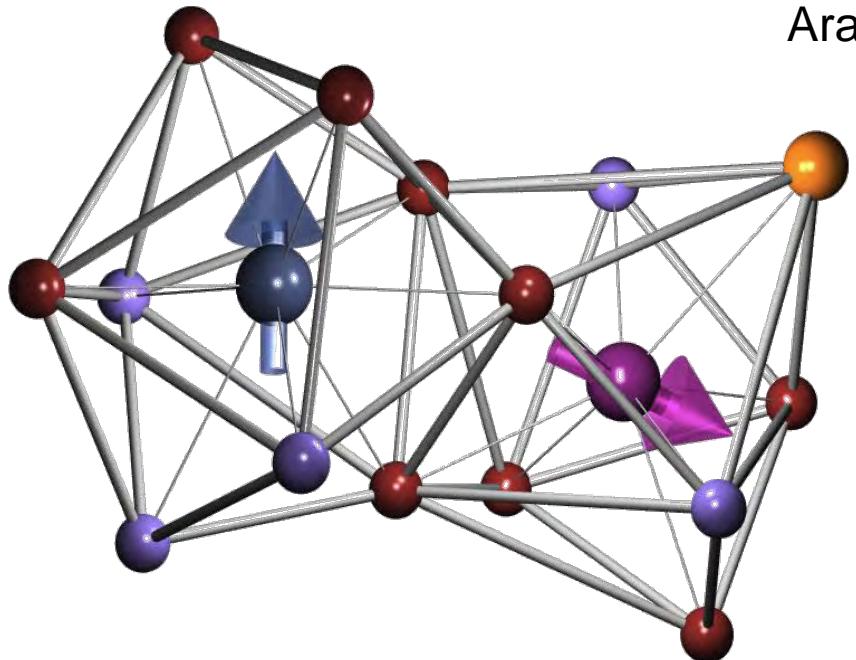




Molecular prototypes for spin-based CNOT and SWAP quantum logic gates



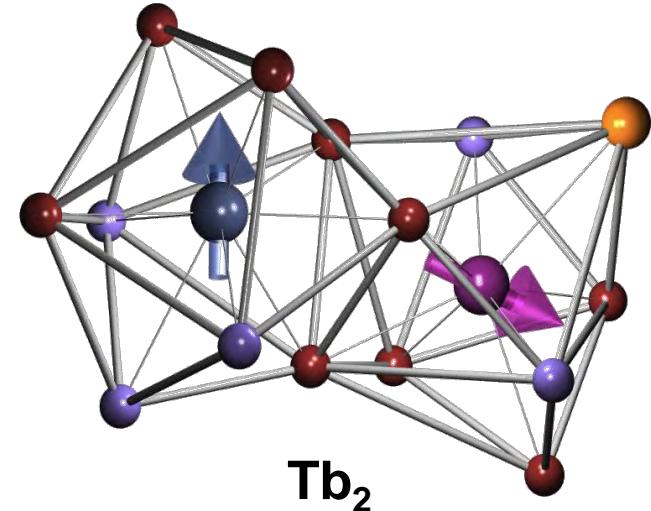
Fernando LUIS

Instituto de Ciencia de Materiales de
Aragón (Zaragoza, Spain)

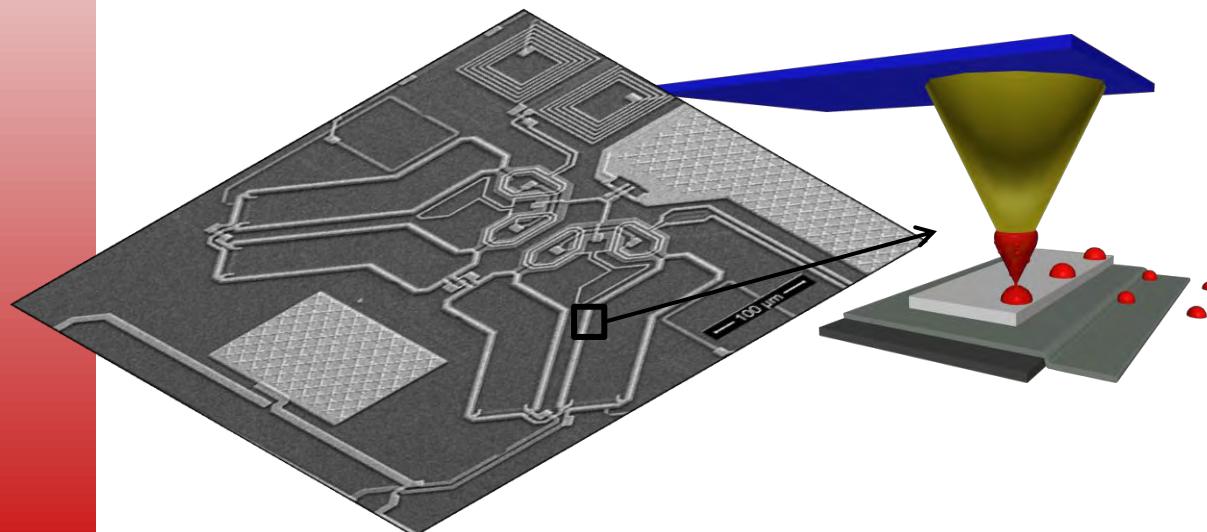


Outline

Molecular design of CNOT and SWAP quantum gates



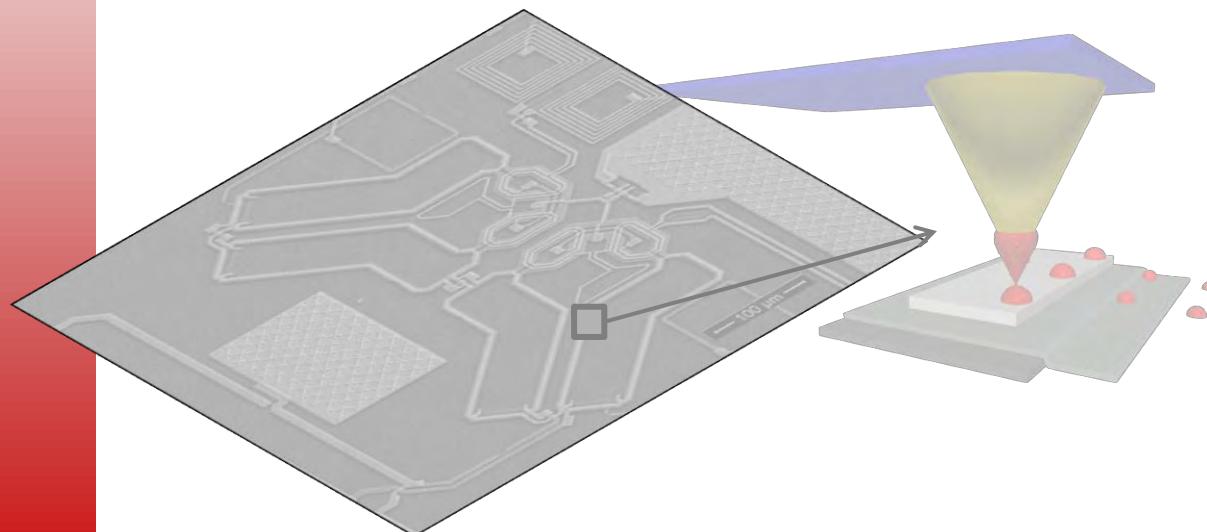
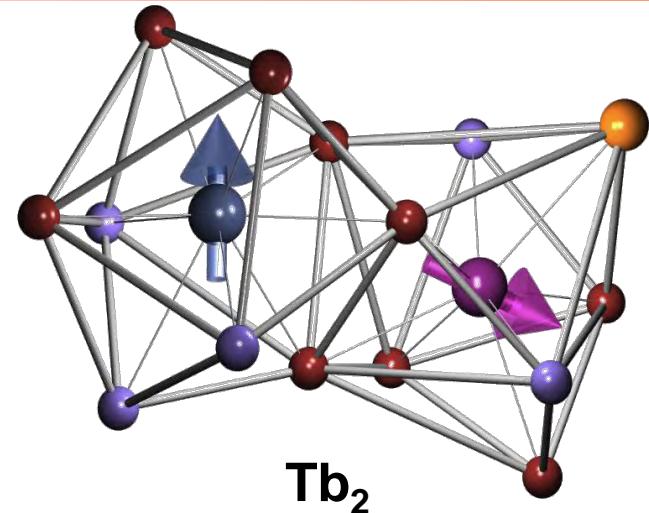
Tb_2



Integration of SMM
into superconducting
microdevices

Outline

Molecular design of CNOT and SWAP quantum gates



Integration of SMM
into superconducting
microdevices

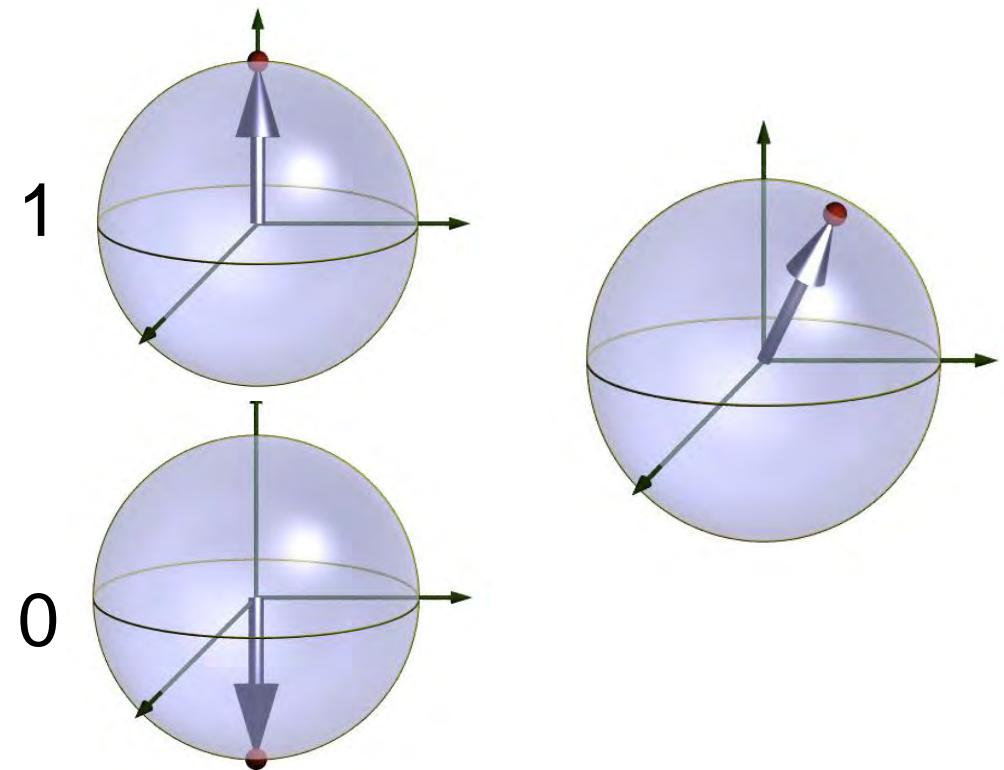
Quantum computers



Richard Feynman, 1982

Quantum processing of information

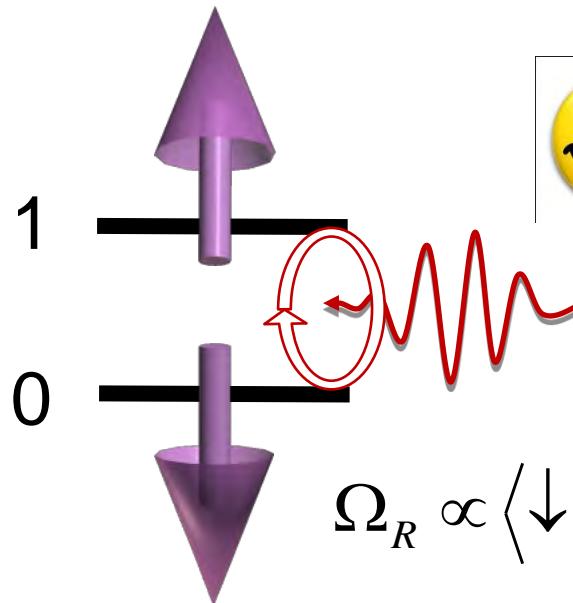
Bit → Qubit



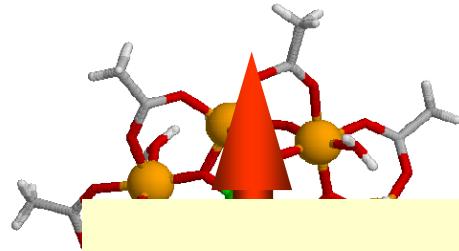
Molecular qubits

Unitary operations

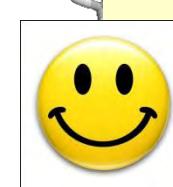
Single qubits



$$|\uparrow\rangle \rightarrow \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$



- Chemically synthesized



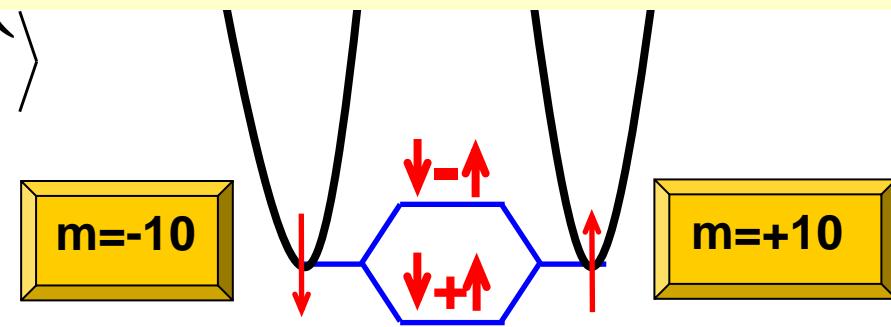
- Carry magnetic moment

Scalability

Identical entities

Read-out

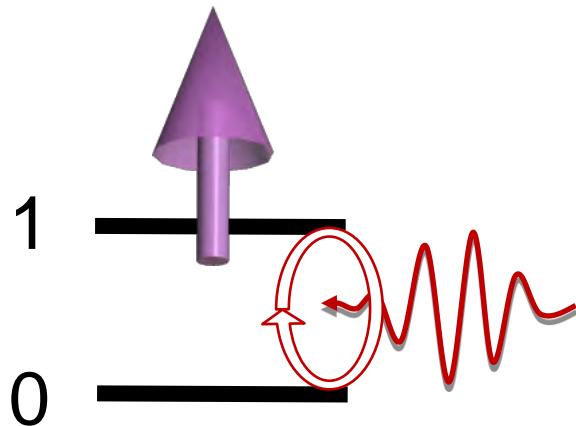
Initialization



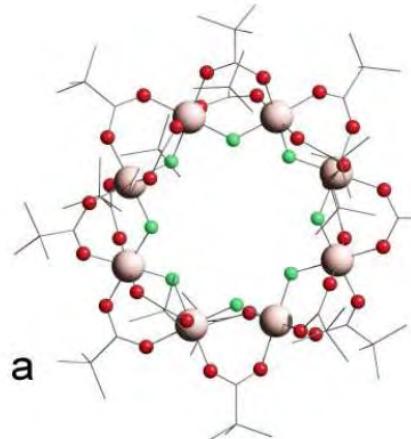
Molecular qubits

Unitary operations

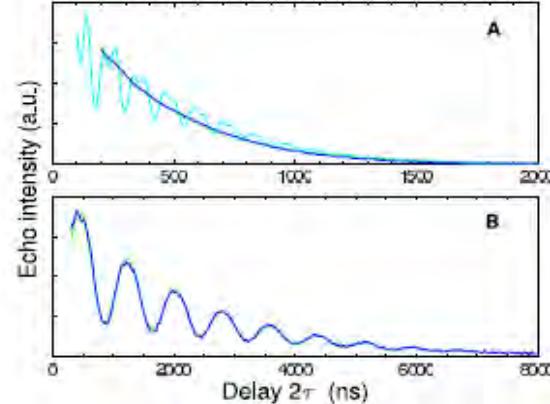
Single qubits



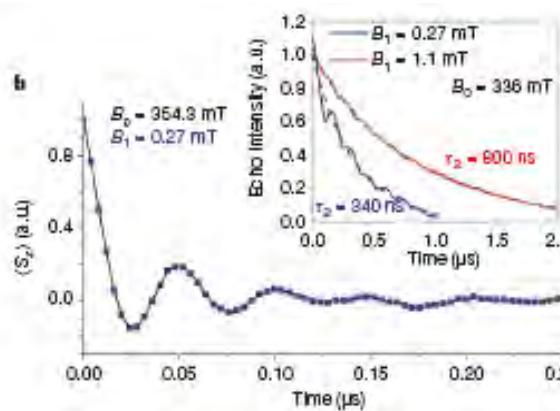
$$|\uparrow\rangle \rightarrow \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$



