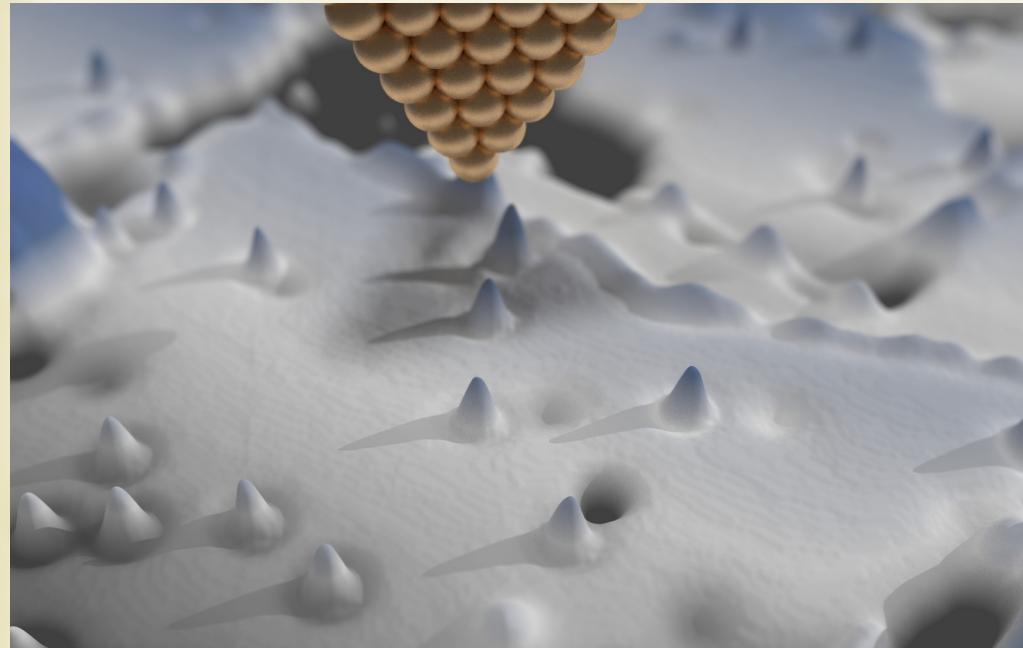


Manipulación de Estados en Cadenas de Átomos Magnéticos Utilizando un Microscopio de Efecto Tunel (Electron Spin Resonance)



