12.1 Energy barrier for bit reversal

Commercial magnetic storage requires that the bits retain their orientation for 10 years.
Calculate the corresponding energy barrier E_{rev} .

12.1 Energy barrier for bit reversal - Solution

EPFL

$$\tau \;=\; \tau_0 \exp(E_{rev}/k_B T) \qquad\qquad \tau_0 \approx 10^{-10}\text{s}$$

τ = 10 years = 3.1536 10^8 s

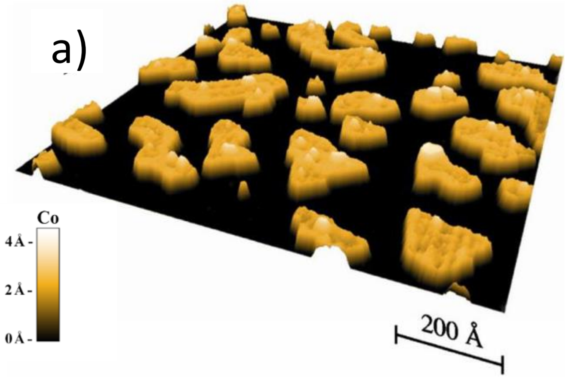
$k_B T \;=\; 0.026$ eV @ RT

$$E_{rev} = k_B T \,\ln\frac{\tau}{\tau_0} \approx 0026 \cdot 42.6 \approx 1.1 \text{ eV}$$

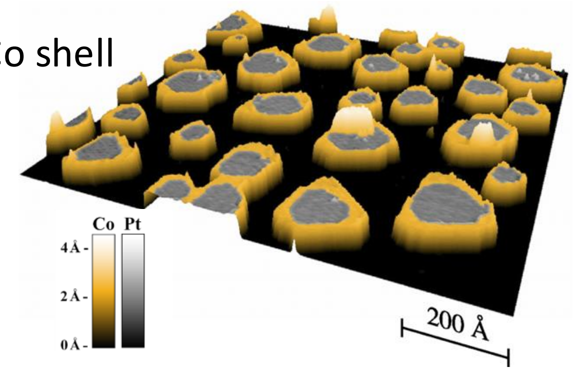
12.2 T_b of Co islands

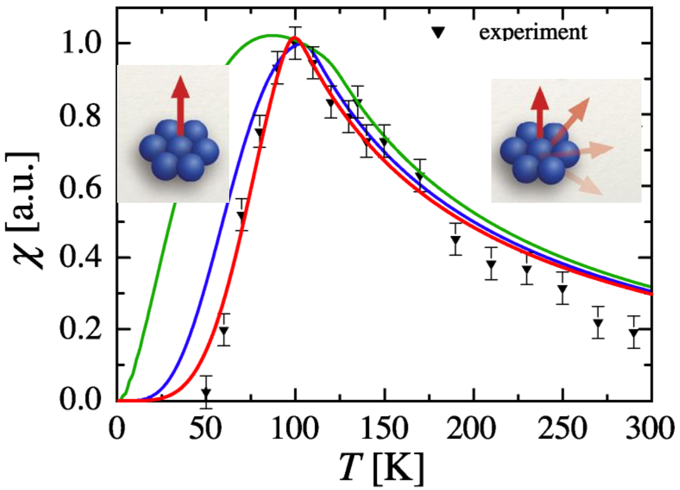
The blocking temperature T_b of 2D islands grown on Pt(111) has been determined by measuring the magnetic susceptibility $\chi = \frac{dM}{dB}$ $(\sim \frac{dM}{dH})$: T_b corresponds to the position of the peak in the magnetic susceptiblity curve vs T.

