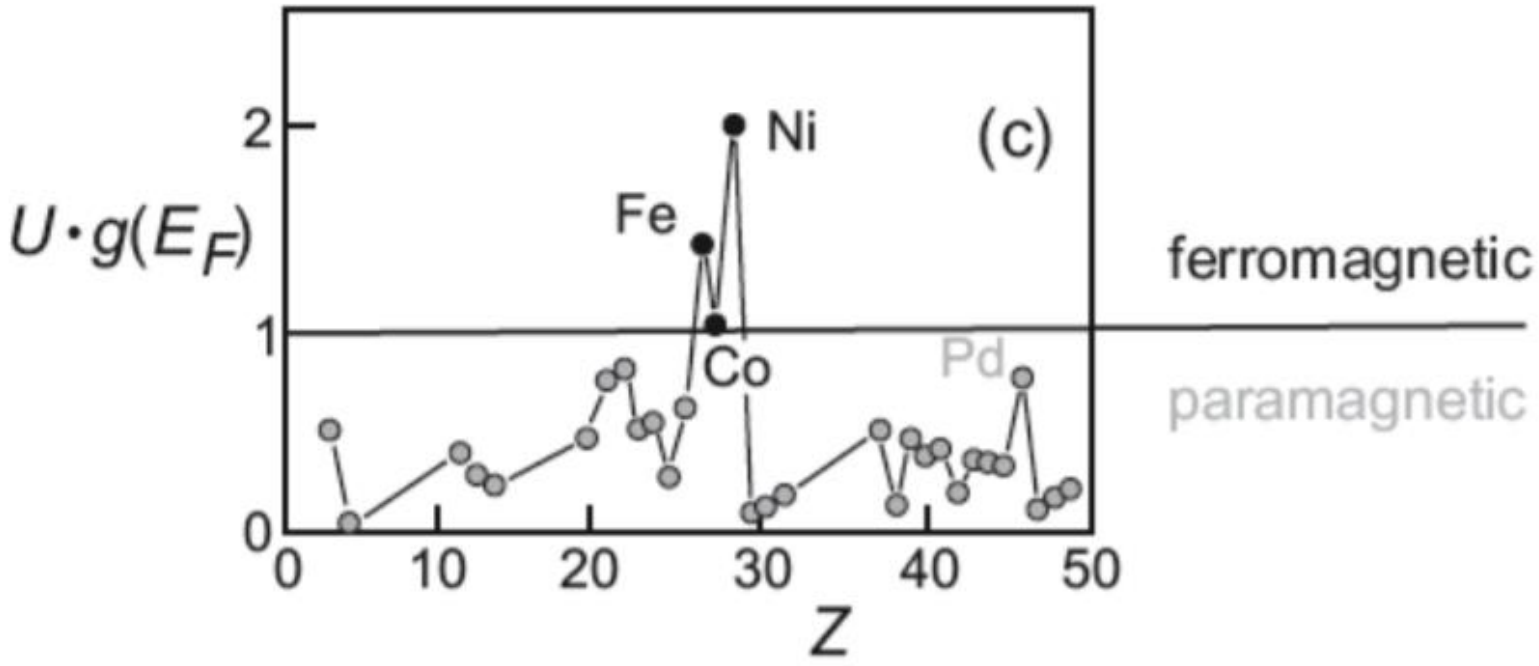
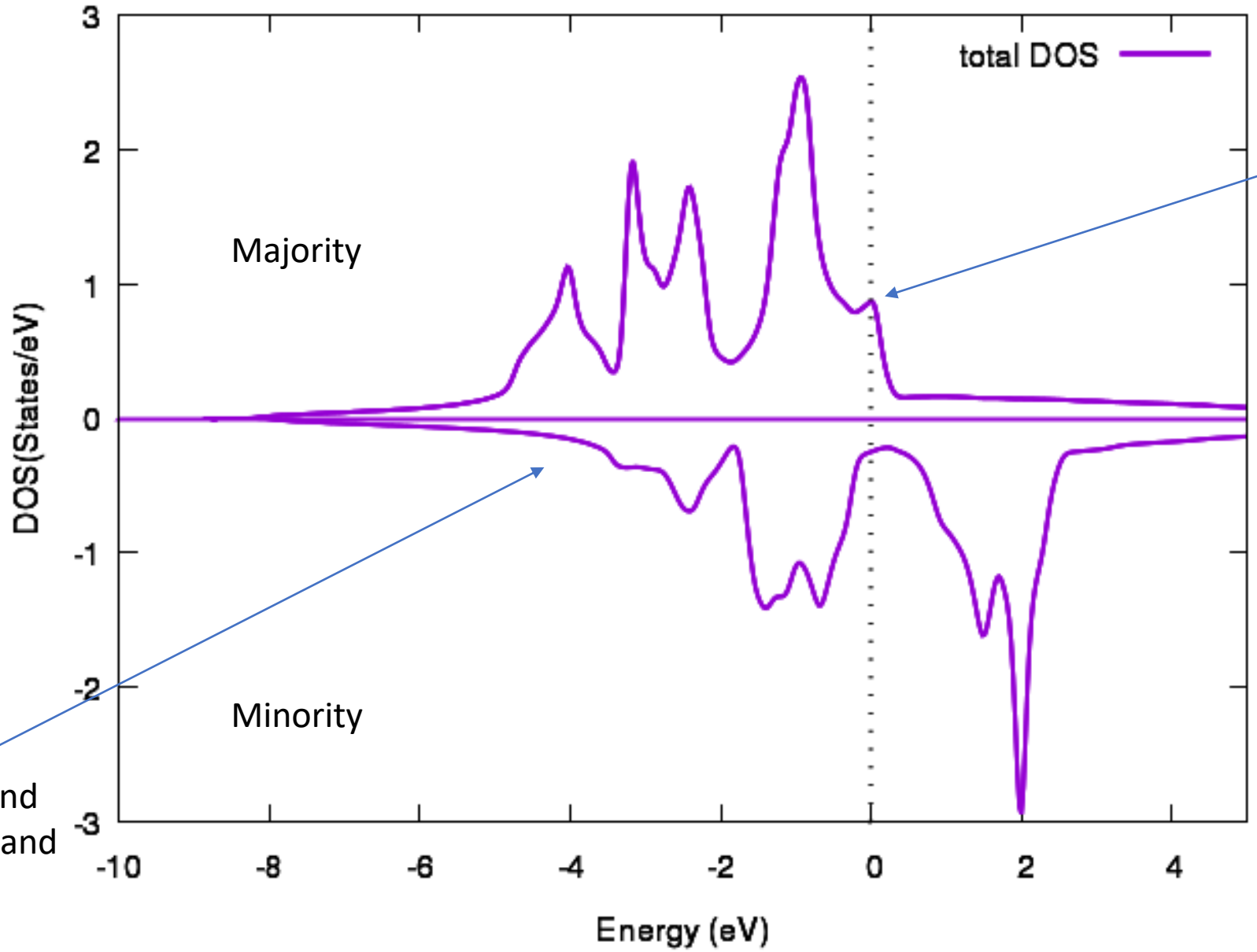
Density of states plots of 3d and 4d elements

