s	-0.223390	0.377449	0.128357	-0.559744
p	0.472838	0.226078	0.585306	-0.768616
d	0.123830	0.178237	0.244239	-0.384825
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

(DW)

s	-0.223317	0.377569	0.127902	-0.559491
p	0.473905	0.226291	0.585192	-0.767790
d	0.123826	0.178211	0.244695	-0.385415
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

II.2) SOLUCAO NAO MAGNETICA

%%

II.2.A) No relax. + no spin-orbit:

%%

Experimental lattice parameter of W: 3.165 \AA

%%%%%%%%%

Emp. Sphere

%%%%%%%%%

Occ.:

s-up	0.021
p-up	0.024
d-up	0.012
s-dw	0.021
p-dw	0.024
d-dw	0.012

Cbar
Dbar1/2
(UP)

s	0.452107	0.216817	0.401671	-1.044749
p	0.526667	0.114156	0.469903	-1.514835
d	0.289442	0.028997	0.205717	-4.527529
	\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%
Fe(S):
 %%%%%%%%%

Occ.:
 s-up 0.343
 p-up 0.300
 d-up 3.334

 s-dw 0.343
 p-dw 0.300
 d-dw 3.334

Cbar
Dbar1/2
 (UP)

-0.059955	0.358579	0.070795	-0.557985
0.486489	0.233078	0.511503	-0.702464
0.091421	0.100813	0.040638	1.189997
\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%
W(S-1)
 %%%%%%%%%

Occ.:
 s-up 0.421
 p-up 0.440
 d-up 2.092
 s-dw 0.421
 p-dw 0.440
 d-dw 2.092

Cbar
Dbar1/2

(UP)

-0.231327	0.390632	0.070656	-0.532772
0.504396	0.234604	0.577725	-0.737344
0.118289	0.181033	0.211841	-0.341167
\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%
 W(S-2)
 %%%%%%%%%

Occ.:

s-up 0.423
 p-up 0.481
 d-up 2.101

s-dw 0.423
 p-dw 0.481
 d-dw 2.101

Cbar

Dbar1/2

(UP)

-0.226435	0.385574	0.094938	-0.543101
0.499843	0.232620	0.580279	-0.744594
0.126014	0.180319	0.227982	-0.360330
\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

%%%%%%%%
 W(S-3)
 %%%%%%%%%

Occ.:

s-up 0.430
 p-up 0.512
 d-up 2.085

s-dw 0.430
 p-dw 0.512
 d-dw 2.085

Cbar

Dbar1/2

(UP)

-0.218636	0.379463	0.120802	-0.555667
0.497383	0.230094	0.582573	-0.753687
0.132964	0.179174	0.239615	-0.376613
\bar{C}	$\bar{\Delta}^{1/2}$	\bar{O}	E_γ

Fe/W(110) with L.S