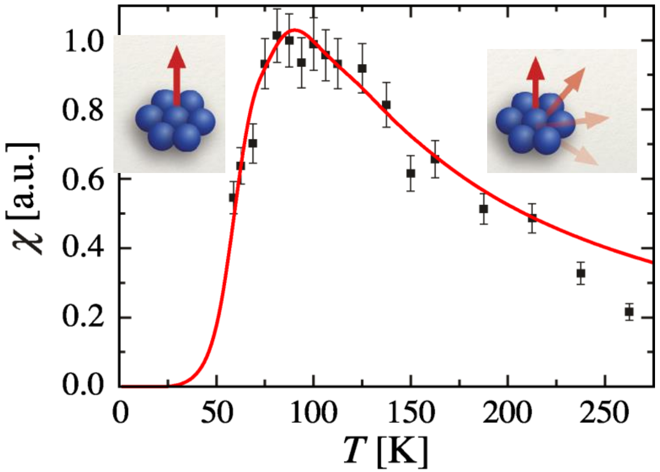
Two different samples have been grown: a) Co 2D islands, b) Pt 2D islands decorated by a Co rim. The islands are 1 atomic layer thick, and have a size of approx 1000 atoms. The magnetic susceptibility curves of the two samples have been recorded (the figures shows also some models, colored liines) .
What can you say about T_b for the two samples, and how can you explain it?



b) Pt core and Co shell





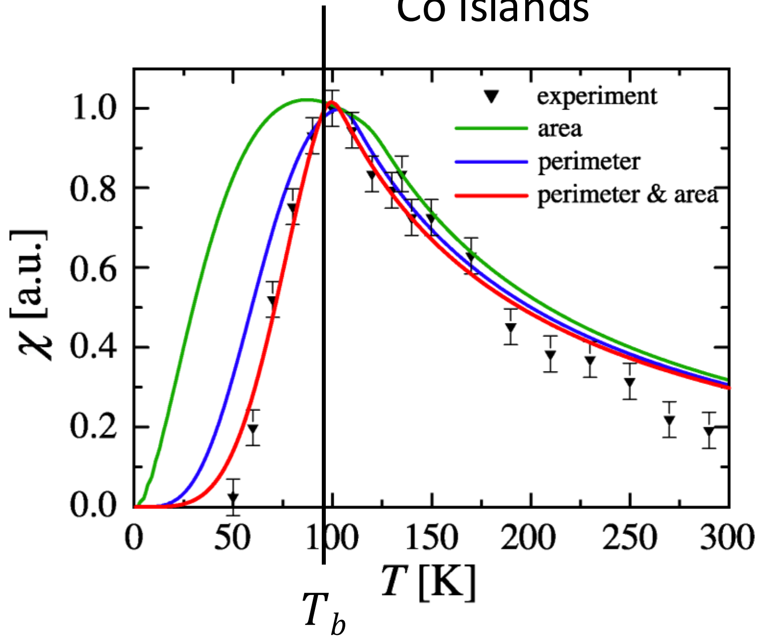


S. Rusponi *et al.*,
Nature Mat. **2**, 546 (2003)

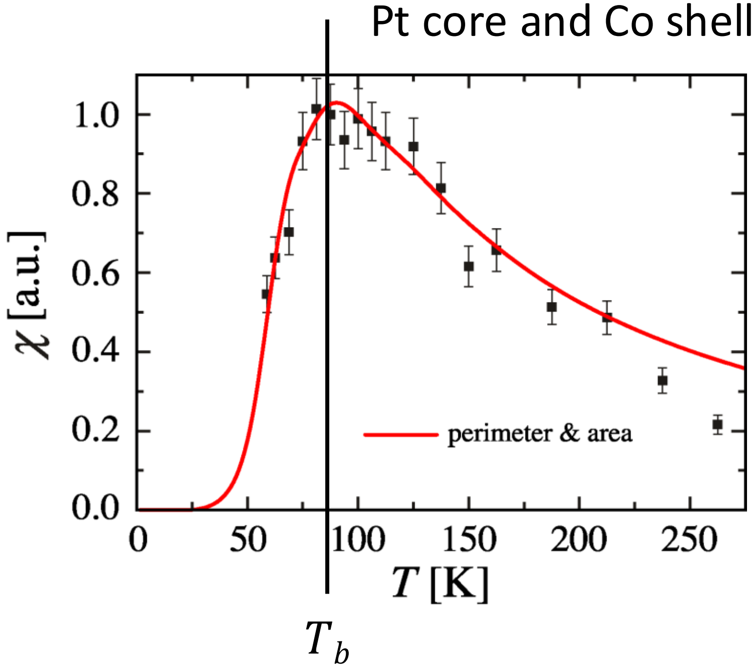
From the position of the peak in the magnetic susceptibility curve, we deduce that the to systems display the same blocking temperature $T_b \approx 100$ K.