Using WIEN2K, implementing Density Functional Theory.

Stoner criterion of ferromagnetism: $Ug(E_F)>1$



Density of states vs energy of Iron

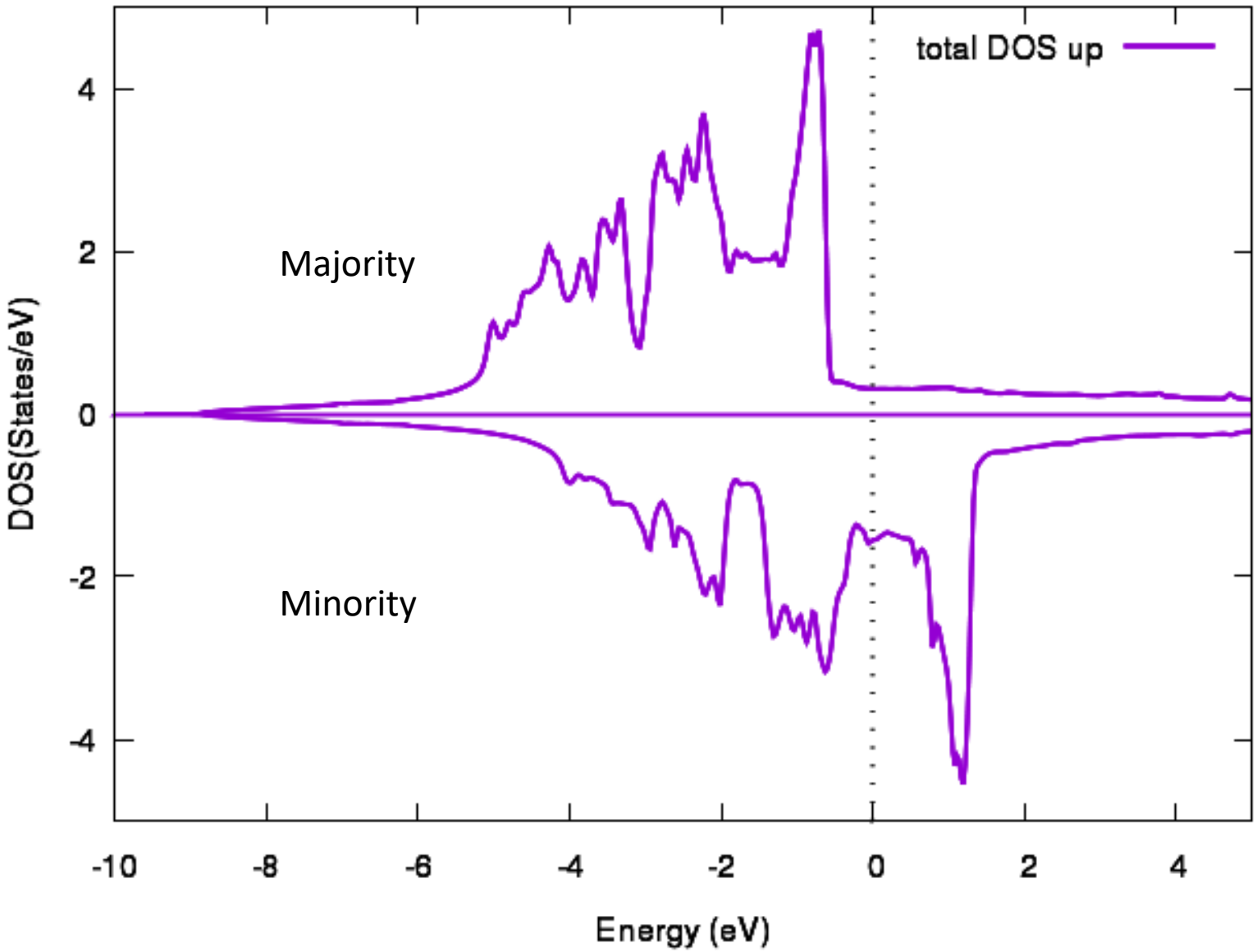


Peak in density of states at Fermi level- enough to satisfy Stoner criterion.