Alejandro Ferrón

Seminario del Grupo Nanofísica
Corrientes 6 de Mayo de 2021
18hs

Grupo y Colaboradores



*Joaquín
Fernandez -Rossier*



Jose L. Lado



I M I T



FaCENA - UNNE



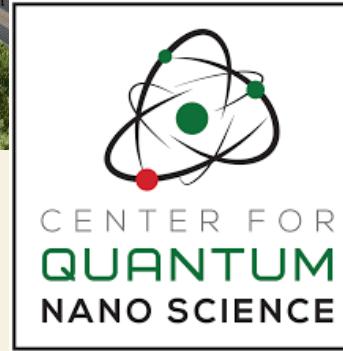
*Alba
Ramos*



*Sergio
Gomez o
Rodriguez*



Grupo y Colaboradores



Christopher Lutz



Andreas Heinrich

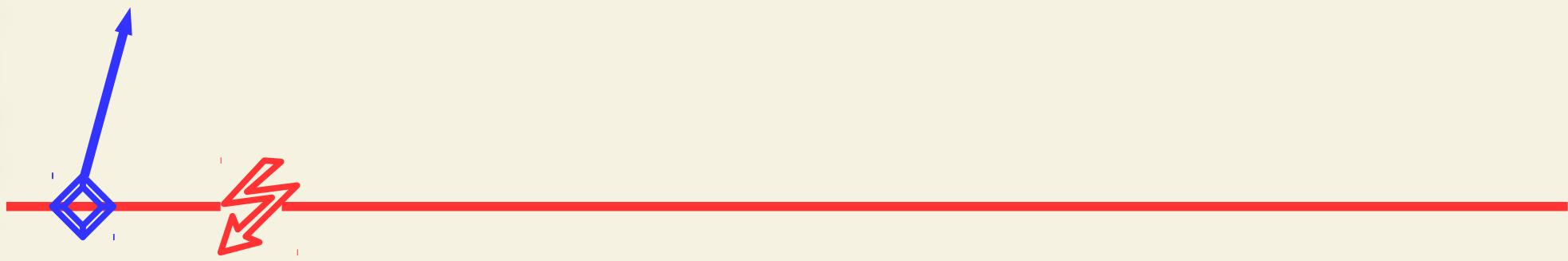
**Grupos
Experimentales**

Outline

Outline

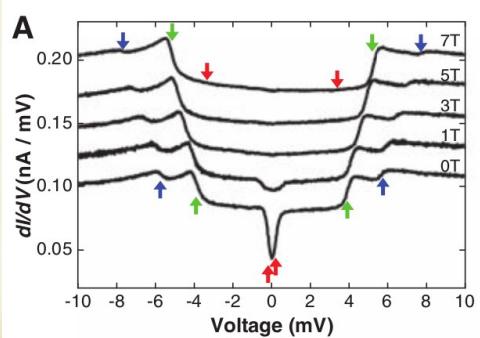
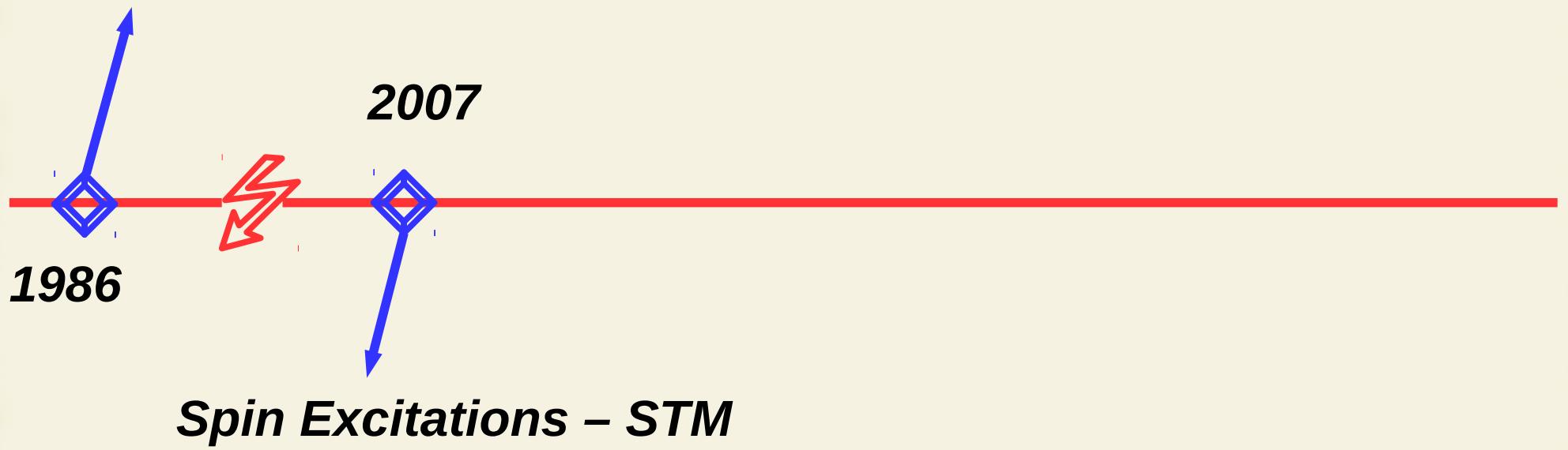
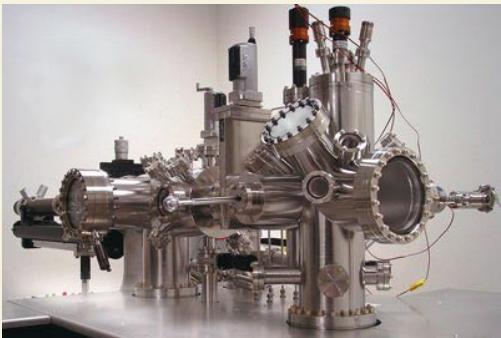


