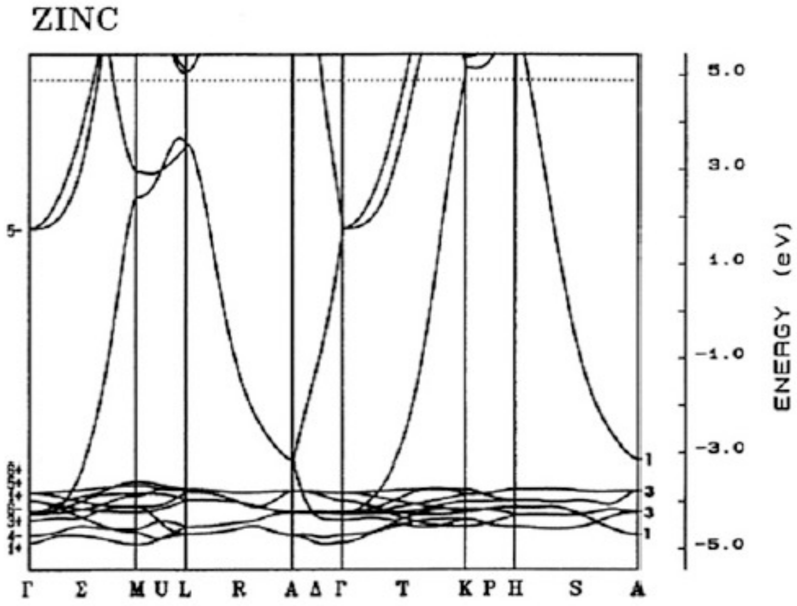
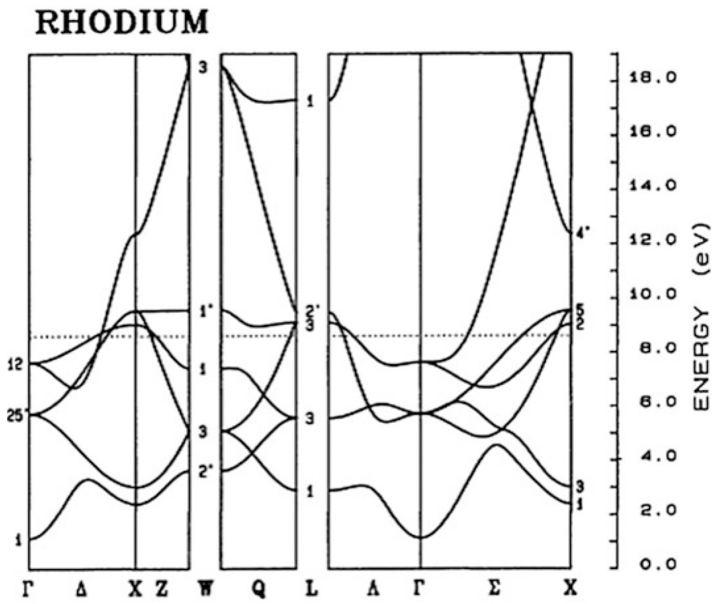
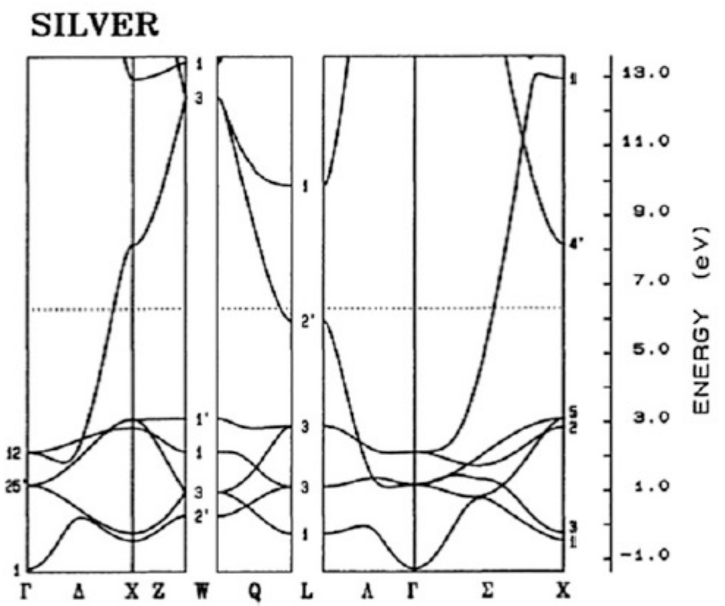
Magnetic alloy

We want to form a magnetic alloy with high magnetic moment mixing Co with one of these three elements, which are not magnetic in bulk: Zn, Rh, Ag.