This means that the barrier for reversal, related to the blocking temperature, originates from the Co atoms at the edge of the islands, i.e from the atoms that have lower coordination. For the atoms with lower coordination the orbital momentum is less quenched, resulting in a larger MAE (strong reduction of L implies a strong reduction of $K_{MAE} = \lambda S \Delta L$, and therefore of E_{rev} and T_b.
The edge does the job!

Co islands



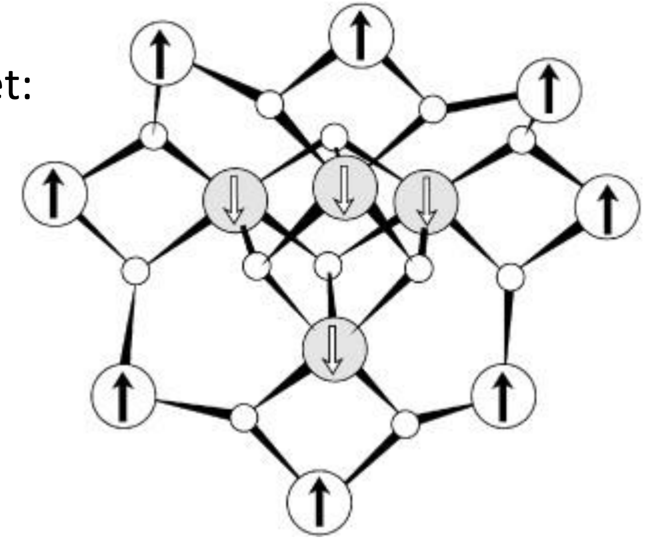
Pt core and Co shell islands



S. Rusponi *et al.*, Nature Mat. **2**, 546 (2003)

12. 3 Quantum tunneling of magnetization in Mn_{12}-acetate

Single molecule magnet:
Mn_{12}-acetate

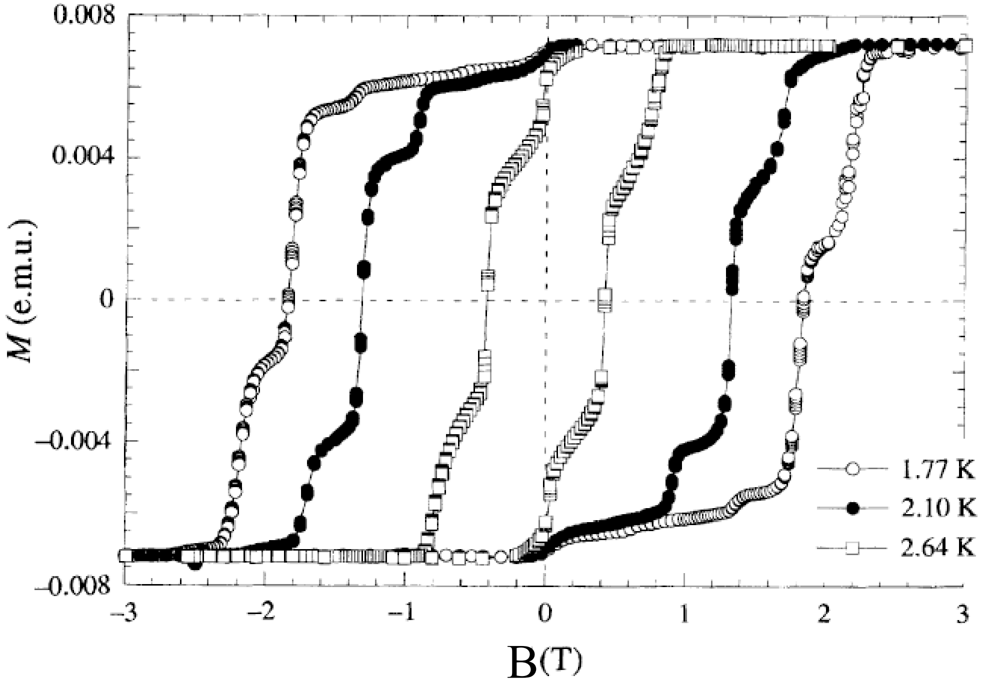


We measure the magnetization curve of a Mn_{12}-acetate.
The molecule consists of 12 Mn atoms, 8 Mn atoms having spin up and 4 Mn atoms having spin down. Each Mn atom has a spin $S = 5/2$ and orbital moment $L = 0$.

For simplicity, to find the energy levels we assume a uniaxial crystal field:
$E = -DM_J{}^2$ at $B = 0$ T.

Calculate the expected difference in magnetic field between two consecutive drops of the magnetization.

$D = 0.052$ meV; $\mu_B = 0.06$ meV/T



Adapted from: L. Thomas *et al.* Nature **383**, 145 (1996); J. R. Friedman *et al.* Phys. Rev. Lett. **76**, 3830 (1996)

The magnetization drop is due to QTM induced by spin-phonon scattering between states with opposite M_J values.

In field the energies are described by $E = -DM_J{}^2 - g_J\,\mu_B M_J \mathrm{B}$

At low T, after saturation at high field only the ground state is occupied. Then, reversing the field, a drop in M(H) is observed when the ground state $M_J = S$ is degenerate with a state with opposite $M_J = -S + n$ i.e.