Scanning Tunneling Microscope:
Premio Nobel

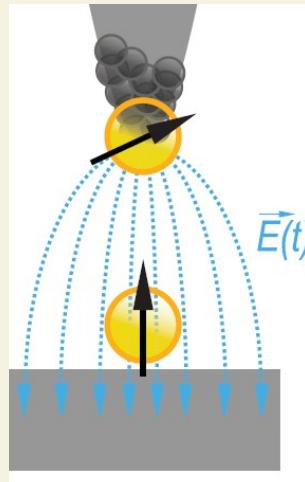
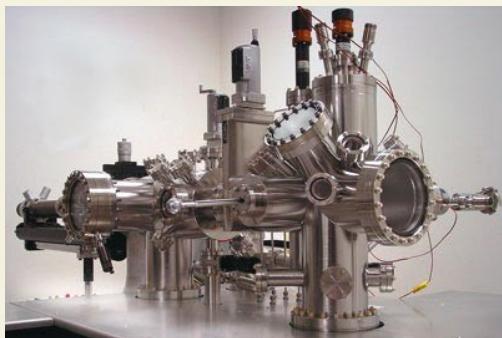


1986

Outline

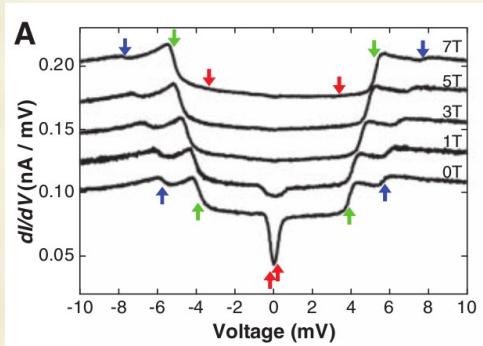
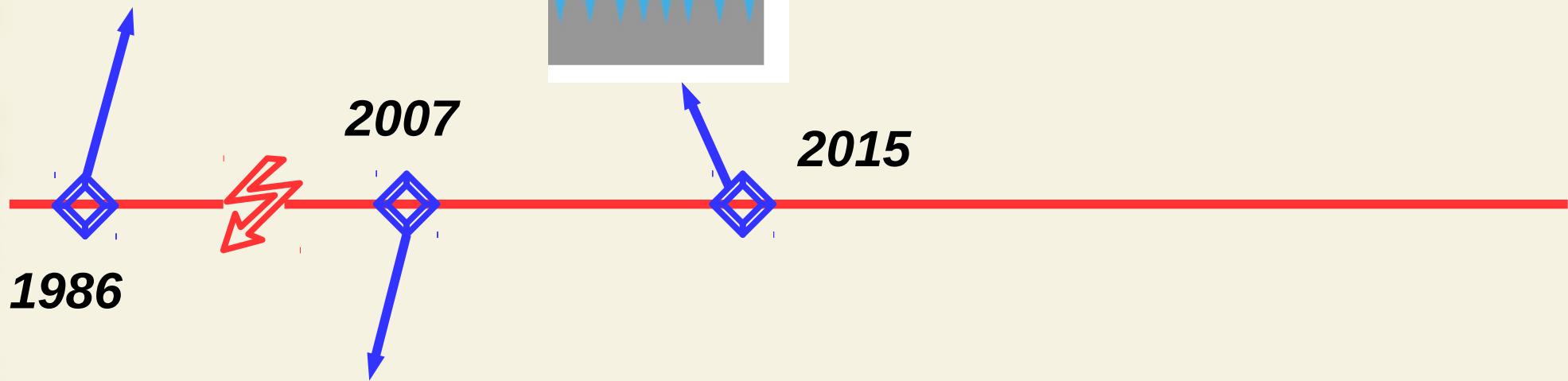