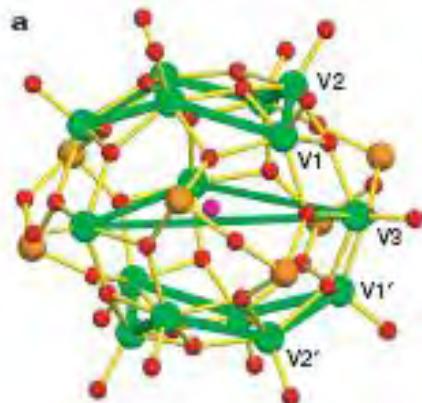
Cr_7Ni , $S = 1/2$



A. Ardavan et al. Phys. Rev. Lett. **98**, 057201 (2007)



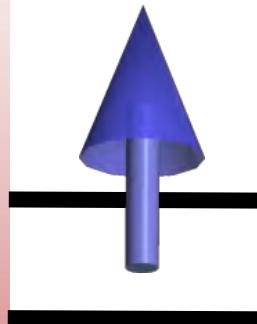
S. Bertaina et al. Nature **453** (2008)



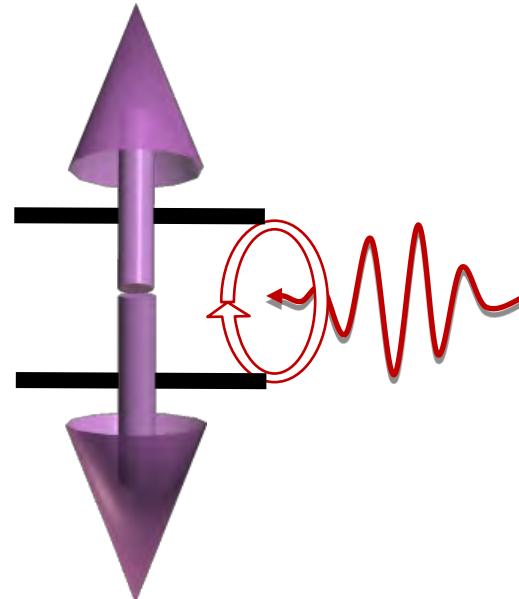
V_{15} , $S = 1/2$

CNOT (universal) quantum logic gate

“control”



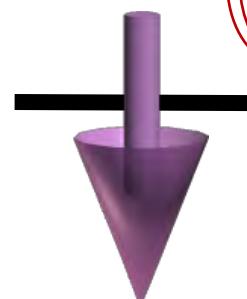
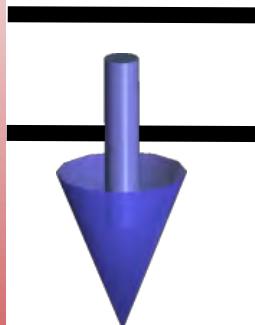
“target”



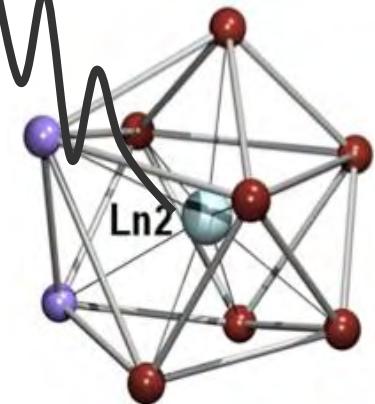
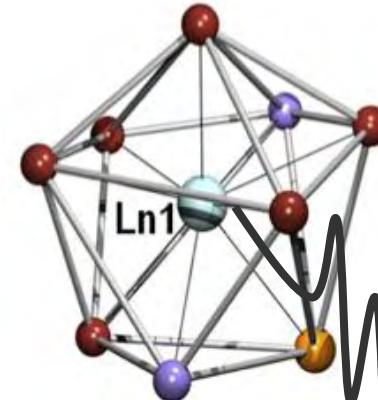
CNOT quantum logic gate

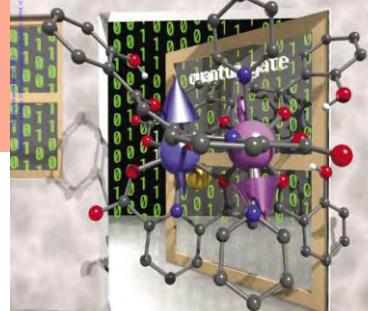
“control”

“target”



- 1. Two qubits
- 2. Coupling
- 3. Asymmetry

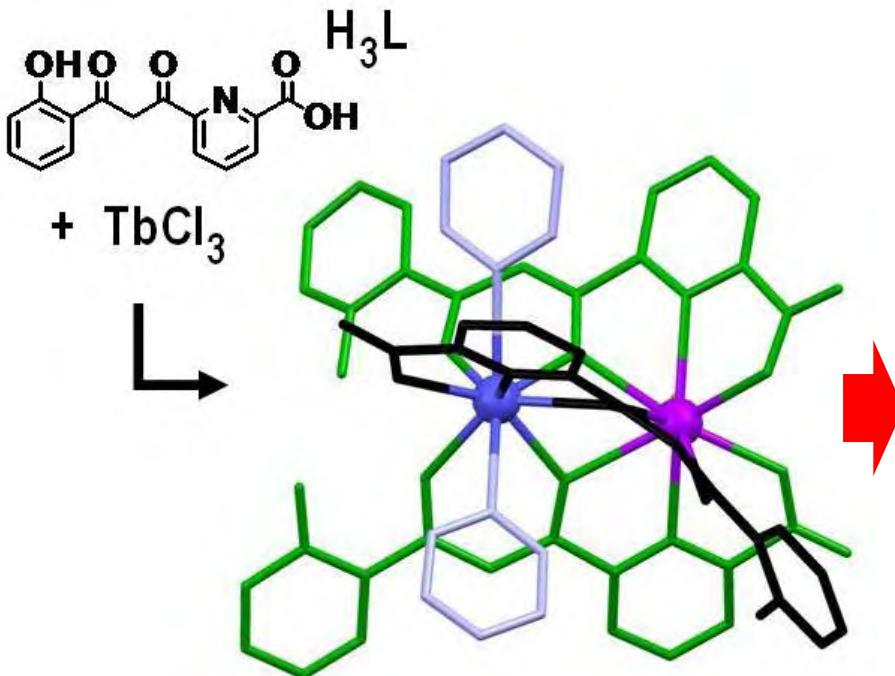




RSC Publishing

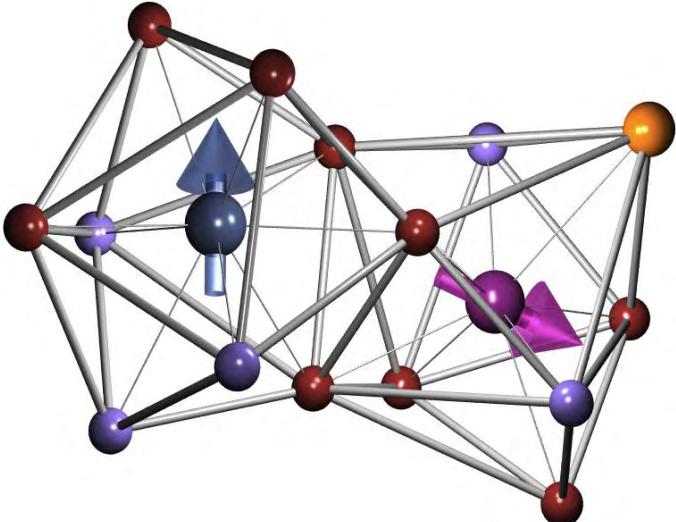
DOI: 10.1039/C1CS15115K

D. Aguilà *et al.*, Inorg. Chem. **49** (2010) 6784
 G. Aromí, D. Aguilà, P. Gámez, F. Luis, and O. Roubéau,
 Chem. Soc. Rev., (2012), DOI: 10.1039/C1CS15115K



Dinuclear $[Tb]_2$ complex

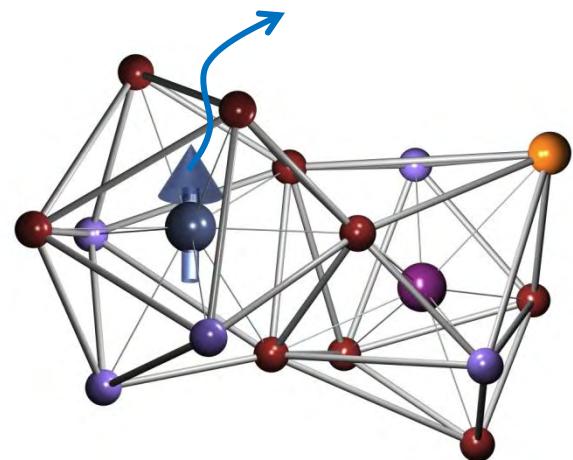
Linked to three asymmetric
 H_3L ligands



Two anisotropic spins in
 different coordinations

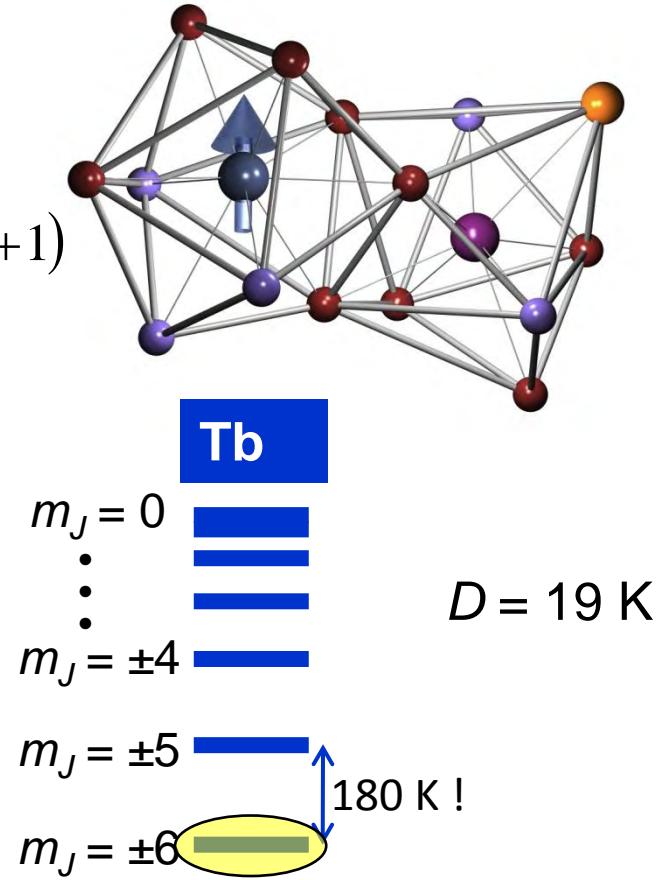
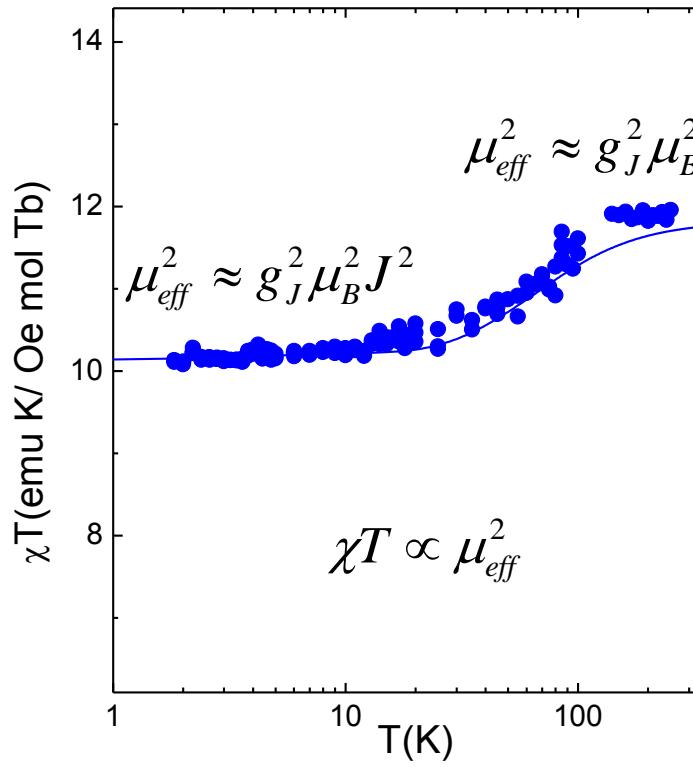
Definition of qubit states