$$-DS^2 - g_J\mu_B\, S\, B = -D(-S+n)^2 - g_J\mu_B(-S+n)\, B$$

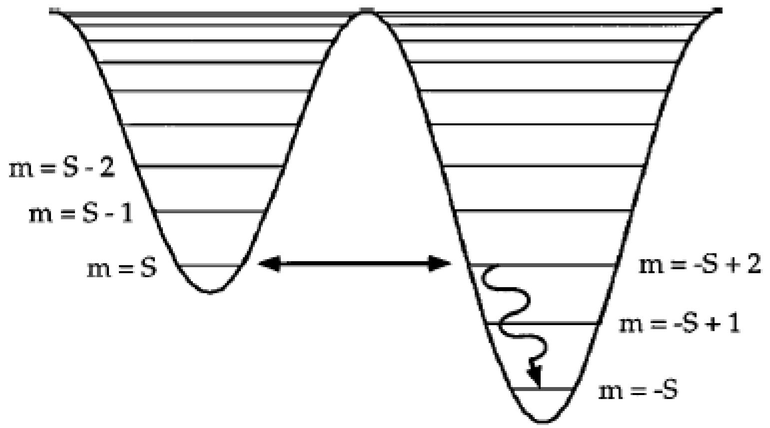
$$B = -\frac{Dn}{g_J\mu_B}$$

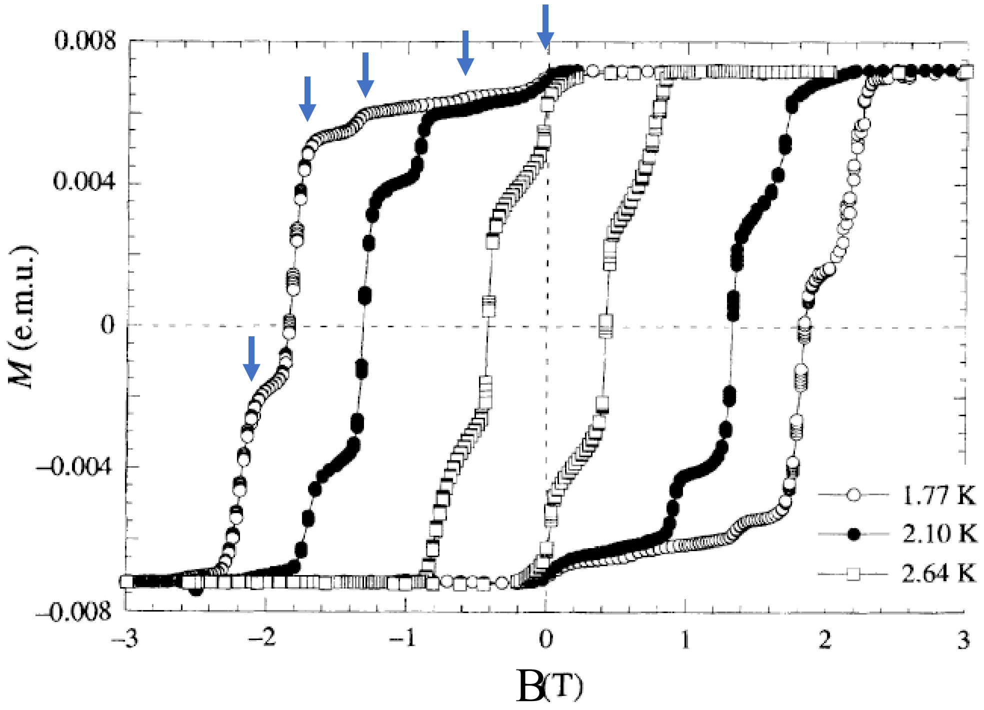
$$\Delta B = -\frac{D(n-1)}{g_J\mu_B} - \frac{Dn}{g_J\mu_B} = \frac{D}{g_J\mu_B}$$

Since $L = 0$, $g_J = 2$

$$\Delta B = \frac{0.052}{2\cdot 0.06} \approx 0.43\ \mathrm{T}$$

here $M_J = M_S$ is called m





12.4 XAS: dipolar selection rules

The electronic structure of 3d metals can be represented as $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{\alpha}\ 4s^{\beta}\ 4p^{\gamma}$
α is between 1 and 10,
$\beta + \gamma$ is between 1 and 2.

The schematic valence DOS of vanadium (V) and copper (Cu) are shown in the figure.

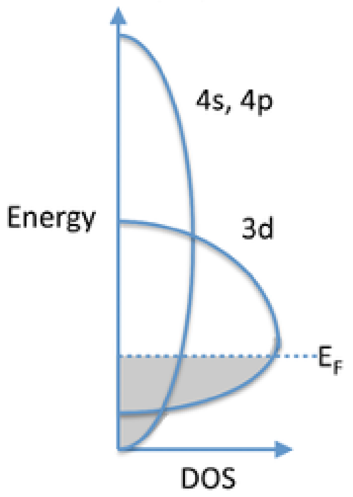
Using the dipolar selection rules and the table of the binding energies at the next page, for both V and Cu:

a) Identify the possible transition in a XAS experiment.

b) At which photon energy will the absorption edges appear ?

c) Which edges are “step-like” and which ones are “peak-like”?

vanadium



copper

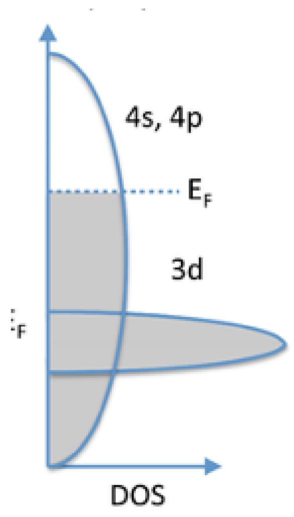


Table 1-1. Electron binding energies, in electron volts, for the elements in their natural forms.