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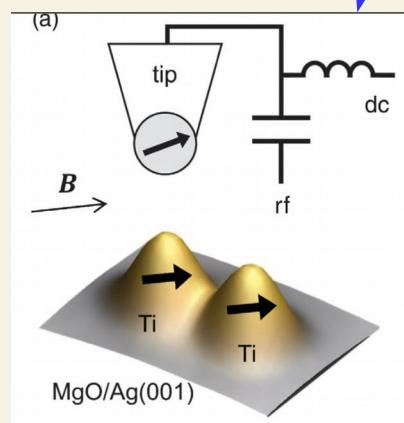
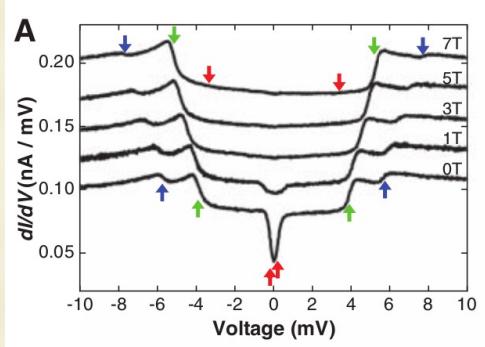
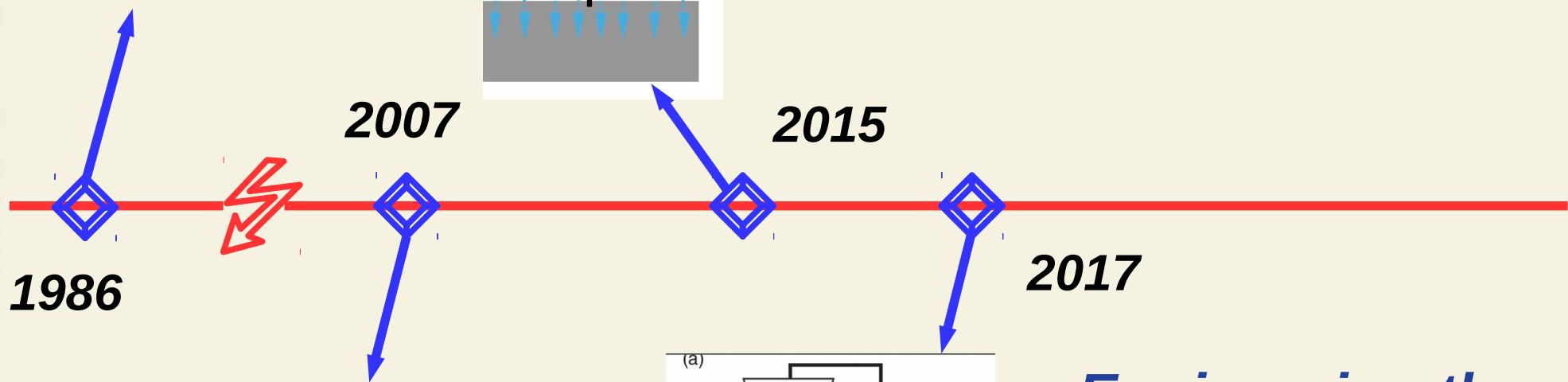
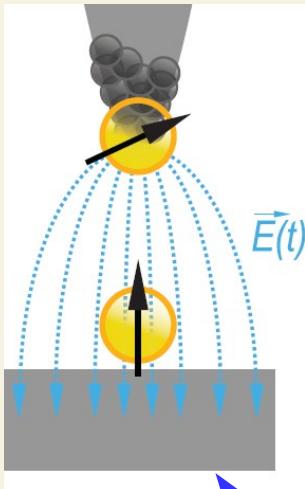


Electron Spin Resonance

Science 350, 417 (2015)