[LaTb] $J = 6$, $g_J = 3/2$



Definition of qubit states

[LaTb] $J = 6, g_J = 3/2$

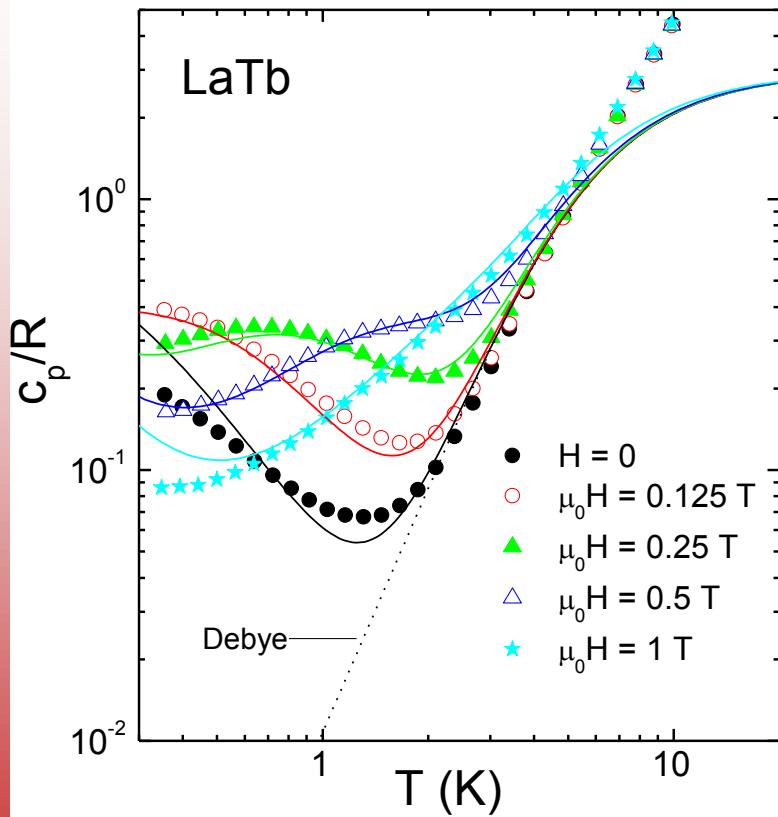


$$\mathcal{H}_{anis} = -DS_z^2 - g_J \mu_B (H_x J_x + H_y J_y + H_z J_z)$$

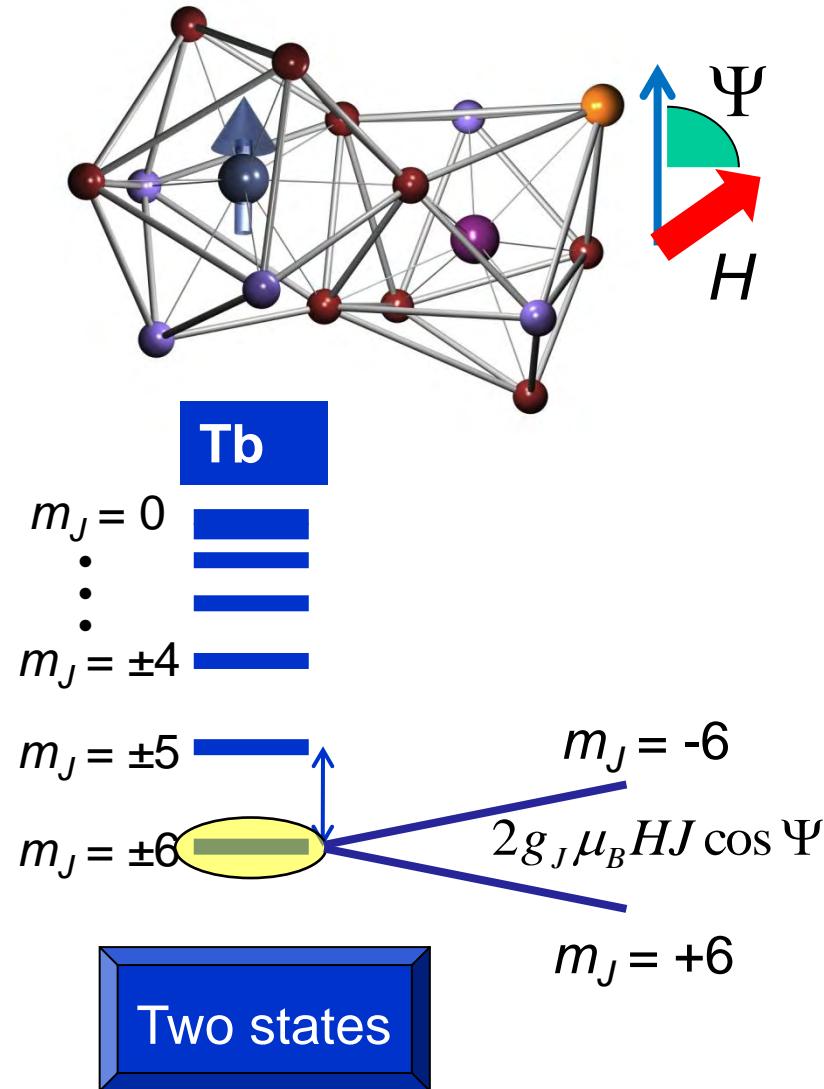
Two states

Definition of qubit states

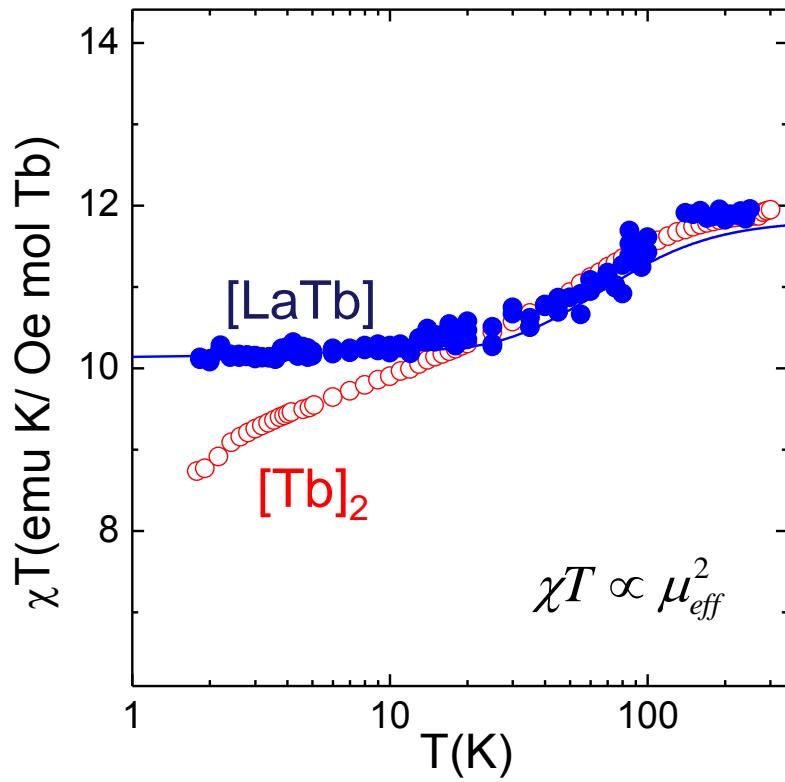
[LaTb] $J = 6, g_J = 3/2$



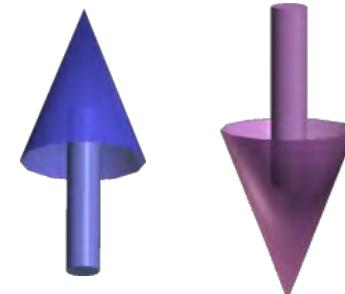
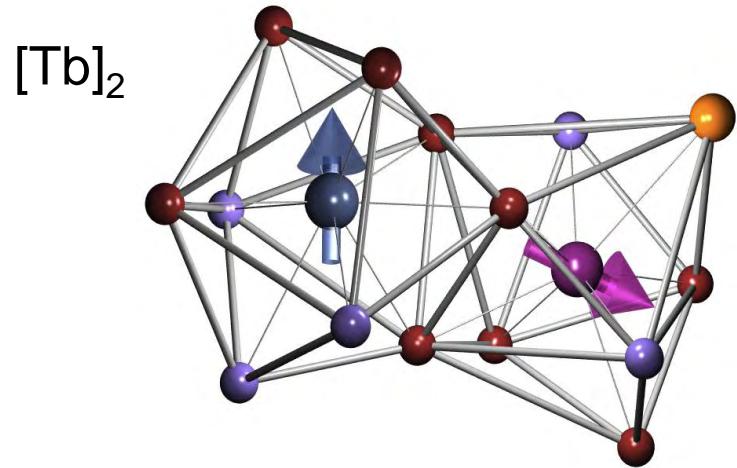
$$\mathcal{H}_{m=\pm 6} = -g_J \mu_B H_z J_z$$



Coupling between the Tb³⁺ qubits

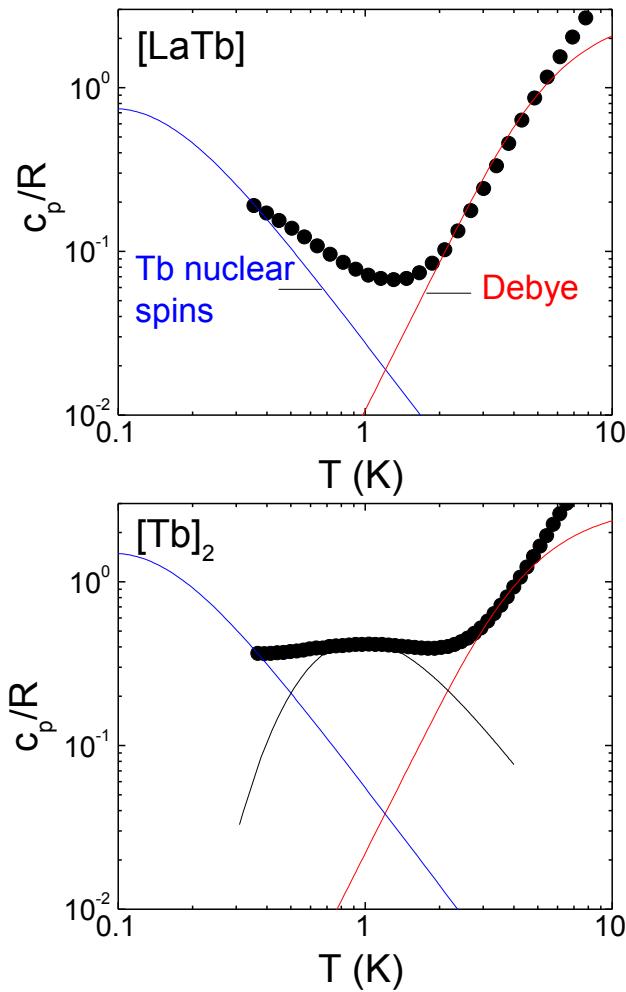


$$\mathcal{H}_{\text{exch}} = -J_{\text{ex}} J_{z1} J_{z2}$$

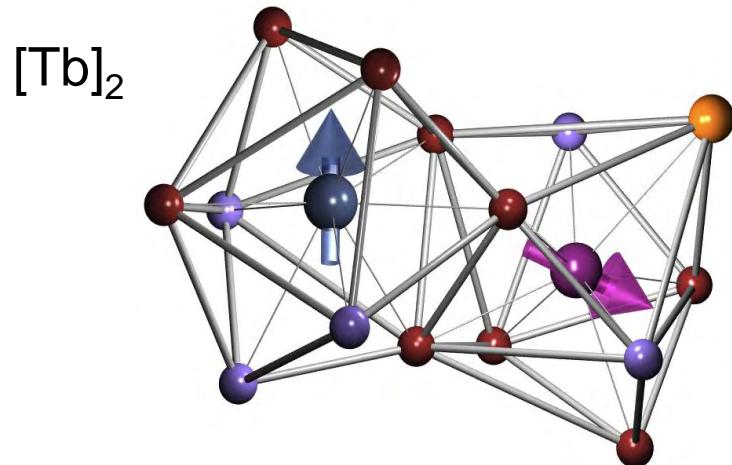


AF coupling

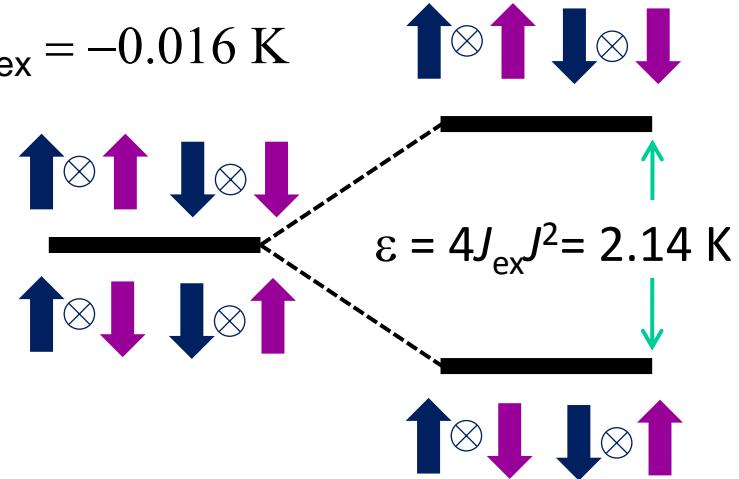
Coupling between the Tb³⁺ qubits



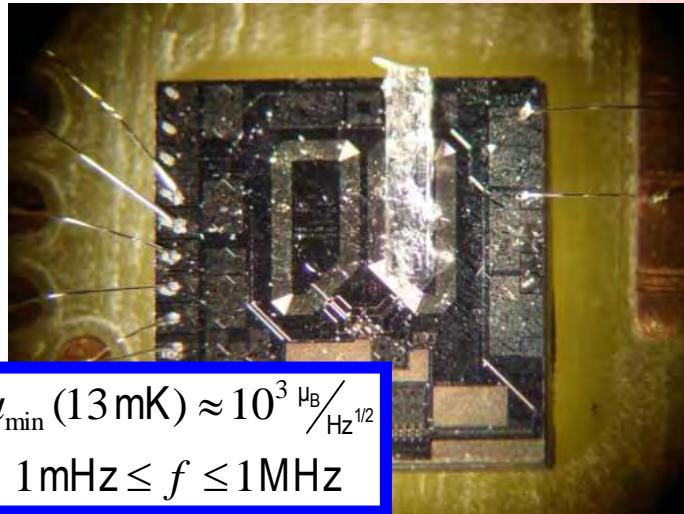
$$\mathcal{H}_{exch} = -J_{ex} J_{z1} J_{z2}$$



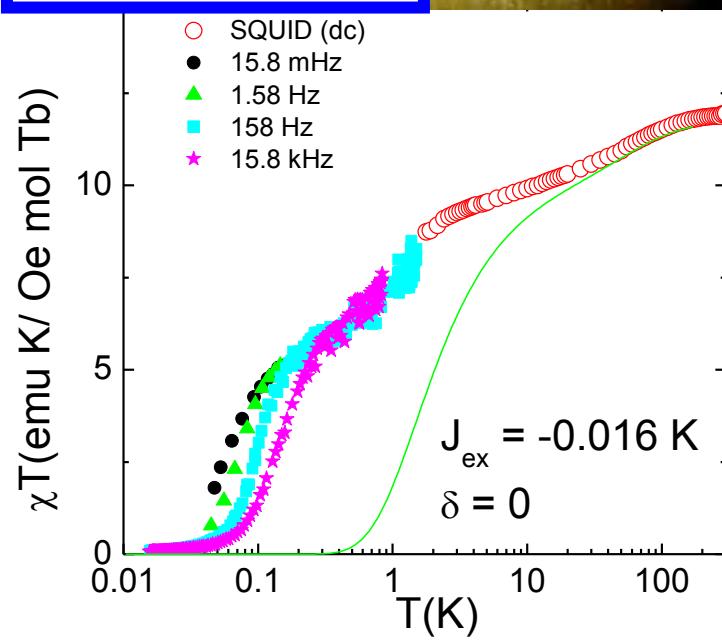
$$J_{ex} = -0.016 \text{ K}$$



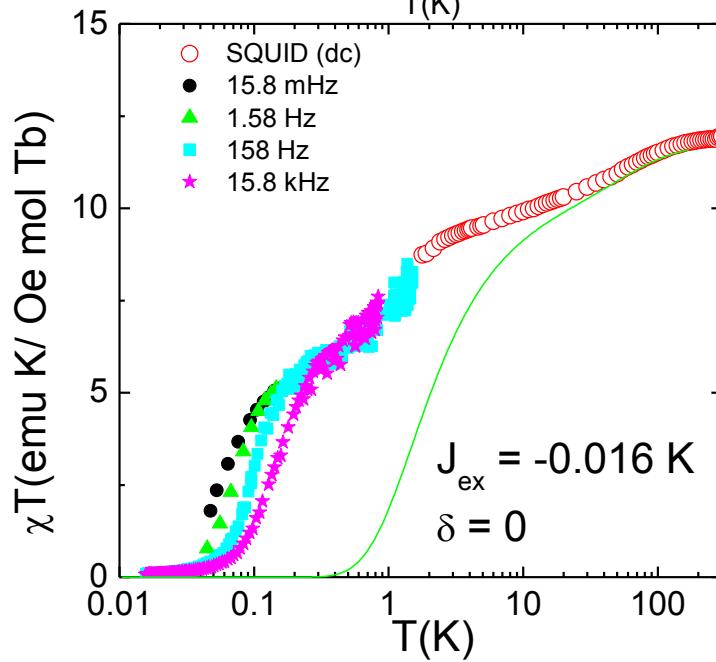
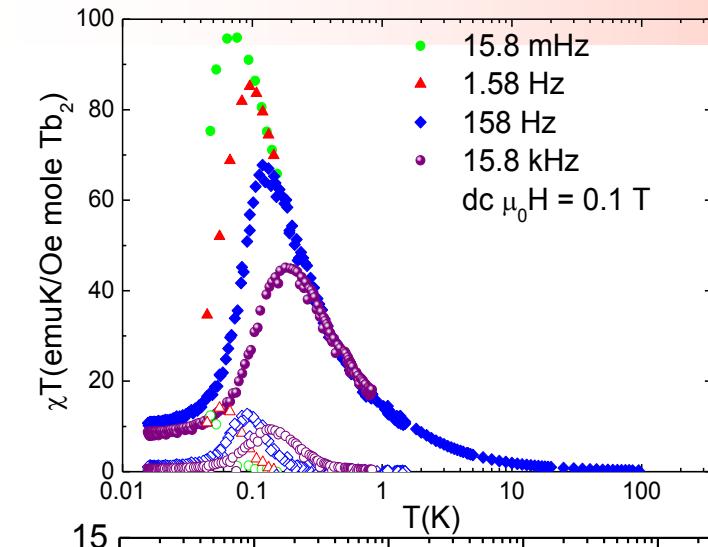
Magnetic asymmetry



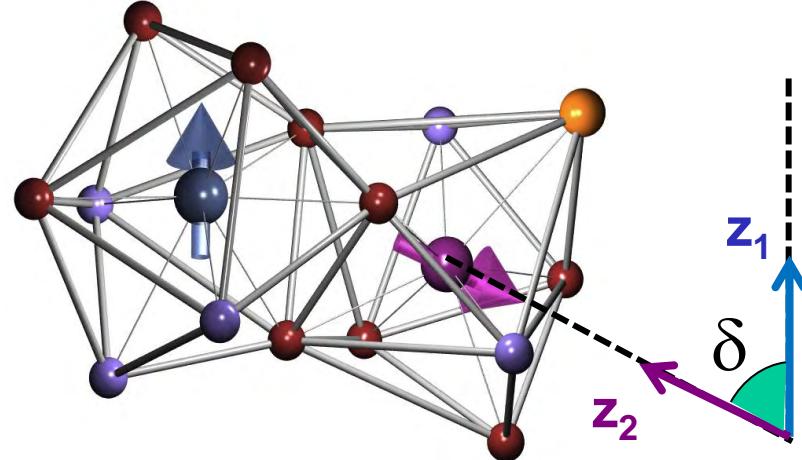
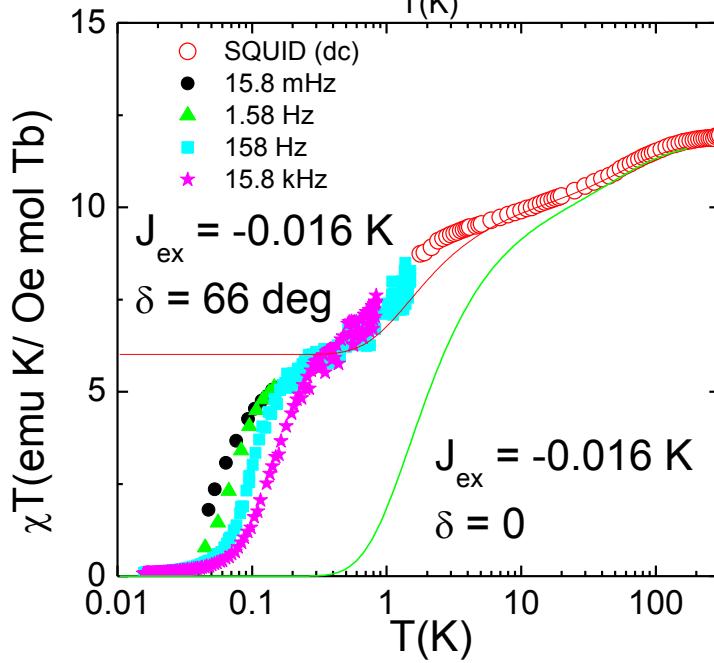
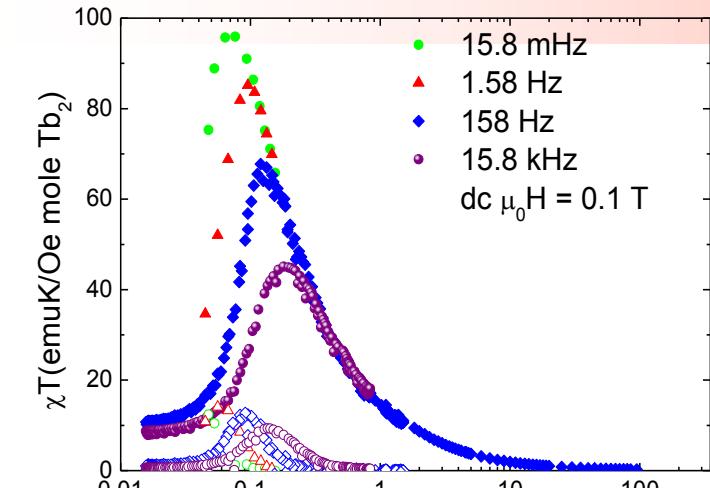
$$\mu_{\min}(13 \text{ mK}) \approx 10^3 \frac{\mu_B}{\text{Hz}^{1/2}}$$
$$1 \text{ mHz} \leq f \leq 1 \text{ MHz}$$