Considering their band structure, class them according to the suitability.





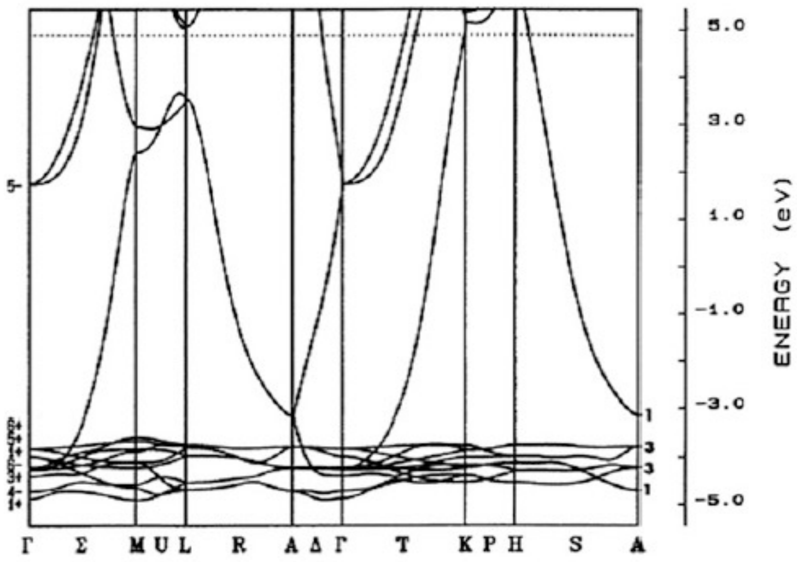


Solution: Magnetic alloy

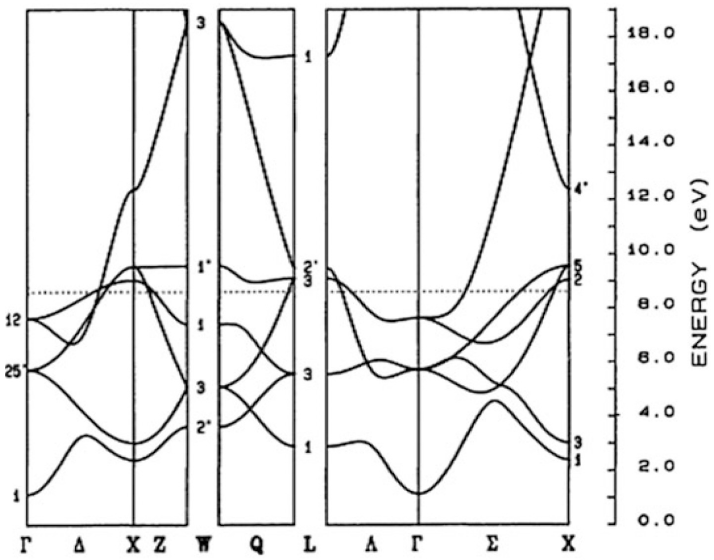
The magnetic moment of the alloy is an average of the magnetic moment of Co and of the second element.
The necessary condition to have a contribution of the second element is a high d-state DOS at the Fermi level.
Then the three elements can be classified in the following order:

Rh
Ag
Zn

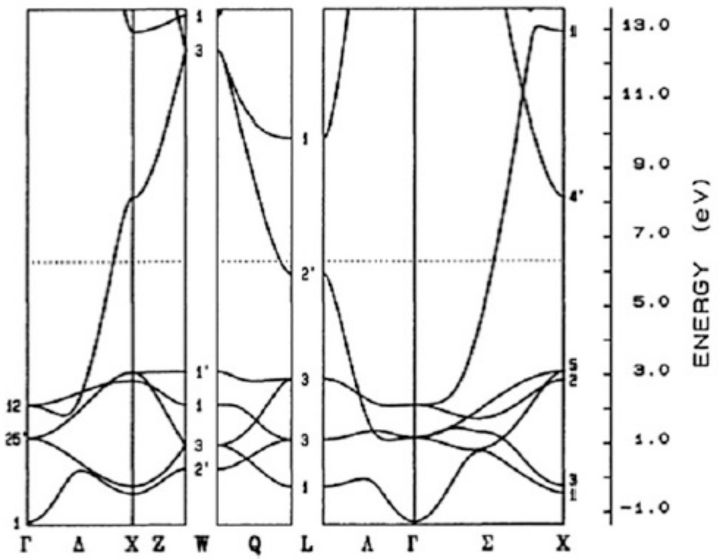
ZINC



RHODIUM



SILVER



Magnetic moments

We want to evaluate the magnetic moment of atoms in several situations. We apply an external magnetic field B applied along the z direction and for simplicity we assume T = 0 K.