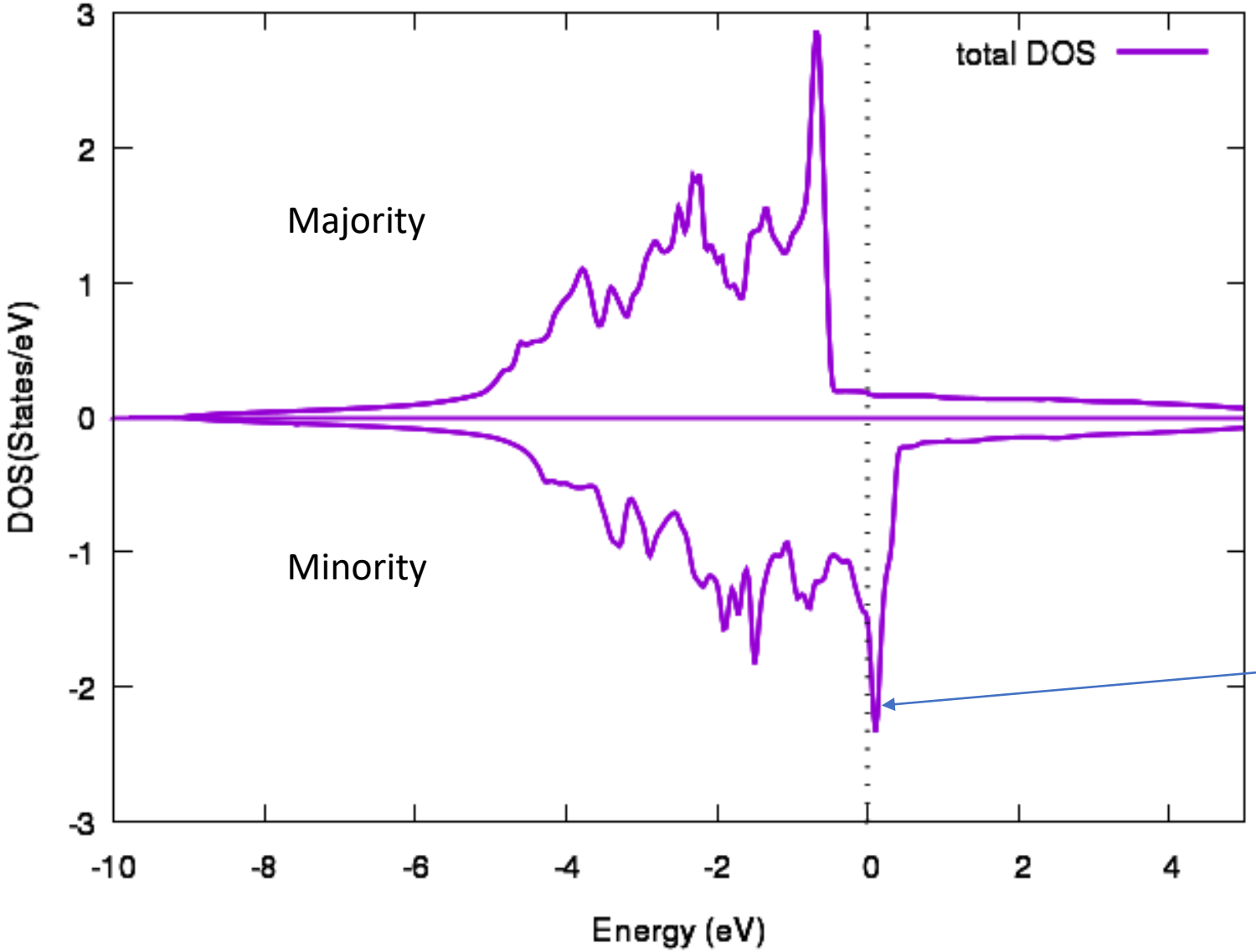
Spin-split bands and unequal majority and minority DOS – signatures of Ferromagnets

E=0 is the Fermi level.
E <0 are the occupied levels (valence band)
E>0 are unoccupied (conduction band)

Cobalt


total DOS up
Majority
Minority
DOS(States/eV)
Energy (eV)
4
2
0
-2
-4
-10
-8
-6
-4
-2
0
2
4