Magnetic asymmetry



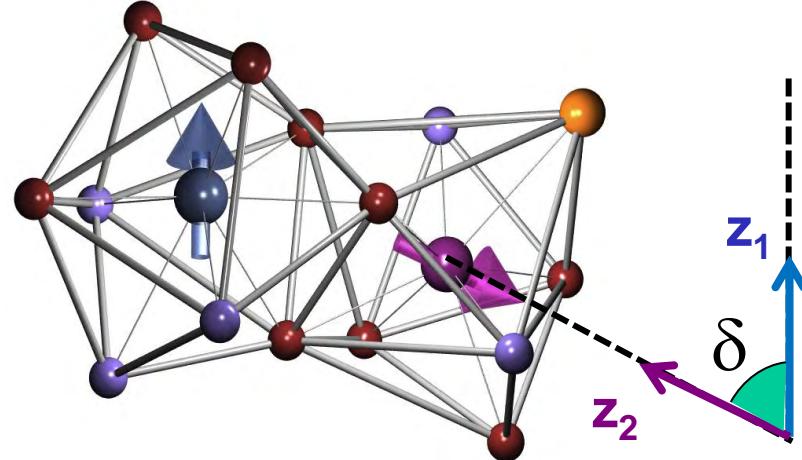
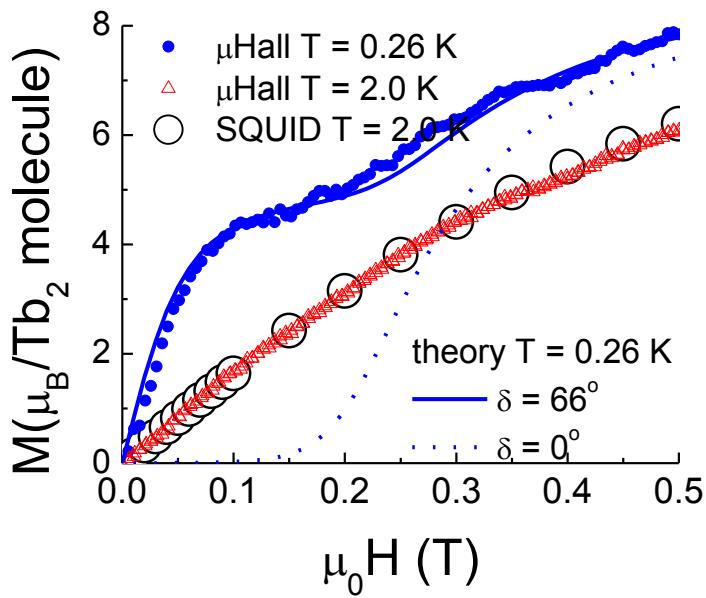
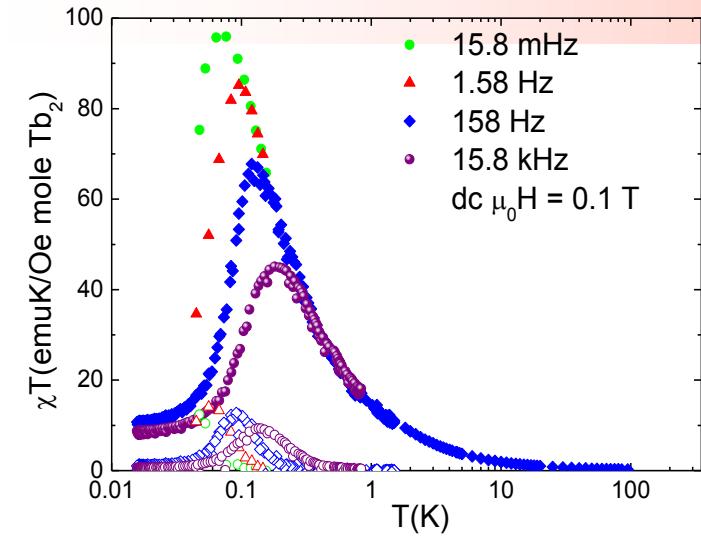
Magnetic asymmetry



$\delta = 66$ degrees

Noncollinear
anisotropy axes

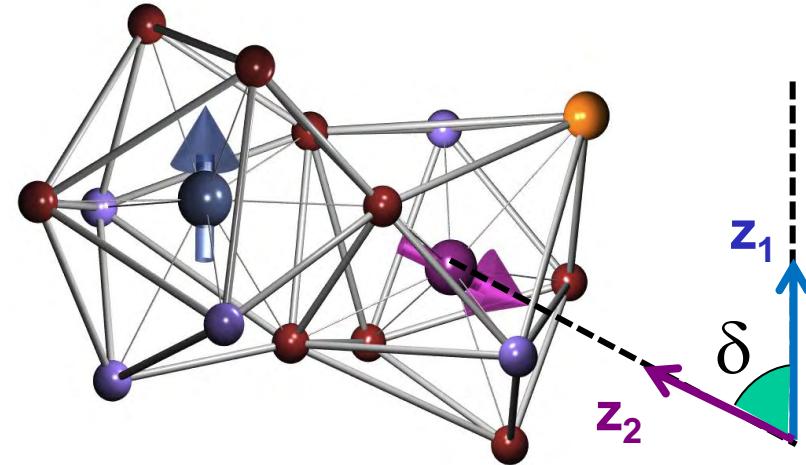
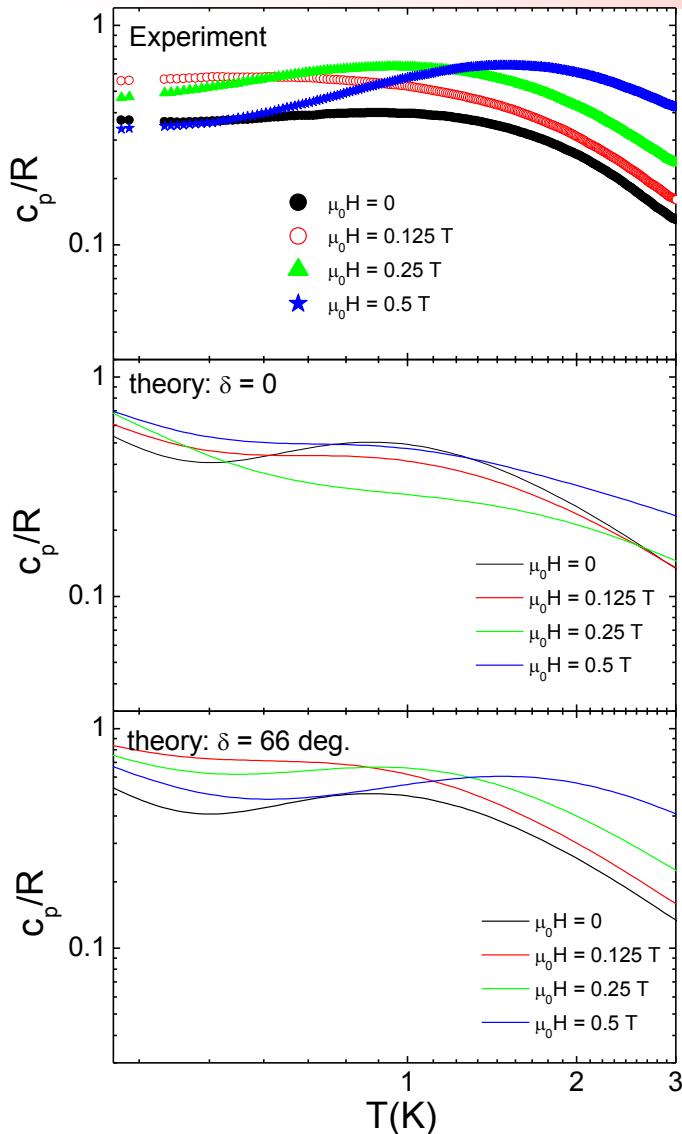
Magnetic asymmetry



$\delta = 66$ degrees

Noncollinear
anisotropy axes

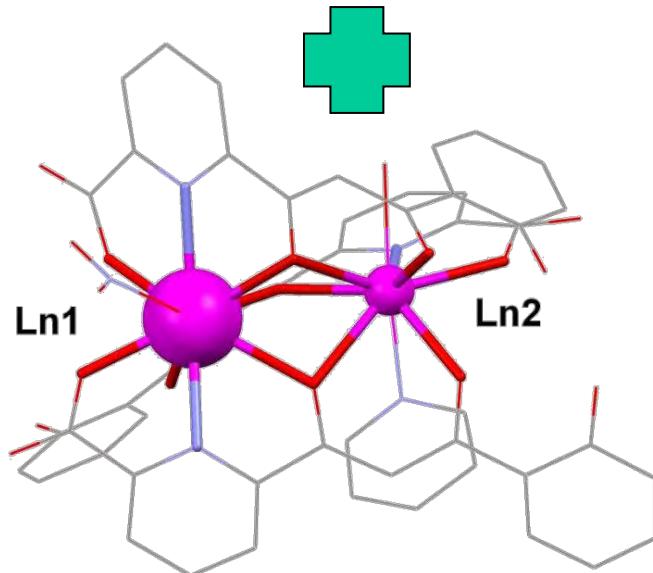
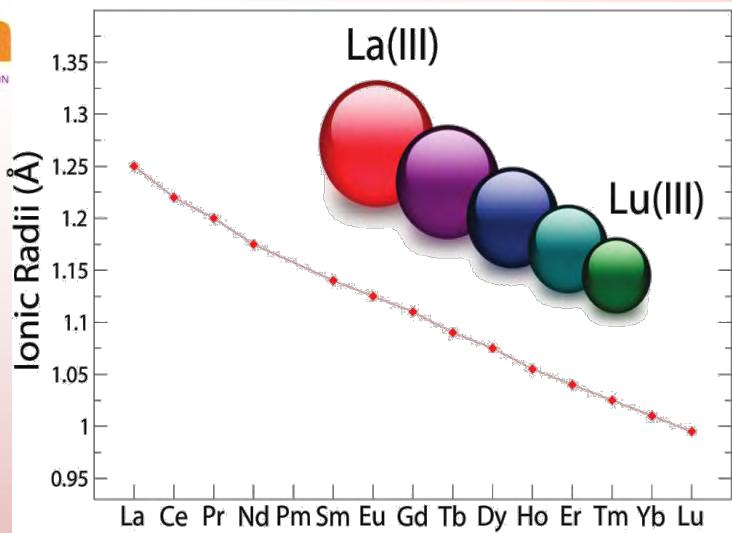
Magnetic asymmetry



$\delta = 66$ degrees

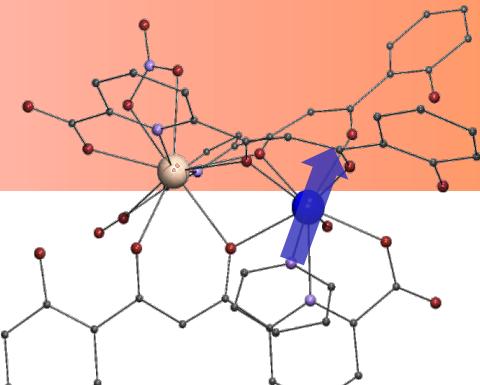
Noncollinear
anisotropy axes

Heterometallic clusters



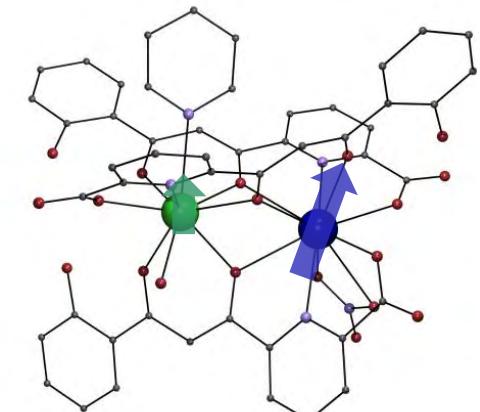
[LaEr]

Er³⁺
 $J = 15/2,$
 $g_J = 6/5$

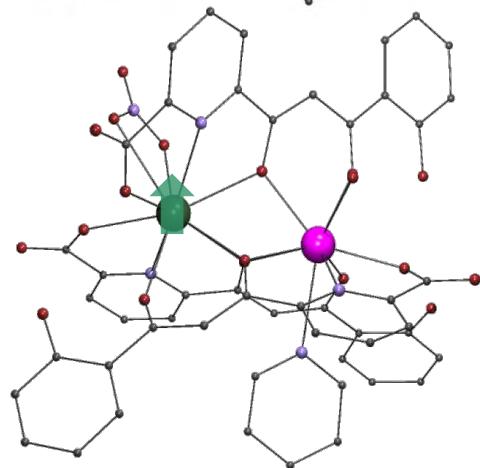


[CeEr]

Ce³⁺
 $J = 5/2,$
 $g_J = 6/7$

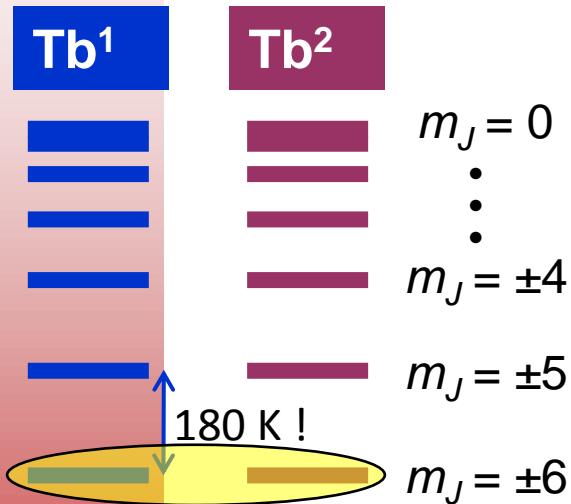


[CeY]



All ingredients are met!