Element	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$	N_1 4s	N_2 $4p_{1/2}$	N_3 $4p_{3/2}$
1 H	13.6											
2 He	24.6*											
3 Li	54.7*											
4 Be	111.5*											
5 B	188*											
6 C	284.2*											
7 N	409.9*	37.3*										
8 O	543.1*	41.6*										
9 F	696.7*											
10 Ne	870.2*	48.5*	21.7*	21.6*								
11 Na	1070.8†	63.5†	30.65	30.81								
12 Mg	1303.0†	88.7	49.78	49.50								
13 Al	1559.6	117.8	72.95	72.55								
14 Si	1839	149.7*b	99.82	99.42								
15 P	2145.5	189*	136*	135*								
16 S	2472	230.9	163.6*	162.5*								
17 Cl	2822.4	270*	202*	200*								
18 Ar	3205.9*	326.3*	250.6†	248.4*	29.3*	15.9*	15.7*					
19 K	3608.4*	378.6*	297.3*	294.6*	34.8*	18.3*	18.3*					
20 Ca	4038.5*	438.4†	349.7†	346.2†	44.3 †	25.4†	25.4†					
21 Sc	4492	498.0*	403.6*	398.7*	51.1*	28.3*	28.3*					
22 Ti	4966	560.9†	460.2†	453.8†	58.7†	32.6†	32.6†					
23 V	5465	626.7†	519.8†	512.1†	66.3†	37.2†	37.2†					
24 Cr	5989	696.0†	583.8†	574.1†	74.1†	42.2†	42.2†					
25 Mn	6539	769.1†	649.9†	638.7†	82.3†	47.2†	47.2†					
26 Fe	7112	844.6†	719.9†	706.8†	91.3†	52.7†	52.7†					
27 Co	7709	925.1†	793.2†	778.1†	101.0†	58.9†	59.9†					
28 Ni	8333	1008.6†	870.0†	852.7†	110.8†	68.0†	66.2†					
29 Cu	8979	1096.7†	952.3†	932.7	122.5†	77.3†	75.1†					
30 Zn	9659	1196.2*	1044.9*	1021.8*	139.8*	91.4*	88.6*	10.2*	10.1*			
31 Ga	10367	1299.0*b	1143.2†	1116.4†	159.5†	103.5†	100.0†	18.7†	18.7†			
32 Ge	11103	1414.6*b	1248.1*b	1217.0*b	180.1*	124.9*	120.8*	29.8	29.2			
33 As	11867	1527.0*b	1359.1*b	1323.6*b	204.7*	146.2*	141.2*	41.7*	41.7*			
34 Se	12658	1652.0*b	1474.3*b	1433.9*b	229.6*	166.5*	160.7*	55.5*	54.6*			
35 Br	13474	1782*	1596*	1550*	257*	189*	182*	70*	69*			
36 Kr	14326	1921	1730.9*	1678.4*	292.8*	222.2*	214.4	95.0*	93.8*	27.5*	14.1*	14.1*
37 Rb	15200	2065	1864	1804	326.7*	248.7*	239.1*	113.0*	112*	30.5*	16.3*	15.3 *
38 Sr	16105	2216	2007	1940	358.7†	280.3†	270.0†	136.0†	134.2†	38.9†	21.3	20.1†
39 Y	17038	2373	2156	2080	392.0*b	310.6*	298.8*	157.7†	155.8†	43.8*	24.4*	23.1*
40 Zr	17998	2532	2307	2223	430.3†	343.5†	329.8†	181.1†	178.8†	50.6†	28.5†	27.1†
41 Nb	18986	2698	2465	2371	466.6†	376.1†	360.6†	205.0†	202.3†	56.4†	32.6†	30.8†
42 Mo	20000	2866	2625	2520	506.3†	411.6†	394.0†	231.1†	227.9†	63.2†	37.6†	35.5†
43 Tc	21044	3043	2793	2677	544*	447.6	417.7	257.6	253.9*	69.5*	42.3*	39.9*
44 Ru	22117	3224	2967	2838	586.1*	483.5†	461.4†	284.2†	280.0†	75.0†	46.3†	43.2†
45 Rh	23220	3412	3146	3004	628.1†	521.3†	496.5†	311.9†	307.2†	81.4*b	50.5†	47.3†
46 Pd	24350	3604	3330	3173	671.6†	559.9†	532.3†	340.5†	335.2†	87.1*b	55.7†a	50.9†
47 Ag	25514	3806	3524	3351	719.0†	603.8†	573.0†	374.0†	368.3	97.0†	63.7†	58.3†