1) Calculate the magnetic moment of a free-standing Co (Ar $3d^7$ $4s^2$), Sm (Xe $4f^6$ $6s^2$) and Dy (Xe $4f^{10}$ $6s^2$) atom
2) Calculate the magnetic moment of a Co atom in bulk Co knowing that $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.3$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$ where n_{3d} and n_{4s} the number of electrons with spin down/up in the respective band
3) Consider the composites $SmCo_5$ and $DyCo_5$. In both composites the magnetic moment of the Co atoms is anti-parallel to the magnetic moment of the rare earth element. Assume for Co the electronic configuration $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.0$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$. For the rare earth assume the standard (Xe $4f^{N-1}$ $5d^1$ $6s^2$) configuration. In addition, the electron in the 5d band occupies the orbital with $L_z = 0$ and its spin is parallel to the spin of the 4f shell. What is the magnetic moment per unit formula?

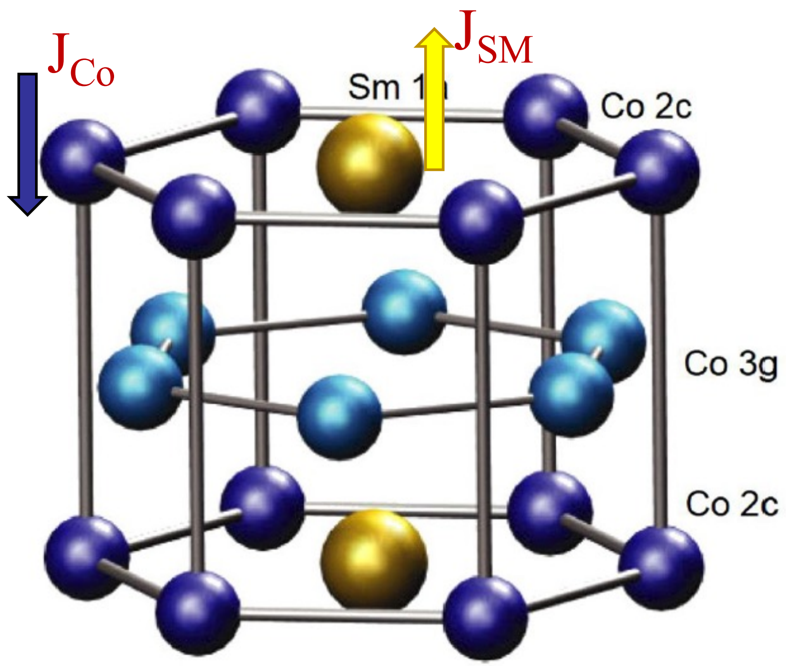


FIG. 1. Unit cell of the hexagonal intermetallic $SmCo_5$.

Adapted from : B. Das *et al.,* Phys. Rev. B **100**, 024419 (2019) DOI: 10.1103/PhysRevB.100.024419

Solution: magnetic moments

1)

Ground state of Co (Ar $3d^7\ 4s^2$)

	+2	+1	0	-1	-2
3d	↑	↑	↑	↑↓	↑↓

4s	↑↓

$L = 3,\ S = 3/2,\ J = 9/2$

$m_L = L\ \mu_B = 3\ \mu_B$,

$m_S = 2\ S\ \mu_B = 3\ \mu_B$,

$m_{at} = g\ J\ \mu_B = 6\ \mu_B$

Ground state of Sm (Xe $4f^{\,6}\ 6s^2$)

	+3	+2	+1	0	-1	-2	-3
4f	↑	↑	↑	↑	↑	↑	

4s	↑↓

$L = 3,\ S = 3,\ J = 0$

$m_L = L\ \mu_B = 3\ \mu_B$,

$m_S = 2\ S\ \mu_B = 6\ \mu_B$,

$m_{at} = g\ J\ \mu_B = 0\ \mu_B$

Ground state of Dy (Xe $4f^{\,10}\ 6s^2$)

