

Exchange coupling in 3d metals

The Curie temperature of bulk Fe, Co and Ni is respectively 1043 K, 1388 K, and 627 K.

Fe has a bcc structure with lattice constant $a = 0.287 \text{ nm}$;

Co has fcc structure (β -Co) with $a = 0.355 \text{ nm}$ (for simplicity; in reality, hcp is the most frequent structure for Co);

Ni has an fcc structure with $a = 0.352 \text{ nm}$.

1) Calculate J_{ex} , the exchange energy between a pair of atoms in each of the mentioned systems.

2) You want to grow a single atomic layer (monolayer) with the highest Curie temperature; which element among Fe, Co and Ni you chose?

Solution: exchange coupling in 3d metals

1) We know that
$$T_c = \frac{2 S(S+1) N J_{ex}}{3 k_B}$$

Fe has a bcc structure; thus each atom has $N = 8$ nearest neighbors.

Fe has a $4s^2 3d^6$ electronic configuration; thus, $S = 2$ and $L = 0$ due to orbital moment quenching in bulk.

$$J_{ex} = \frac{3k_B T_c}{2 S(S+1)N} = 2.8 \text{ meV}$$

Co has a fcc structure; thus each atom has $N = 12$ nearest neighbors.

Co has a $4s^2 3d^7$ electronic configuration; thus, $S = 3/2$ and $L = 0$ due to orbital moment quenching in bulk.

$$J_{ex} = \frac{3k_B T_c}{2 S(S+1)N} = 4 \text{ meV}$$

Ni has a fcc structure; thus each atom has $N = 12$ nearest neighbors.

Ni has a $4s^2 3d^8$ electronic configuration; thus, $S = 1$ and $L = 0$ due to orbital moment quenching in bulk.

$$J_{ex} = \frac{3k_B T_c}{2 S(S+1)N} = 3.4 \text{ meV}$$

2) In a monolayer, $N = 4$; then we can use the previously calculated values of J_{ex} to calculate T_c for each element

We have $T_c(\text{Fe}) = 521 \text{ K}$; $T_c(\text{Co}) = 465 \text{ K}$; $T_c(\text{Ni}) = 211 \text{ K}$.

Then in the monolayer regime Fe is the element with the highest Curie temperature (while in bulk is Co)

Spin coupling

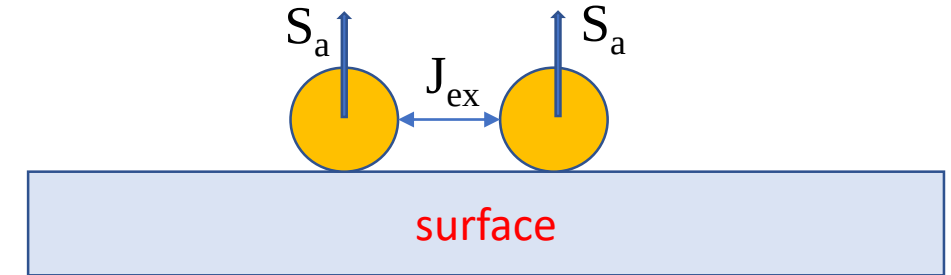
Consider two atoms on a surface. For simplicity we assume that each atom has a spin $S_a=1/2$ which can point up or down. Using the standard notation $|S,m\rangle$, each atom can then assume the states $|1/2,1/2\rangle$ or $|1/2,-1/2\rangle$.

With an STM tip we approach the two atoms to form a dimer. An exchange coupling couples the two spins: the dimer is then described by an Hamiltonian of the form $H = -2J_{\text{ex}} S_a S_a$, where J_{ex} is the exchange constant.