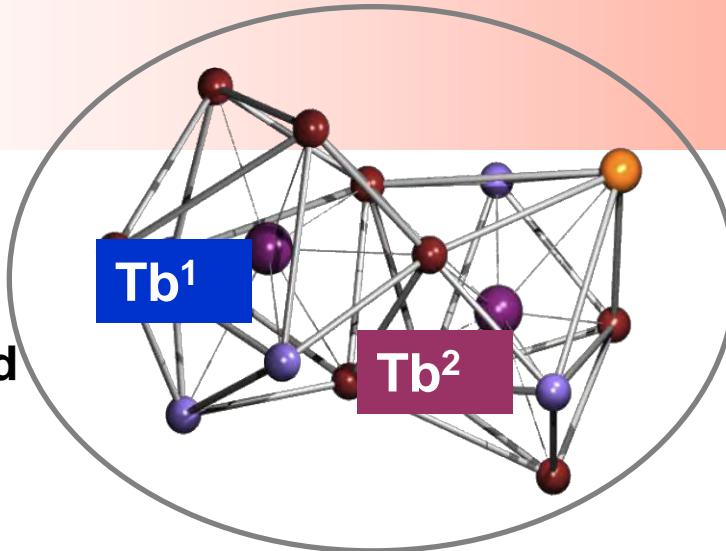
99.99% lie in the ground state below 20 K



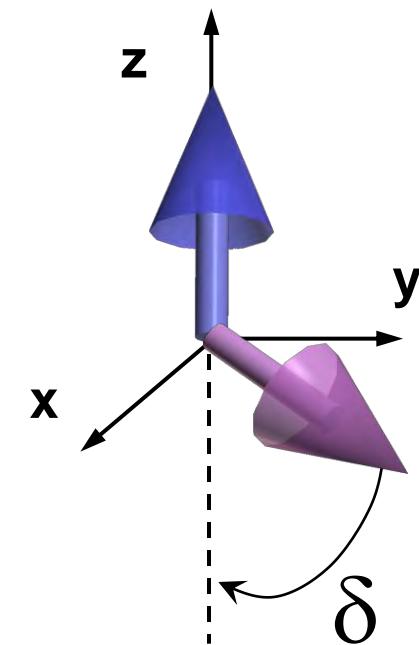
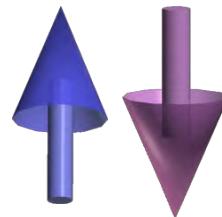
two qubits ✓

interaction ✓

$\delta = 66$ deg ✓



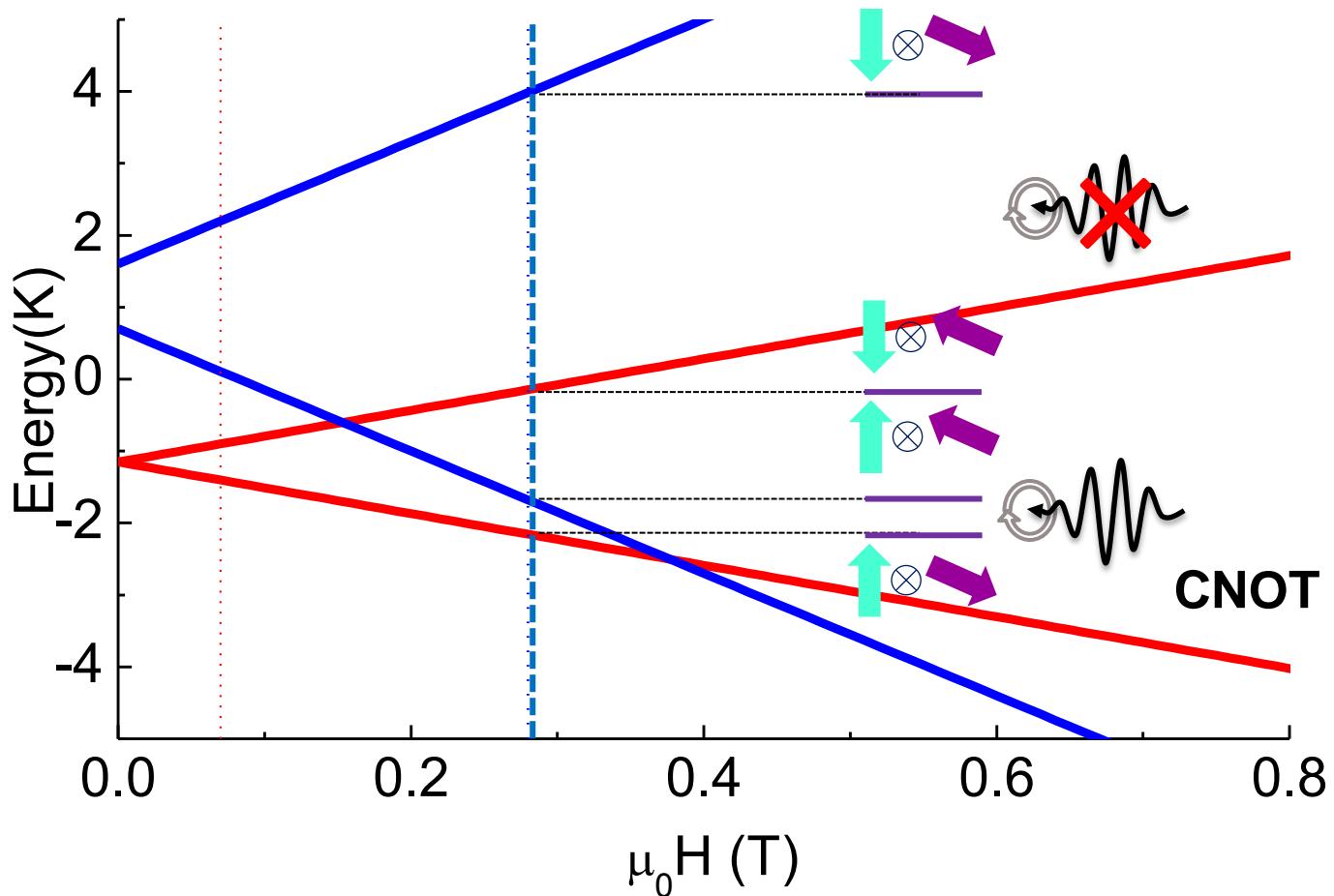
Antiferromagnetic exchange below 3 K



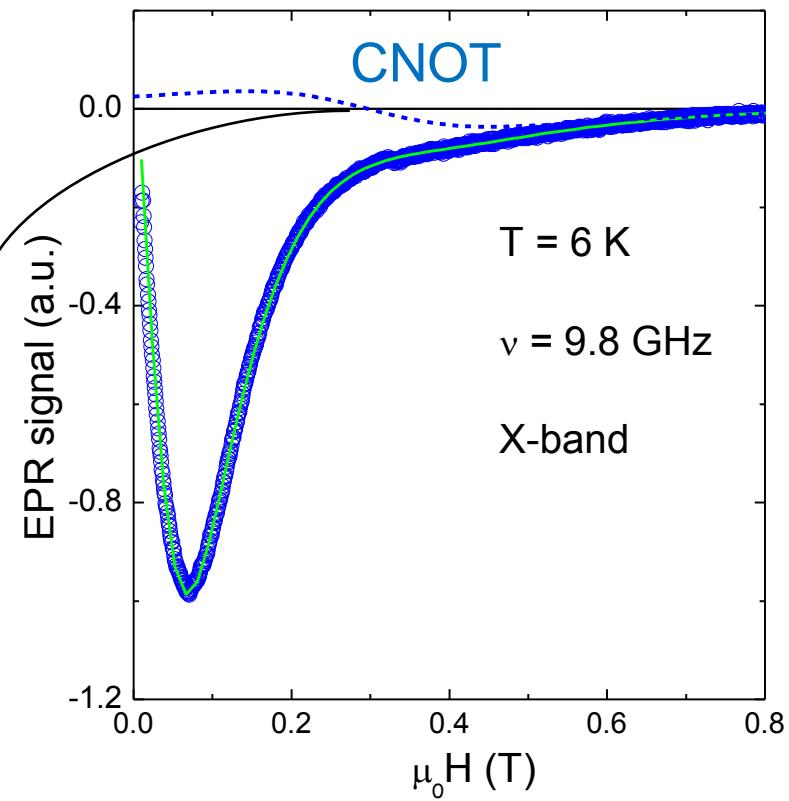
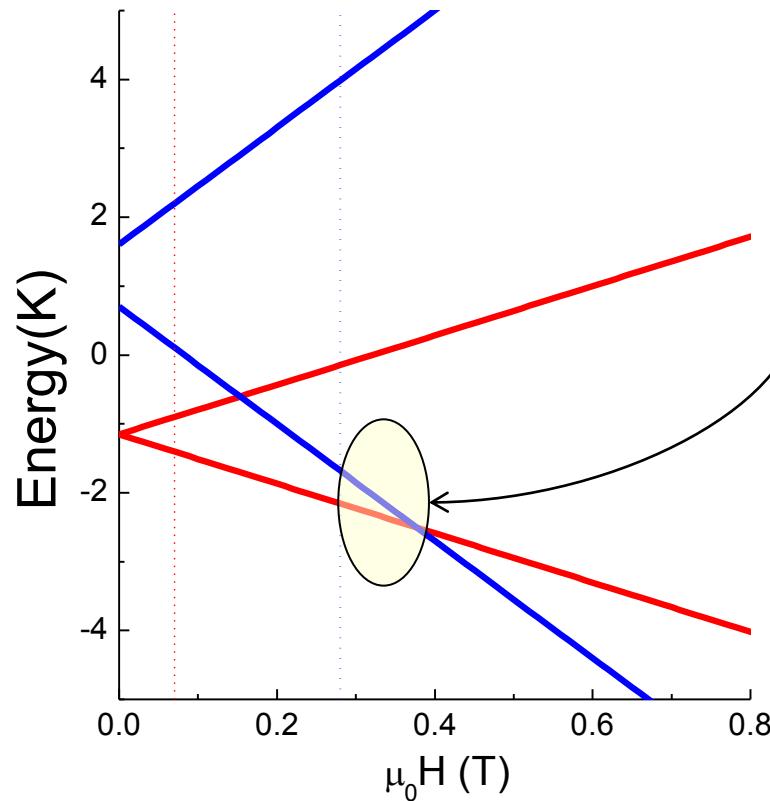
Non-collinear easy axes or different ions

$[\text{Tb}]_2$ as a CNOT logic gate

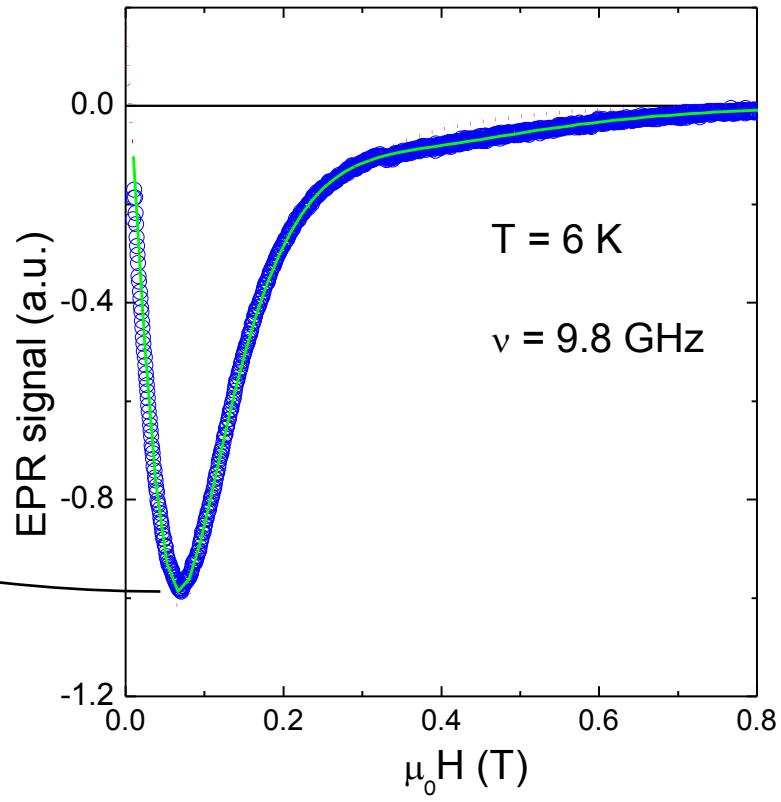
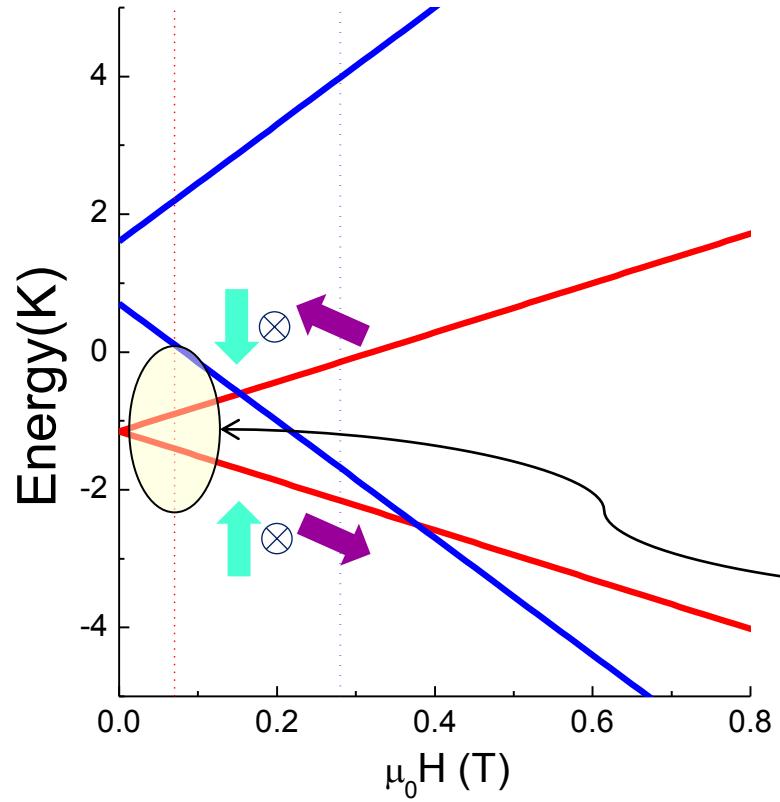
$$\mathcal{H}_{m=\pm 6} = -2J_{ex}J_{z1}J_{z2} - g_J\mu_B(H_{z1}J_{z1} + H_{z2}J_{z2}) + A_{hf}(J_{z1}I_{z1} + J_{z2}I_{z2})$$



Implementation by EPR



CNOT transitions are not forbidden



SWAP gate operations are also possible!

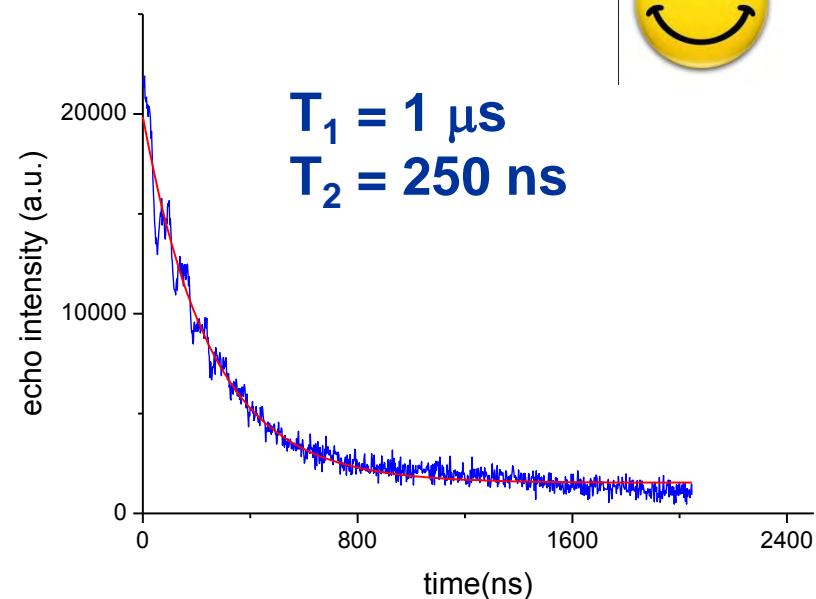
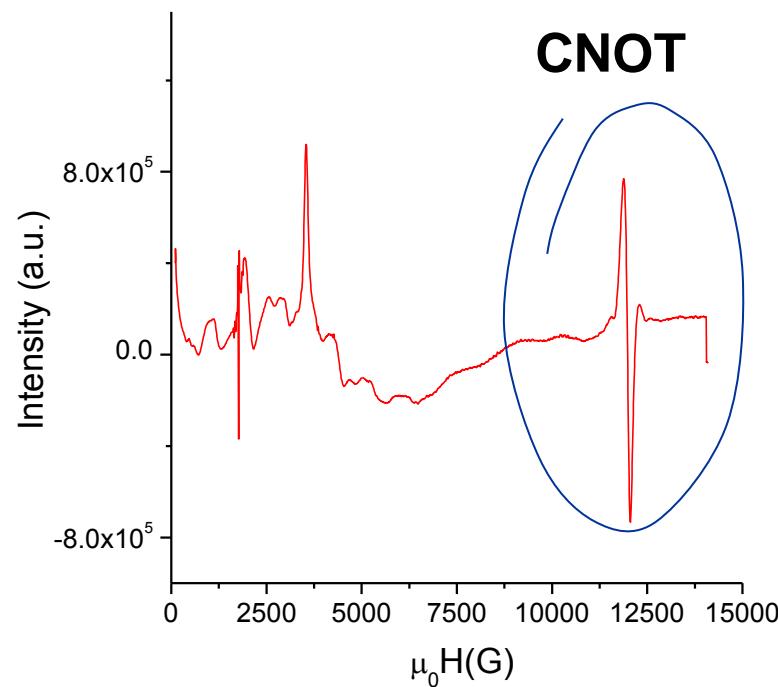
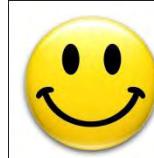
Quantum coherence? (X-band pulsed EPR)



ECHO?
NOT OBSERVED



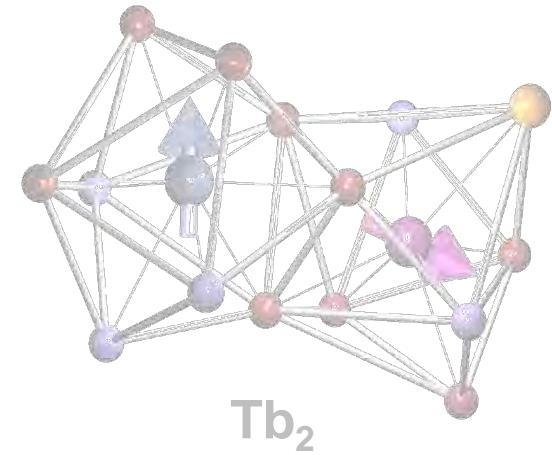
OBSERVED!!



