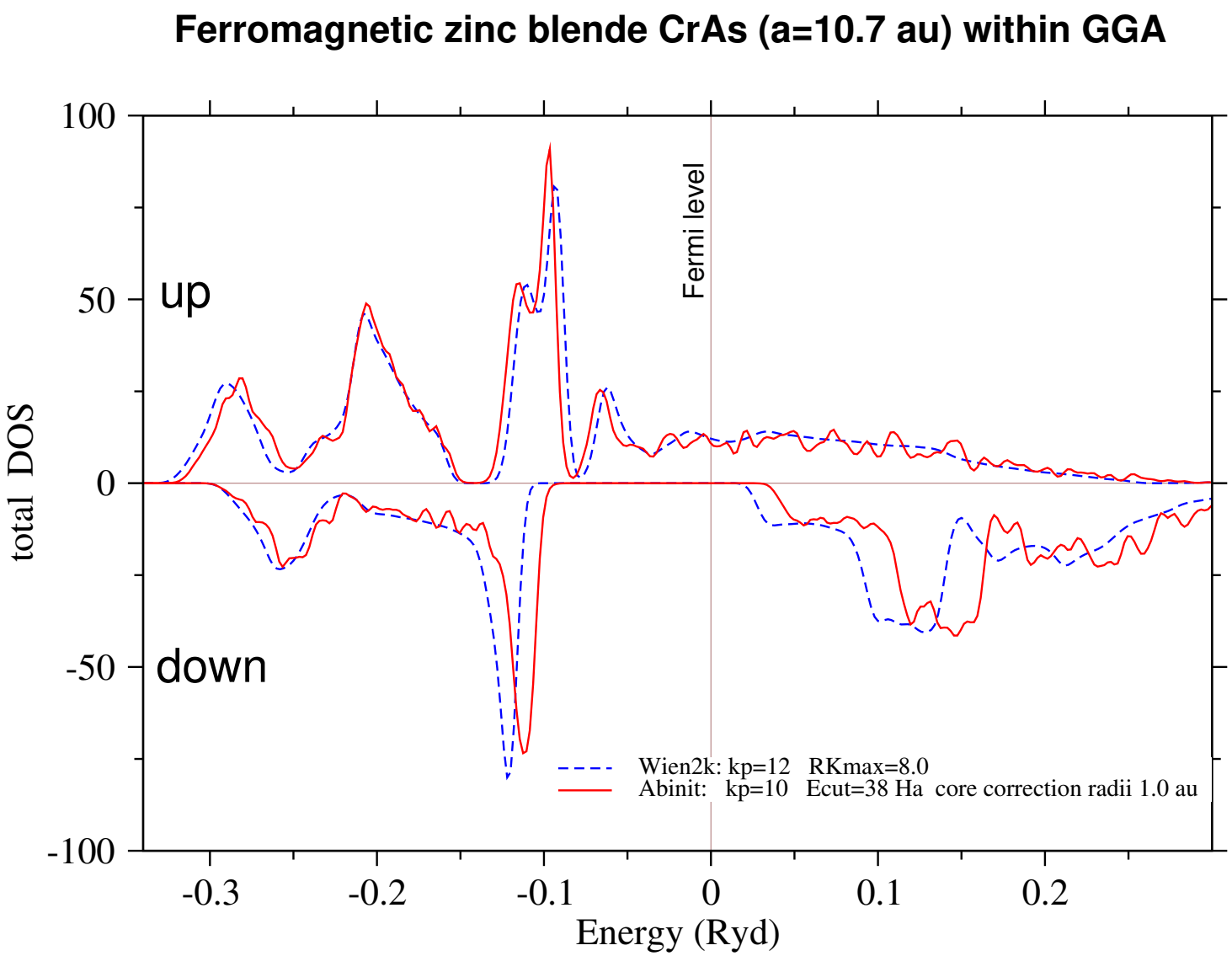
Ferromagnetic zinc blende CrAs (a=10.7 au) within GGA
100
50
0
-50
-100
total DOS
up
down
Fermi level
Wien2k: kp=12 RKmax=8.0
Abinit: kp=10 Ecut=38 Ha core correction radii 1.0 au
-0.3
-0.2
-0.1
0
0.1
0.2
Energy (Ryd)