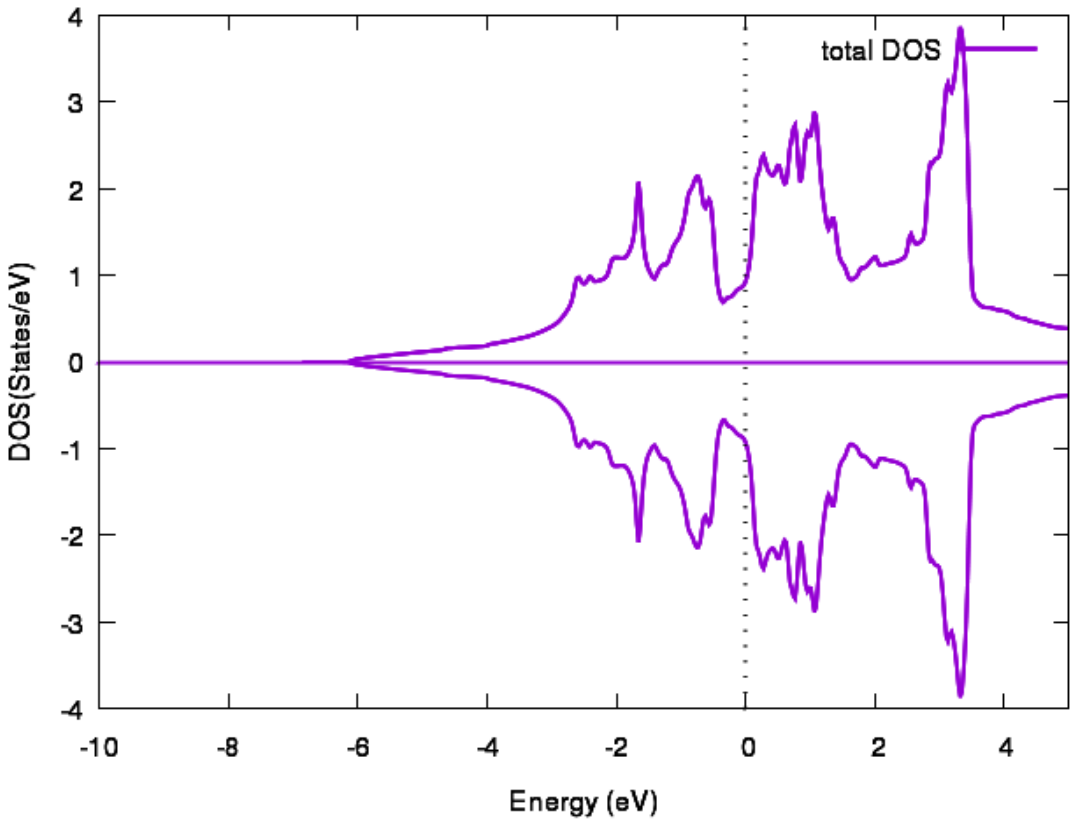
Nickel



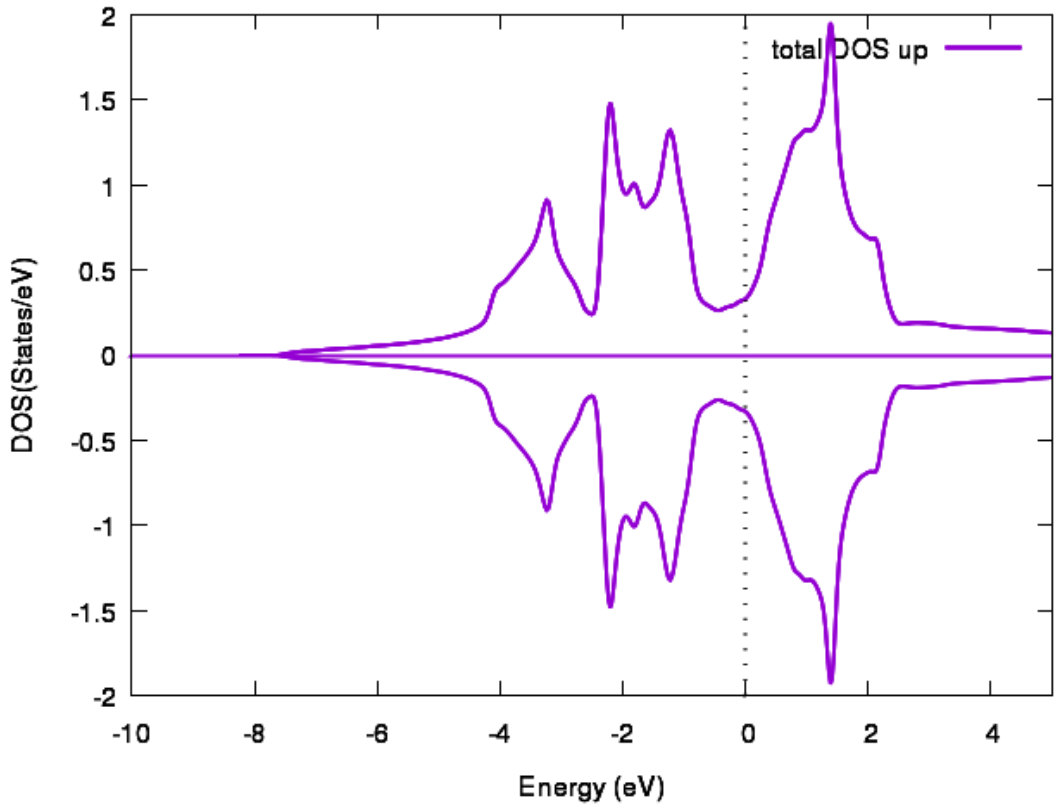
Peak in density of states at Fermi level- satisfies Stoner Criterion.

Low density of states at the Fermi level
– do not satisfy the Stoner criterion –
Pauli Paramagnets