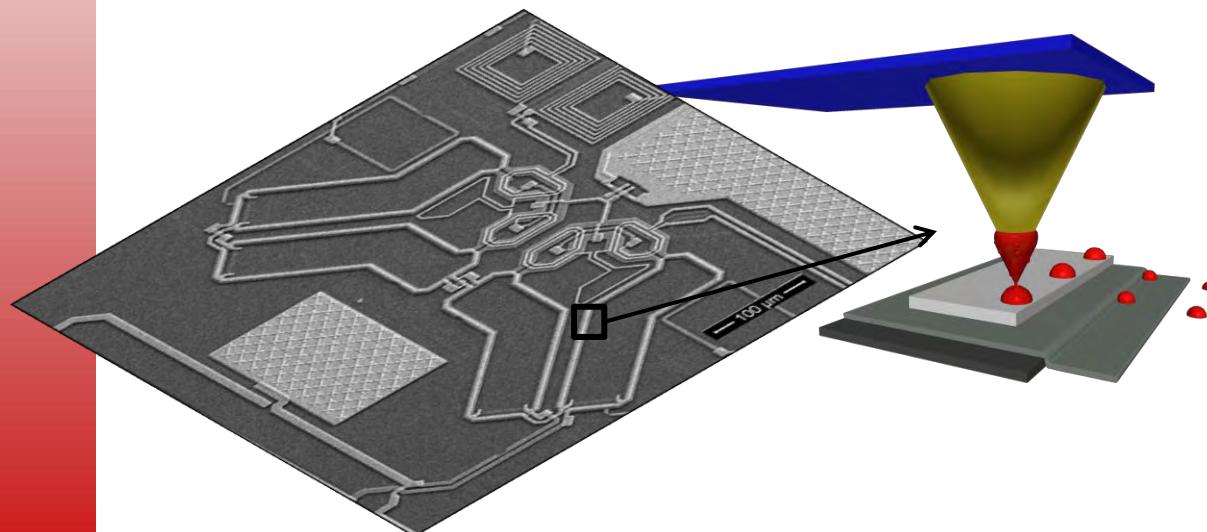
Outline



Molecular design of CNOT and SWAP quantum gates



Tb_2



Integration of SMM
into superconducting
microdevices

Hybrid quantum computation architectures

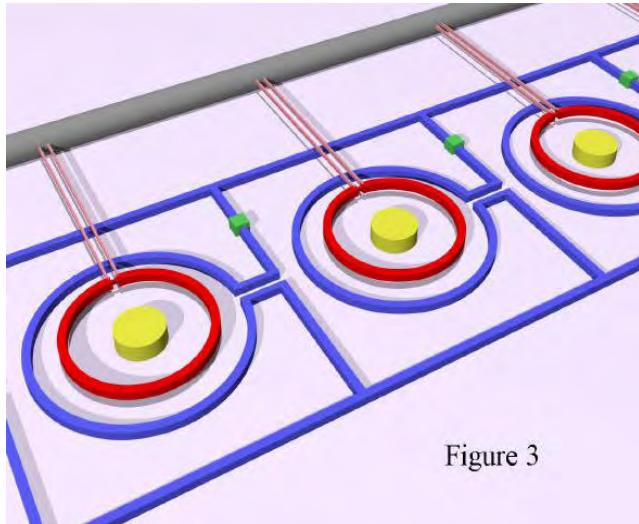
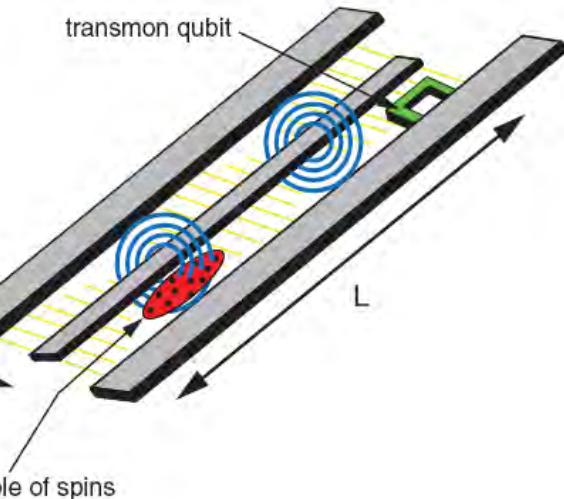


Figure 3

Magnetic qubits as hardware for quantum computers.

J. Tejada, E. M. Chudnovsky, E. del Barco, J. M. Hernandez and T. P. Spiller, Nanotechnology **12** (2001) 181–186

Molecule-based
qubits and qugates

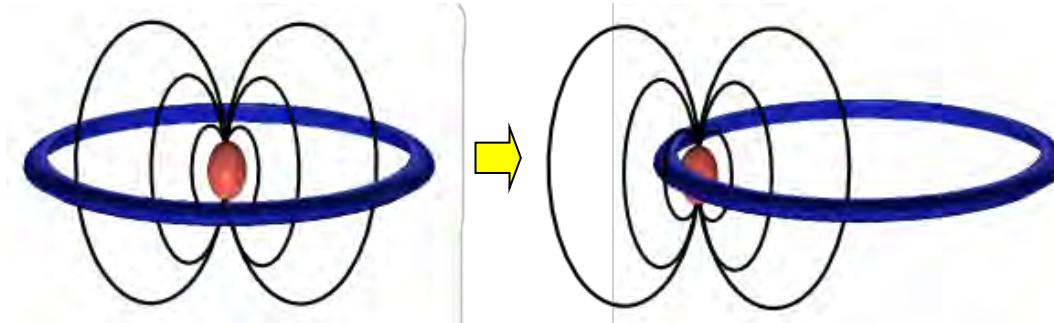
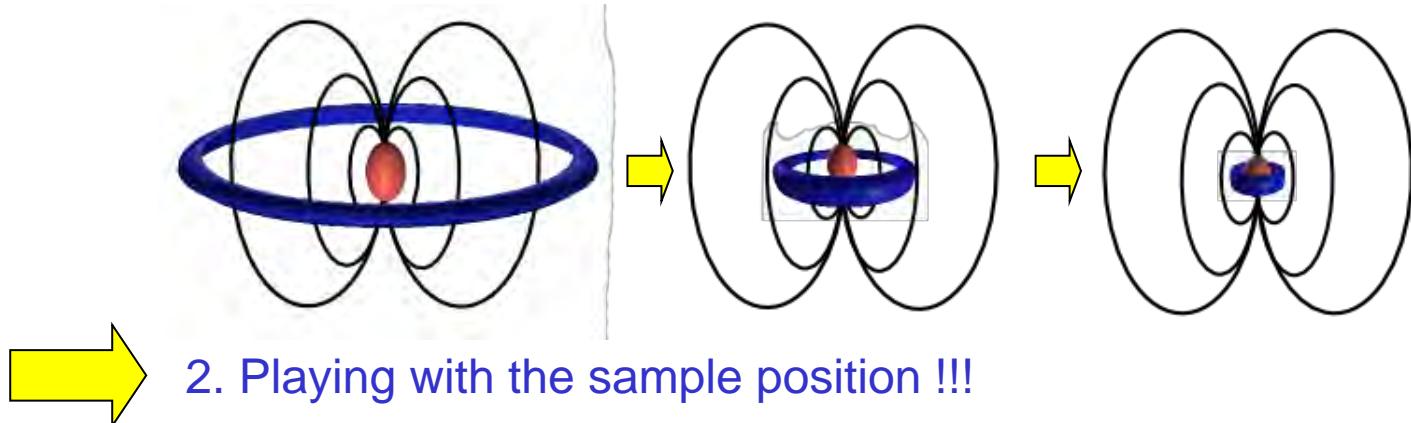


Cavity QED Based on Collective Magnetic Dipole Coupling:
Spin Ensembles as Hybrid Two-Level Systems.
Atac Imamoglu, PRL **102**, 083602 (2009)

Superconducting
μcircuits

The goal: maximizing the flux coupling

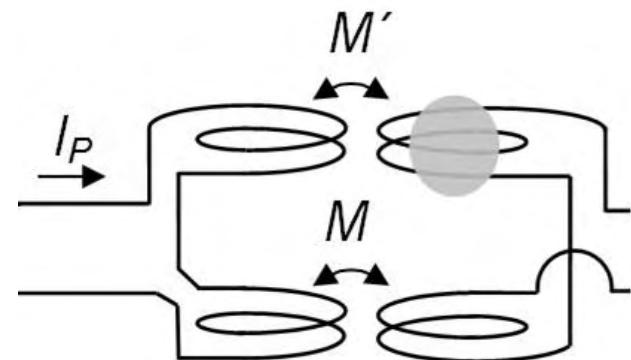
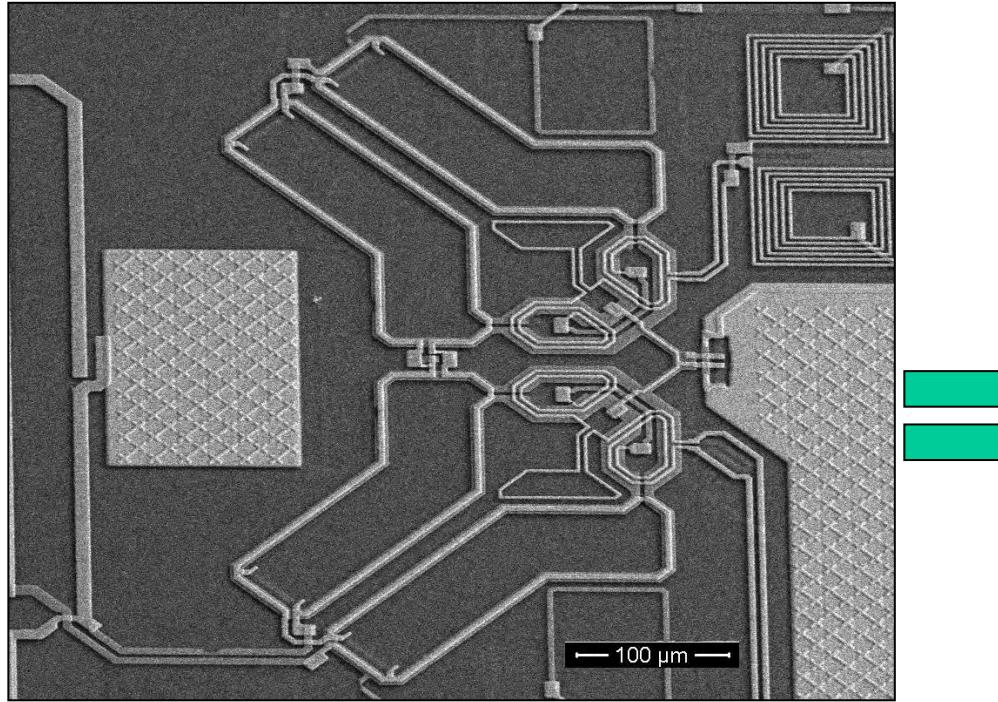
1. Scaling down the dimensions of the loop



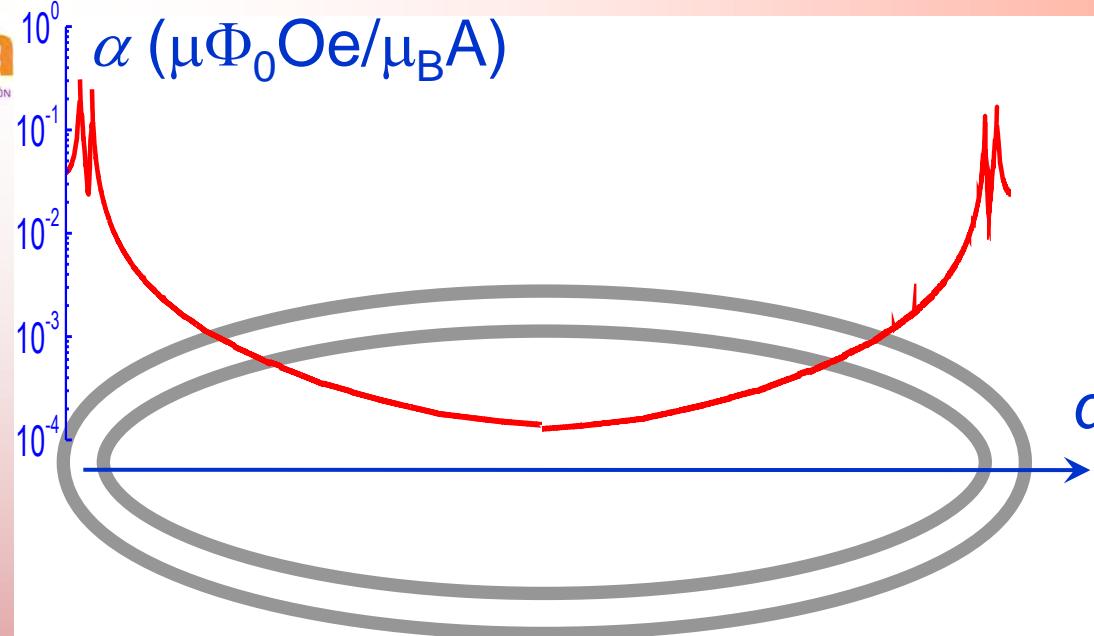
“The first challenge is the placement of a single nanoparticle close to the nanoSQUID while achieving sufficient magnetic coupling between the particle and the device”

C. P. Foley and H. Hilgenkamp. Supercond. Sci. Technol. **22**, 064001 (2009).

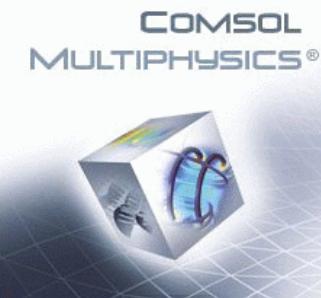
The device: microSQUID ac susceptometer



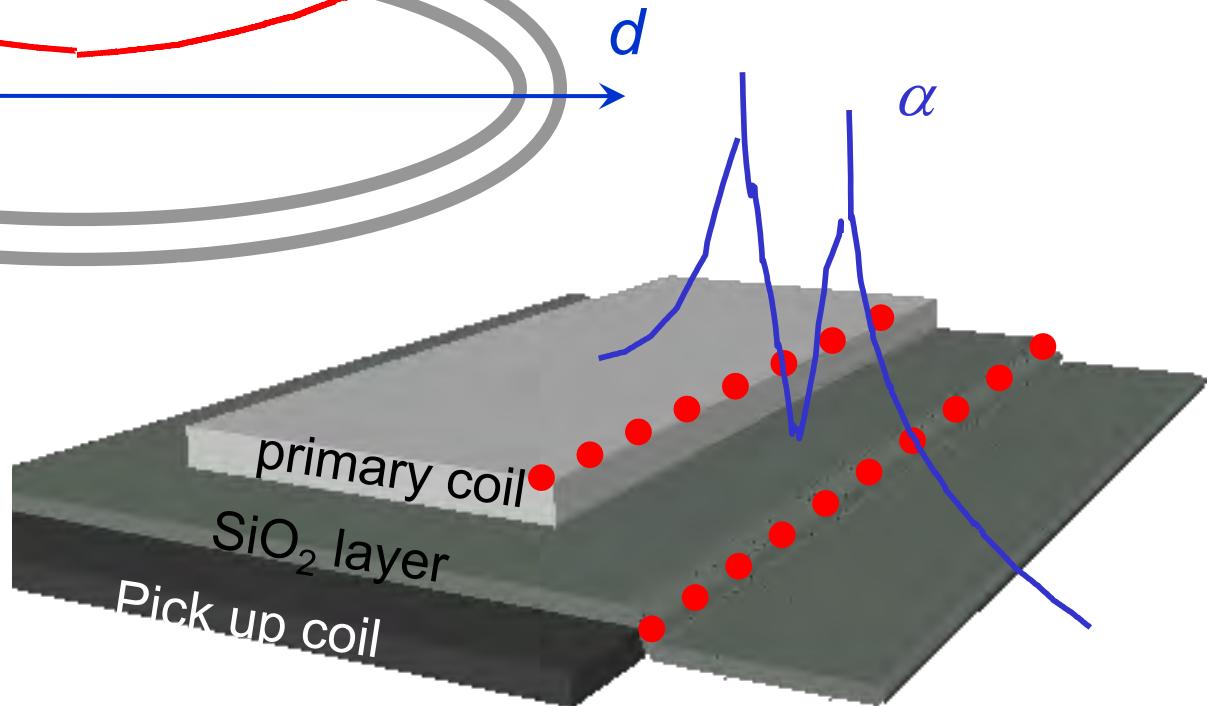
$\alpha (\mu\Phi_0 \text{Oe}/\mu_B \text{A})$