12.4 XAS: dipolar selection rules - Solution

a, b) The dipolar selection rule: $\Delta l = \pm 1$

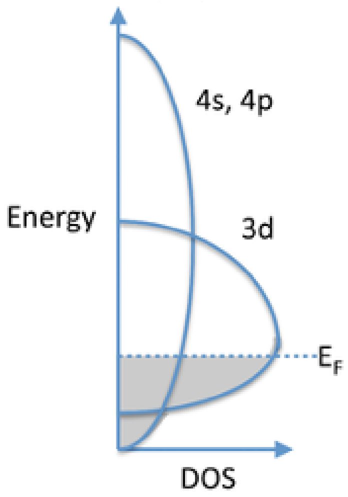
vanadium:

K	1s → 4p	5465 eV
L_1	2s → 4p	627 eV
$L_{2,3}$	2p → 3d, 4s	L_2 : 520 eV, L_3 : 512 eV

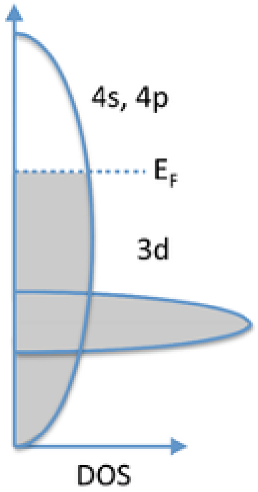
copper:

K	1s → 4p	8979 eV
L_1	2s → 4p	1097 eV
$L_{2,3}$	2p → 4s	L_2 : 952 eV, L_3 : 933 eV