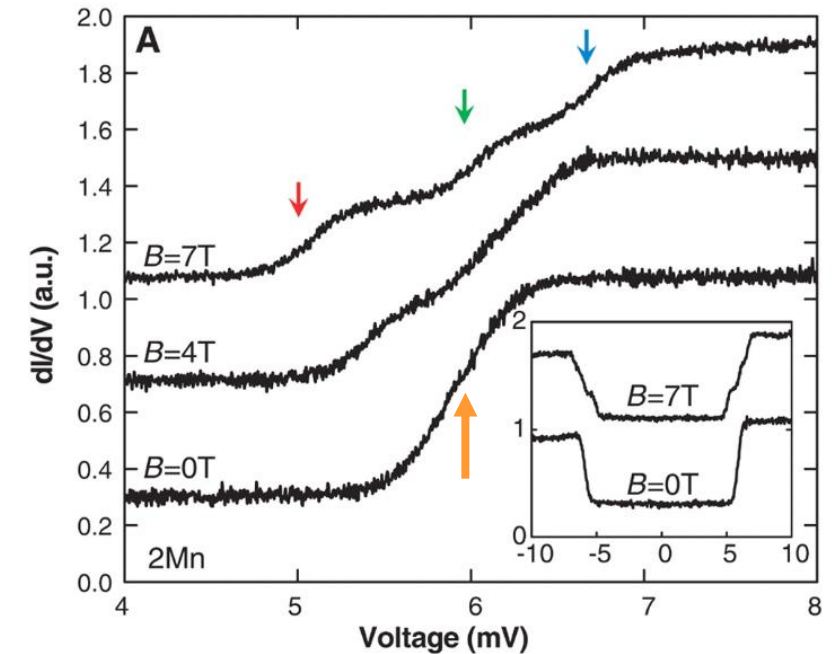
What is the total spin S_d of the dimer? Assuming J_{ex} negative (antiferromagnetic coupling) and $B = 0$, describe the ground and excited states of the dimer and their energy separation.

We go with the STM tip on top of the dimer and we perform an IETS experiment. The result is shown in the figure here on the side.

Why at $B = 0$ only one excitation (orange arrow) is observed while in field three excitations (red, green, and blue arrows) are observed? Use the experimental data to estimate roughly the exchange constant J_{ex} .



IETS spectra at different magnetic field B on a Mn dimer



Solution: Spin coupling

Using the standard notation $|S,m\rangle$, each atom can assume the states $|1/2,1/2\rangle$ or $|1/2,-1/2\rangle$

The atom spins in the dimer can be:

parallel to give $S_d = 1$ corresponding to the triplet $|1,-1\rangle$, $|1,0\rangle$ and $|1,1\rangle$ (ferromagnetic coupling) or antiparallel to give $S_d = 0$ corresponding to the singlet $|0,0\rangle$ (antiferromagnetic coupling).

At $B = 0$ the ground state is given by the singlet $|0,0\rangle$ and the excited state by the three states of the triplet ($|1,m\rangle$ $m = -1, 0, 1$) which are degenerate in energy.

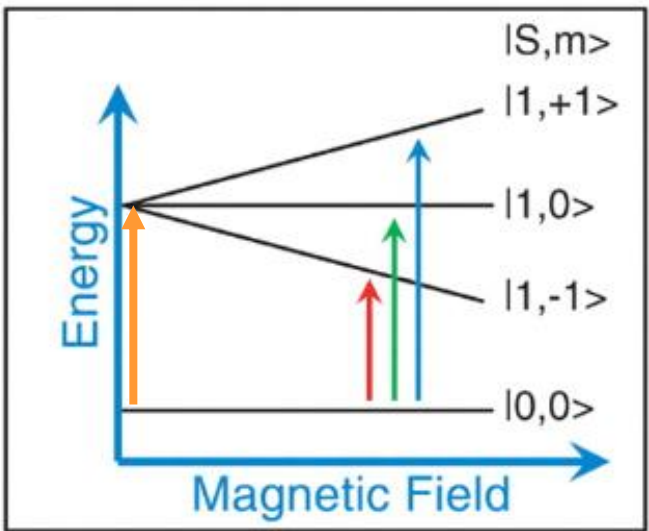
The energy separation between the singlet and the triplet is equal to $2J_{\text{ex}}$.

The spin of the tunneling electron σ , while scattering with the dimer, undergoes a change in the spin of $\Delta\sigma = \pm 1, 0$. To conserve the total moment, all the transitions in the sketch are possible for the dimer spin: red ($\Delta m = -1$), green ($\Delta m = 0$) and blue ($\Delta m = +1$).

At $B = 0$ the three states of the triplet are degenerate in energy and then only the transition corresponding to the orange arrow is observed.

In an external magnetic field, the Zeeman energy splits the three states of the triplet.

The exchange constant can be estimated by the position of the step in the IETS spectrum acquired at $B = 0$, which is roughly 6 meV. This corresponds to $J_{\text{ex}} = 3 \text{ meV}$



IETS energies vs B field