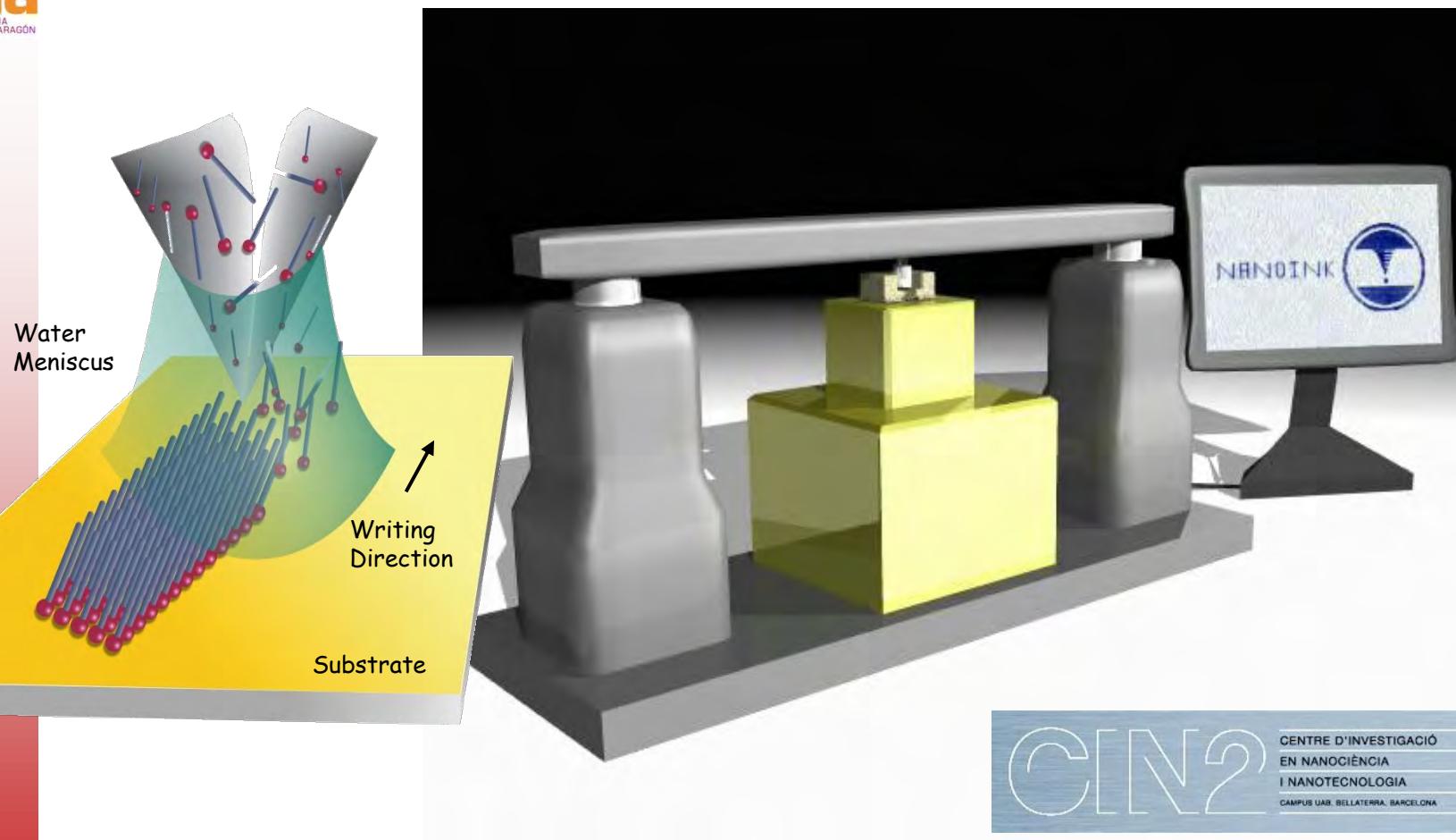
d



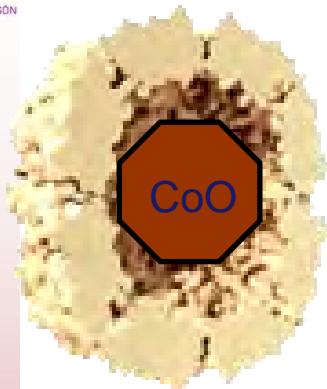
$$\alpha = \frac{\phi_{coupled}}{n\mu_i} \frac{B_P}{i_P}$$



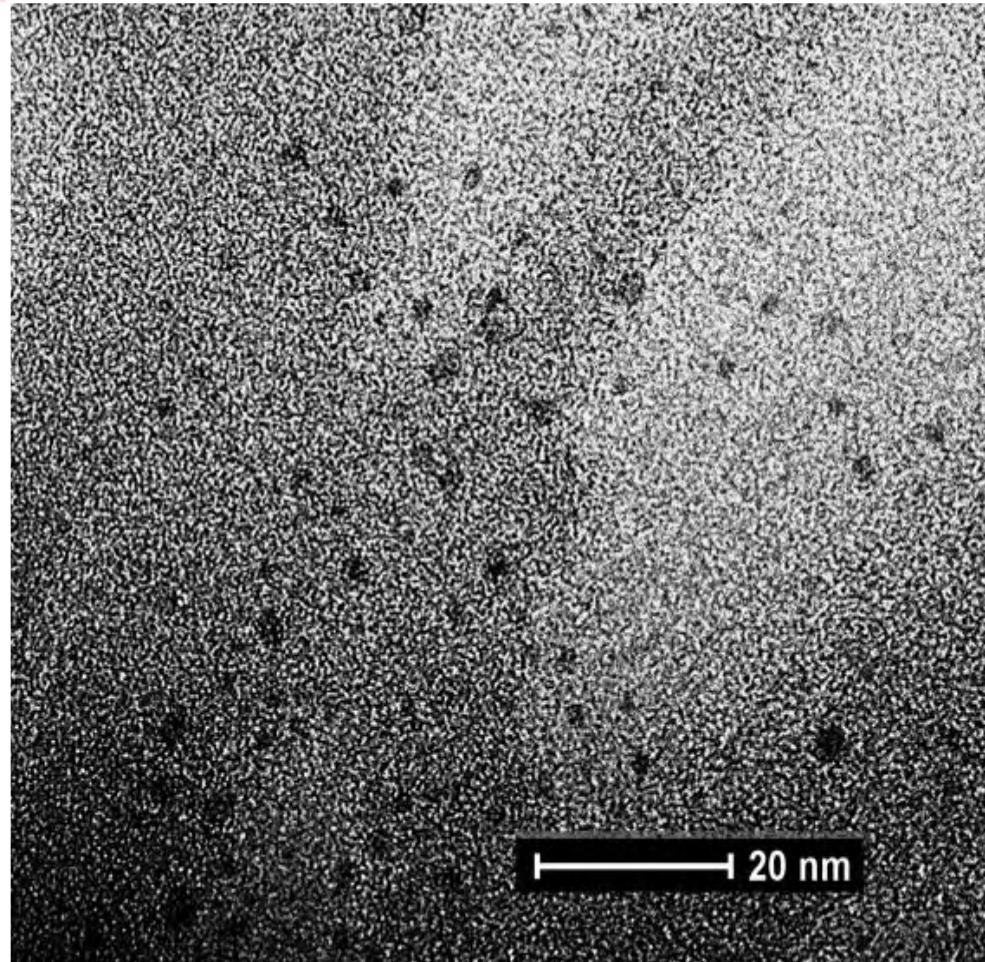
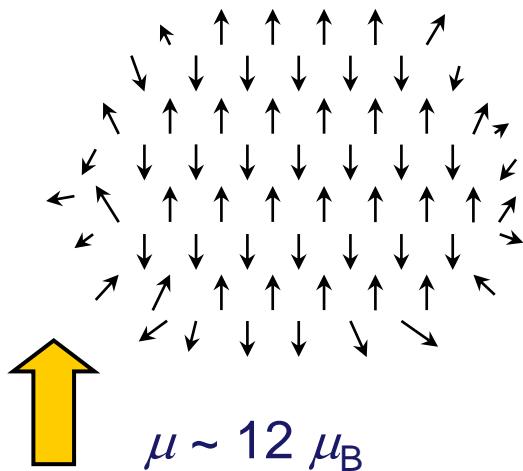
The tool: Dip pen nanolithography

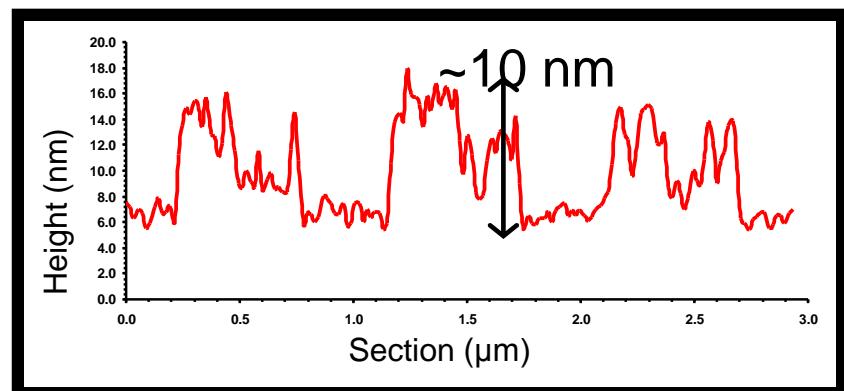
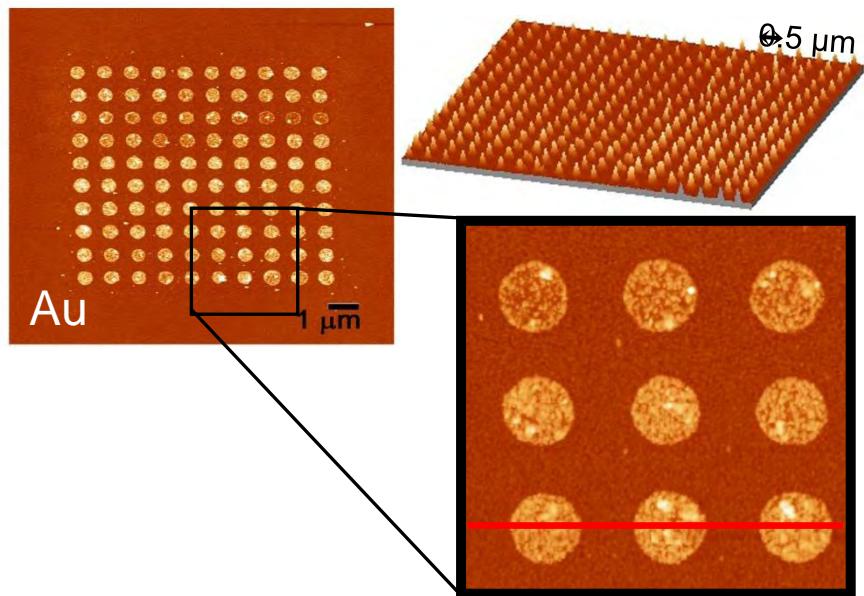
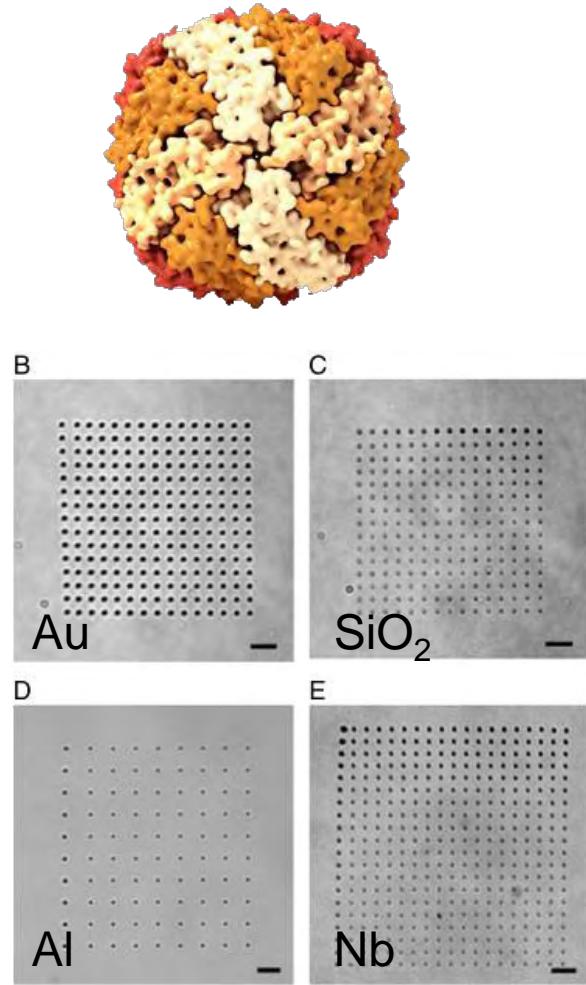


The sample: ferritin-based nanomagnets (CoO)