	+3	+2	+1	0	-1	-2	-3
4f	↑	↑	↑	↑	↑↓	↑↓	↑↓

4s	↑↓

$L = 6,\ S = 2,\ J = 8$

$m_L = L\ \mu_B = 6\ \mu_B$,

$m_S = 2\ S\ \mu_B = 4\ \mu_B$,

$m_{at} = g\ J\ \mu_B = 10\ \mu_B$

2)

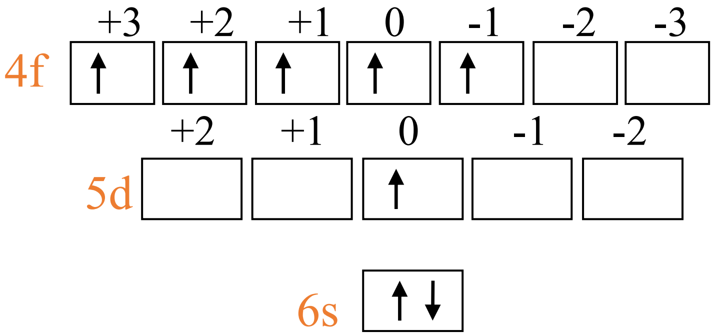
In bulk the orbital moment is quenched; thus, L = 0

Using the occupation number $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.3$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$, for the spin we obtain a contribution of $m_S = 2\ ½\ 1.7 = 1.7\ \mu_B$ from the 3d band and a contribution of $m_S = 0$ from the 4s band. Thus, $m_{at} = 1.7\ \mu_B$

Solution: magnetic moments

3) Co contribution: in bulk the orbital moment is quenched thus L = 0
Using the occupation number $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.0$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$, for the spin we obtain a contribution of $m_S = 2\ \tfrac{1}{2}\ 2 = 2.0\ \mu_B$ from the 3d band and a contribution of $m_S = 0$ from the 4s band. Thus, $m_{Co} = 2\ \mu_B$ in both composite.
Rare earth contribution can be calculated with Hund's rules

Ground state of Sm (Xe $4f^{5}\ 5d^{1}\ 6s^{2}$)



4f: $L = 5$, $S = 5/2$, $J = 5/2$

$m_{4f} = g\ J\ \mu_B = 5/7\ \mu_B$

5d: $L = 0$, $S = 1/2$, $J = 1/2$

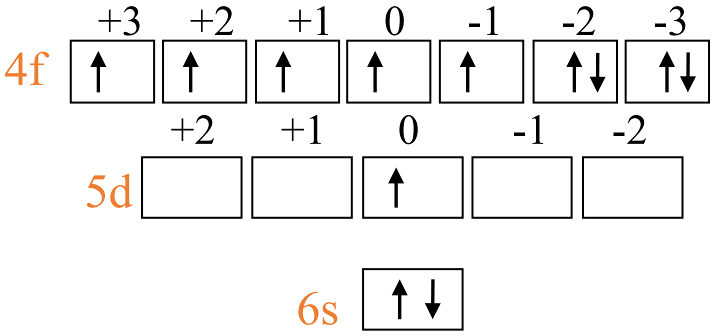
$m_{5d} = g\ J\ \mu_B = 1\ \mu_B$

$m_{6s} = g\ J\ \mu_B = 0\ \mu_B$

$m_{Sm} = 2/7\mu_B$ (S_{5d} is parallel to S_{4f} but since $L_{4f} > S_{4f}$, J_{4f} is parallel to L_{4f} and antiparallel to S_{4f})

$m_{u.f.} = 5\ m_{Co} - m_{Sm} = 68/7\mu_B$

Ground state of Dy (Xe $4f^{9}\ 5d^{1}\ 6s^{2}$)



4f: $L = 5$, $S = 5/2$, $J = 15/2$

$m_{4f} = g\ J\ \mu_B = 10\ \mu_B$

5d: $L = 0$, $S = 1/2$, $J = 1/2$

$m_{5d} = g\ J\ \mu_B = 1\ \mu_B$

$m_{6s} = g\ J\ \mu_B = 0\ \mu_B$

$m_{Dy} = 11\mu_B$

$m_{u.f.} = 5\ m_{Co} - m_{Dy} = -1\mu_B$