Chromium

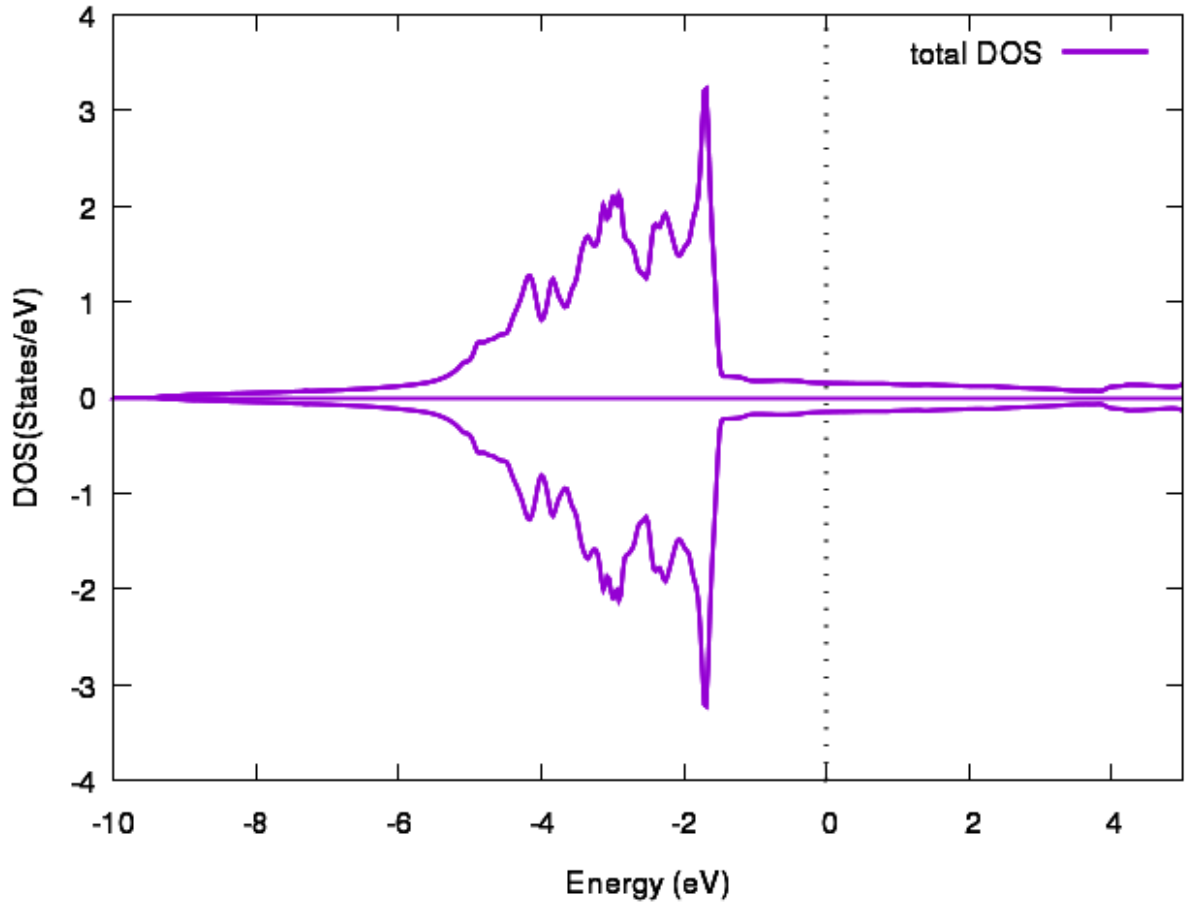


Titanium



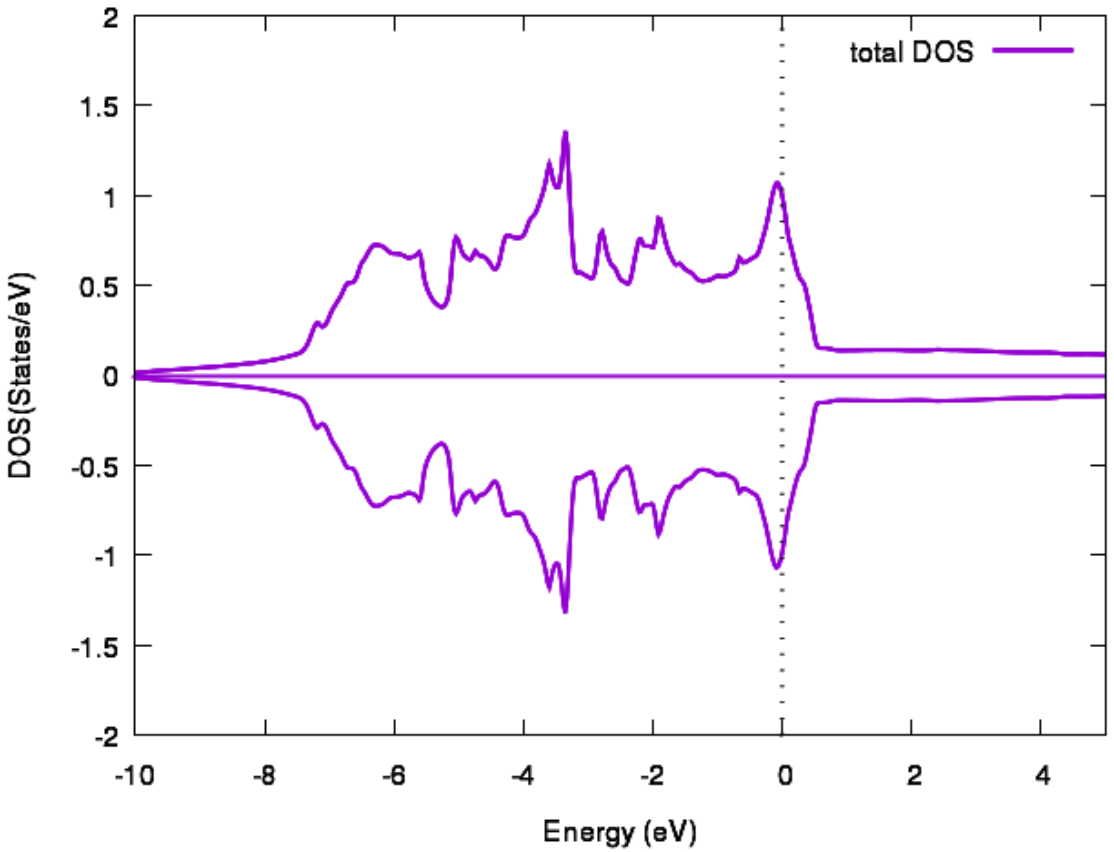
Also note the symmetric nature of density of state – indicates non-ferromagnetic ground state