vanadium



copper

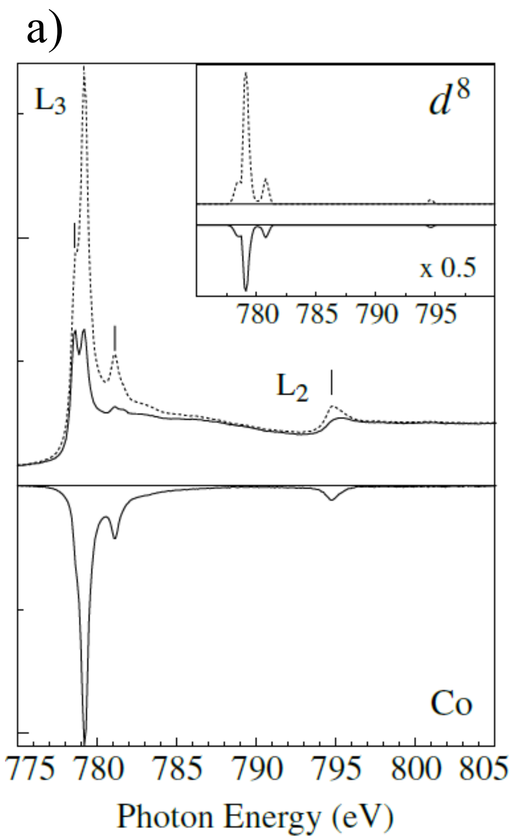


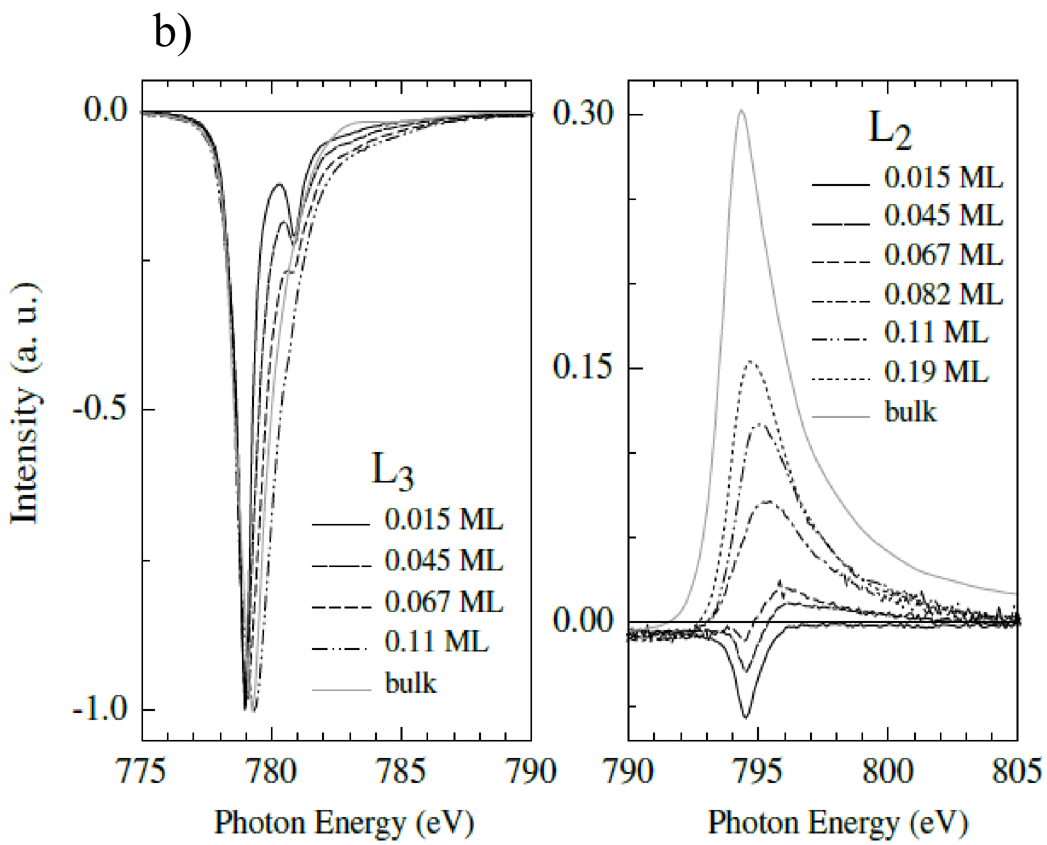
c) Vanadium K edge and L_1 edge are step-like, while the $L_{2,3}$ has peak-like shape because of the 3d contribution to the absorption. Note that the 2p → 4s contribution appears at the same energy, but as step like.
For Cu, all the edges have a step-like shape (no empty 3d DOS).

The XAS and XMCD spectra acquired at (L_2,L_3) edges of Co deposited on K (potassium) are shown in figure a).

Figure b) shows the evolution of the XMCD signal at the L_3 and L_2 edges as a function of the amount of deposited Co.

With a qualitative use of the sum rules, which kind of information we can deduce concerning the evolution of the orbital moment with the amount of deposited Co?





Source: doi.org/10.1103/PhysRevLett.88.047202

From the sum rules we know that:

$$L = -\frac{4}{3} h_d \frac{\int_{L3+L2} (\mu_+ - \mu_-) dE}{\int_{L3+L2} (\mu_+ + \mu_-) dE} = -\frac{4}{3} h_d \frac{q}{t}$$

i.e., the orbital moment is proportional to the total XMCD area (q).

The spectra show that for a Co coverage < 0.06 ML, the area of the XMCD peaks at both L_3 and L_2 have the same sign (both are pointing down) thus giving an additive contribution to the above integral, while for a Co coverage > 0.07 ML the L_2 peak is reversed with respect to the L_3 one, thus giving opposite contributions.

In addition, the area of the L_3 peak stays approximately constant, while the area of the L_2 peak rapidly increases, in particular above 0.08 ML, with the Co coverage. This implies that for Co coverages > 0.08 ML the orbital moment rapidly decreases → quenching of the orbital momentum