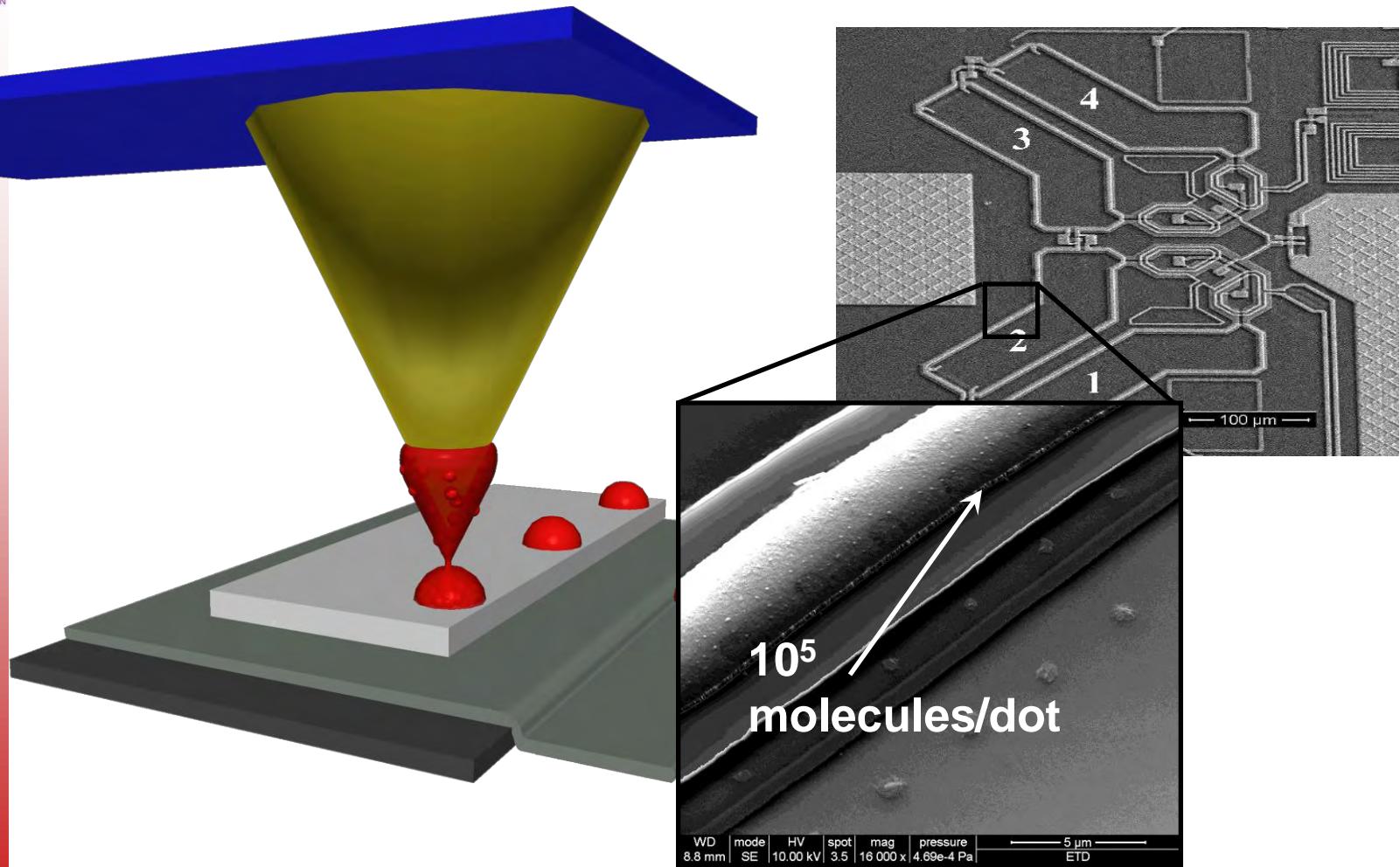


2 nm sized
Antiferromagnetic particle



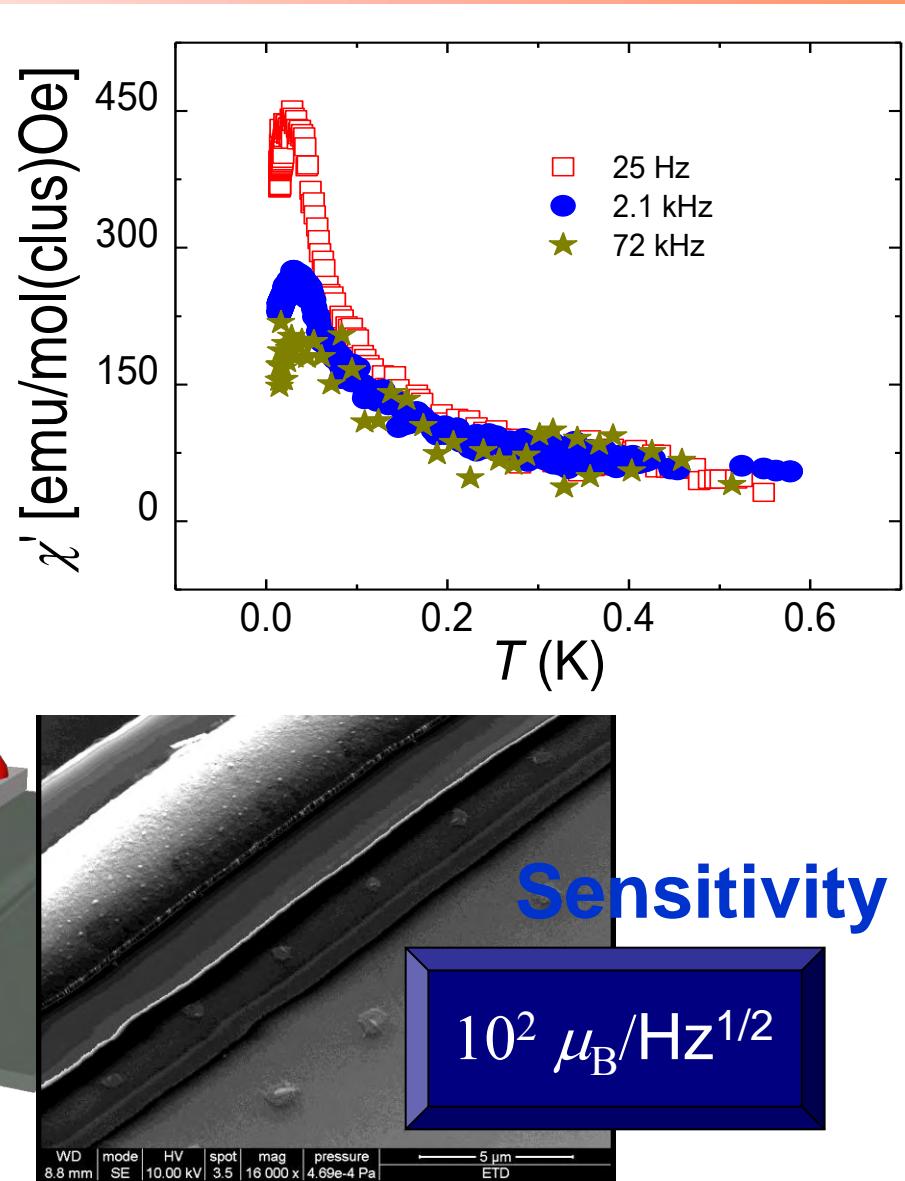
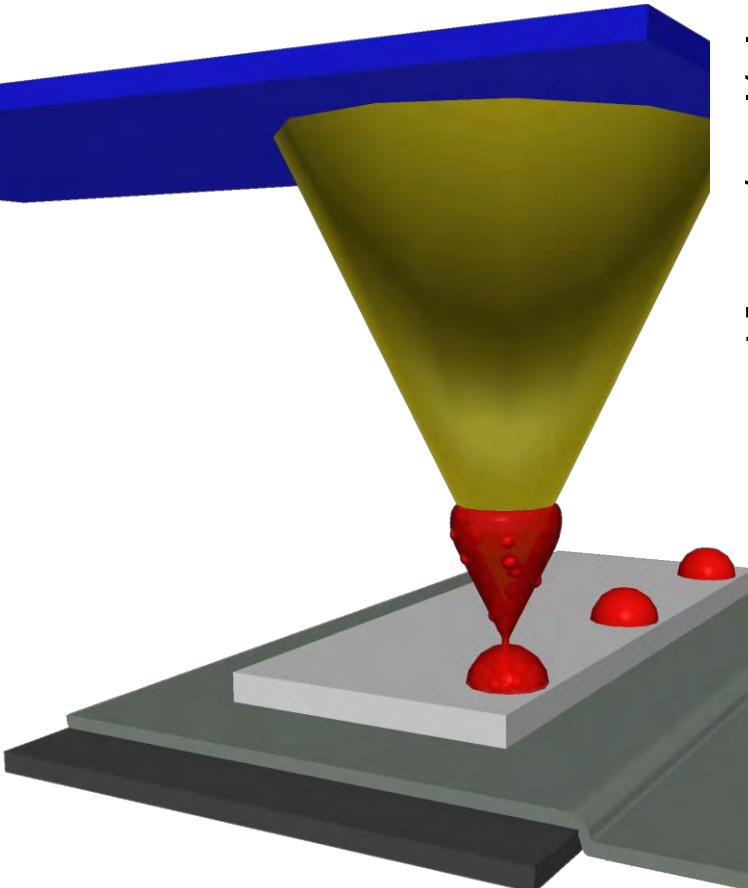


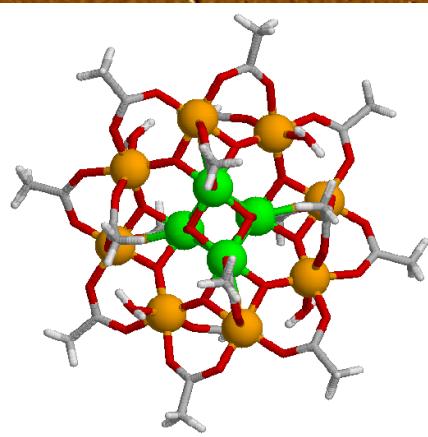
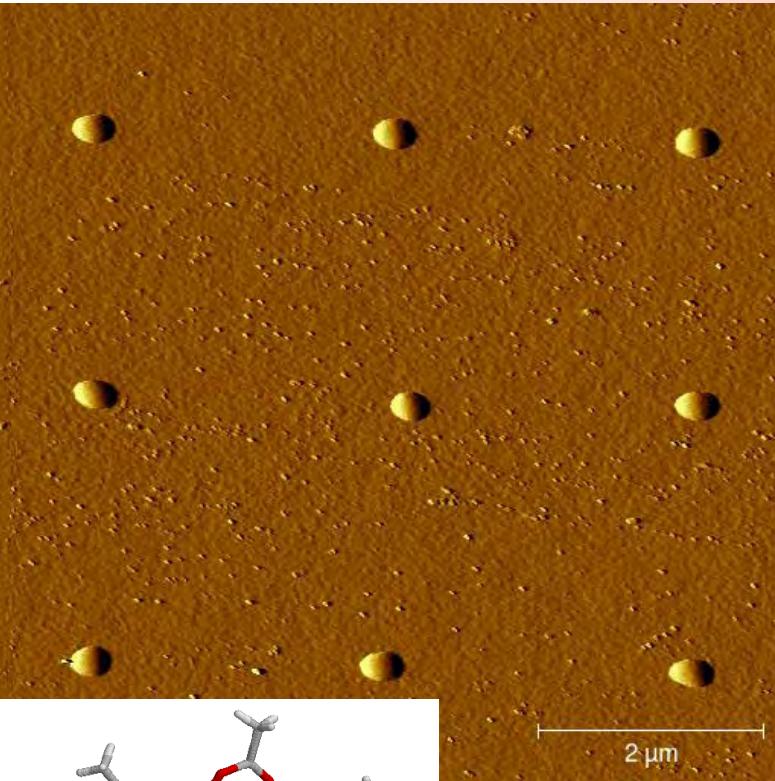
Direct deposition on the most sensitive areas



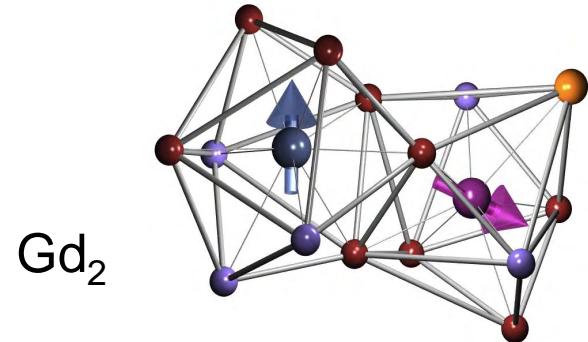
Detection of the linear response of a SMM monolayer

M. J. Martínez-Pérez, E. Bellido, R.. De Miguel, J. Sese', A. Lostao, C. Gómez-Moreno, D. Drung, T. Schurig, D. Ruiz-Molina, and F. Luis, *APL*, **99**, 032504 (2011)

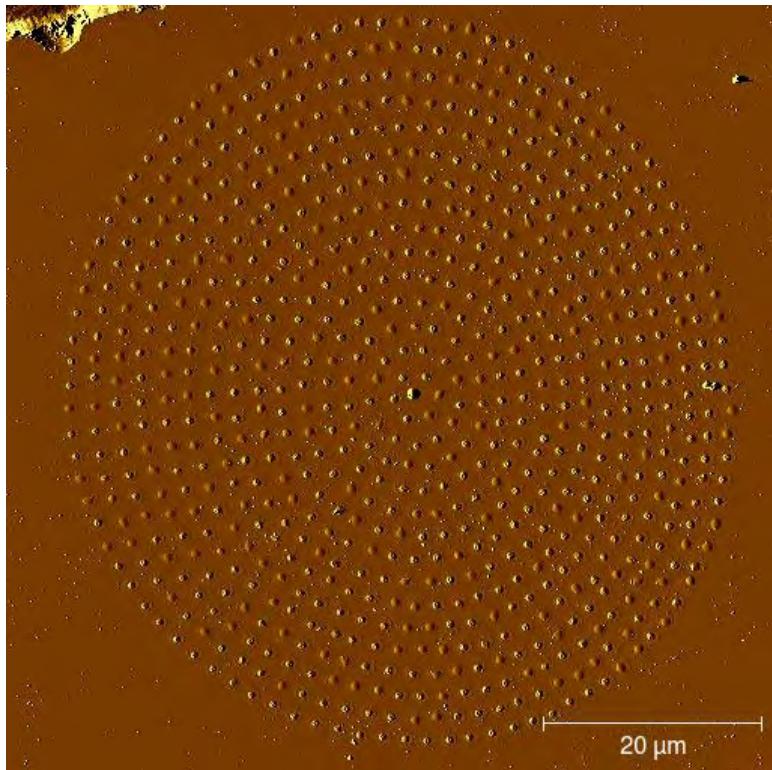




Mn_{12}



Gd_2



20 μm

Towards the implementation of quantum computation architectures

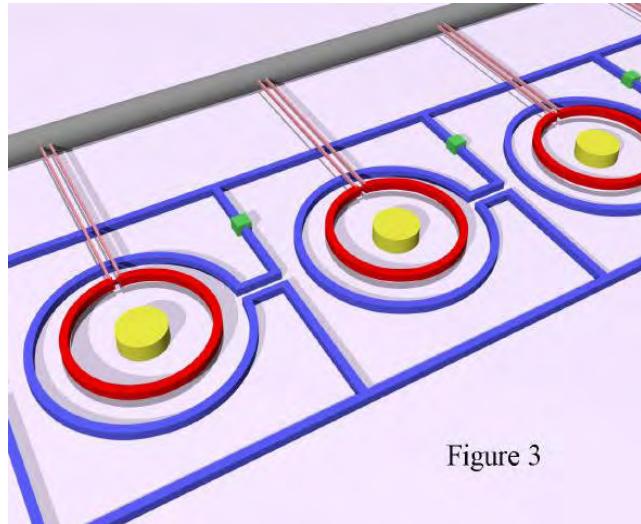
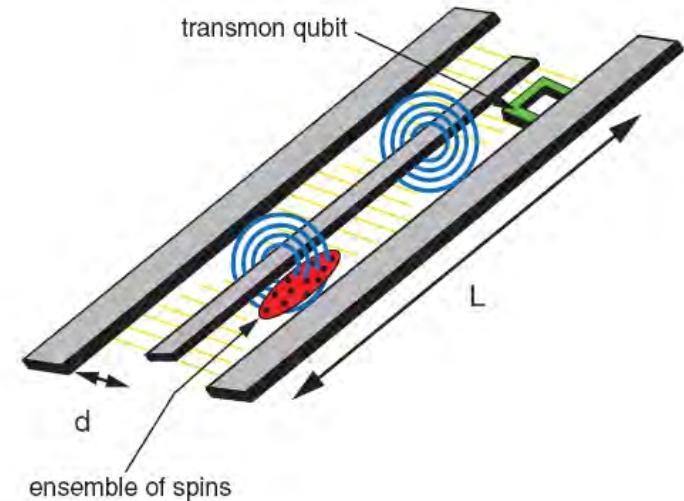


Figure 3

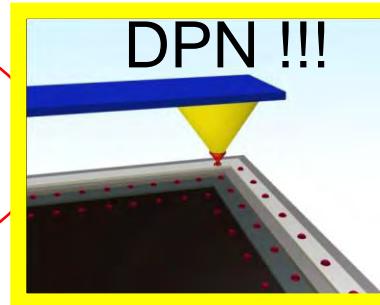
Magnetic qubits as hardware for quantum computers.

J. Tejada, E. M. Chudnovsky, E. del Barco, J. M. Hernandez and T. P. Spiller, Nanotechnology **12** (2001) 181–186



Cavity QED Based on Collective Magnetic Dipole Coupling:
Spin Ensembles as Hybrid Two-Level Systems.
Atac Imamoglu, PRL **102**, 083602 (2009)

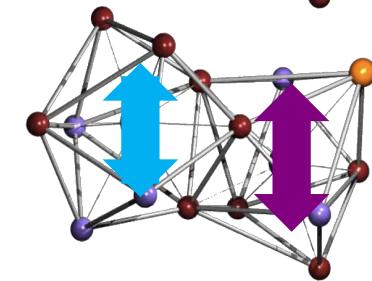
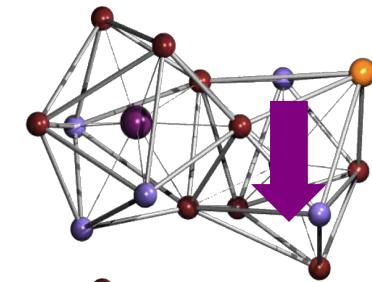
Molecule-based
qubits and qugates



Superconducting
μcircuits

CONCLUSIONS

- [LnLn'] clusters, designed and synthesized via coordination chemistry, meet the following ingredients
 - proper definition of **qubit** states
 - weak AF coupling between qubits
 - magnetic asymmetry
 - molecular prototypes for CNOT quantum gates
 - **SWAP** gate operations can be performed in the same molecule
- Dip pen nanolithography offers a very attractive tool to integrate molecular qubits into superconducting microdevices: **towards the implementation of quantum architectures**





Ana
Repollés



Olivier
Roubeau



Marco
Evangelisti



María José
Martínez



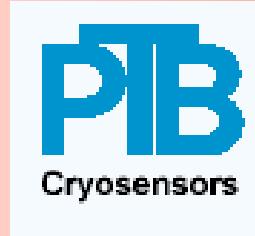
David
Zueco



Agustín
Camón



Guillem Aromí
(et al.)



Dietmar
Drung



Thomas
Schurig



Javier
Sesé



Rosa
Cordoba



Rocío de
Miguel



Ana Isabel
Lostao



Elena
Bellido



Daniel
Ruiz