Copper- very low density of states at E_F

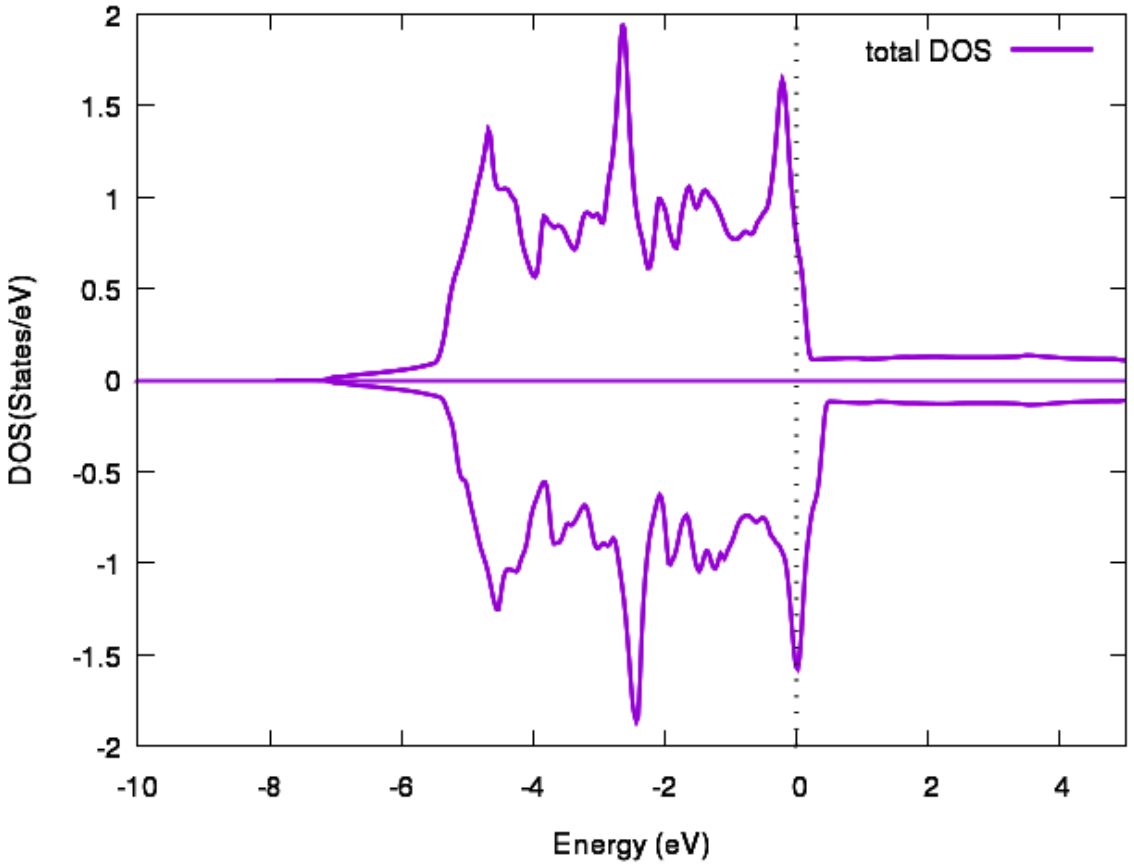


Incipient Ferromagnets- Stoner paramagnets

Platinum



Palladium



Relatively high density of states at the Fermi level – but not enough to satisfy Stoner criterion.