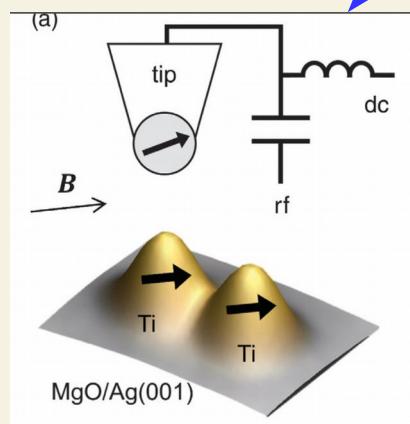
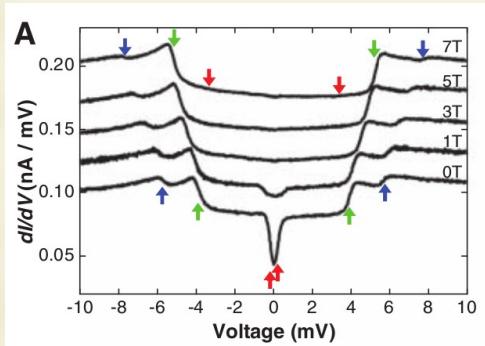
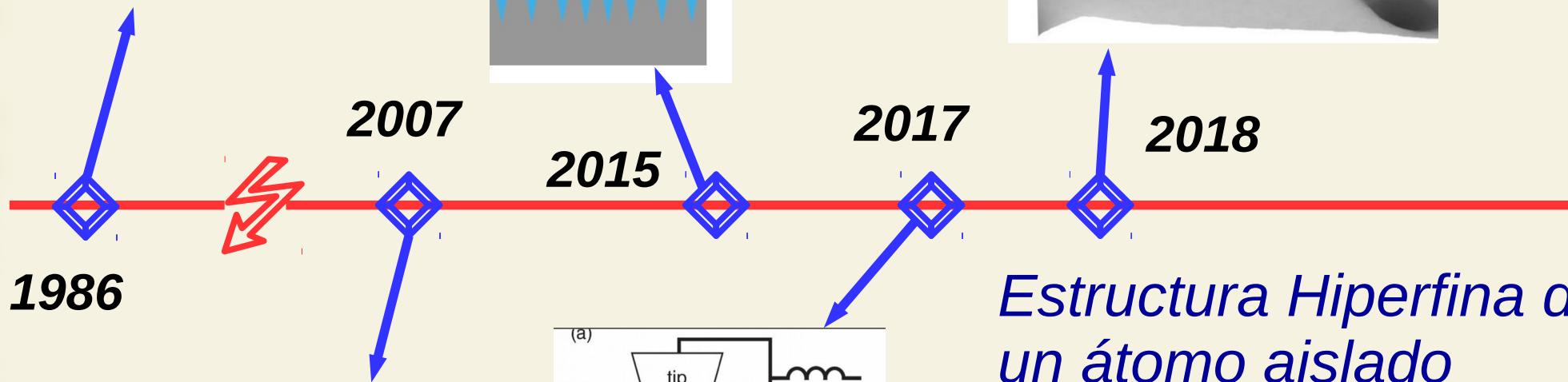
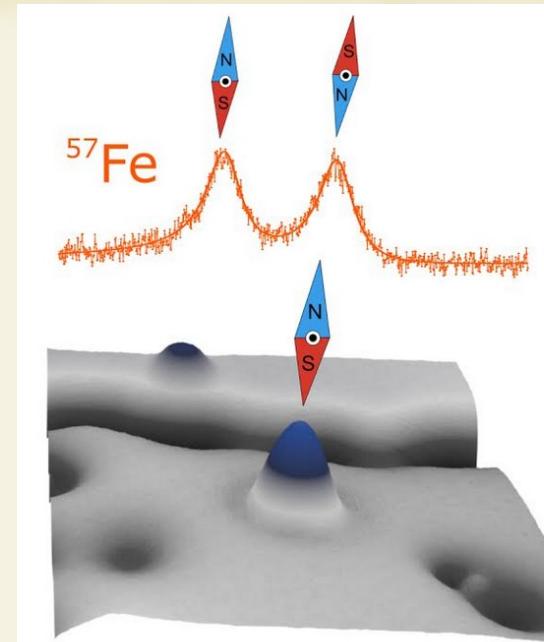
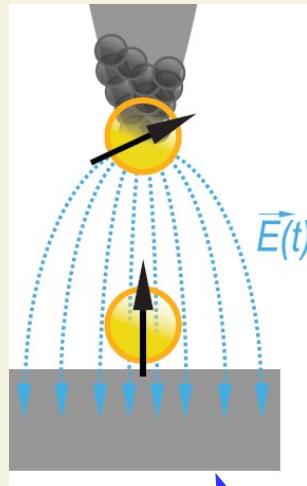
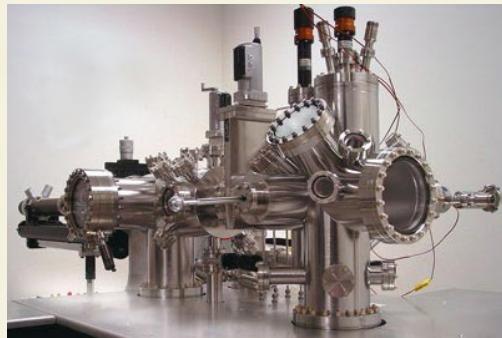
Outline



Engineering the Eigenstates of Coupled Atoms on a Surface

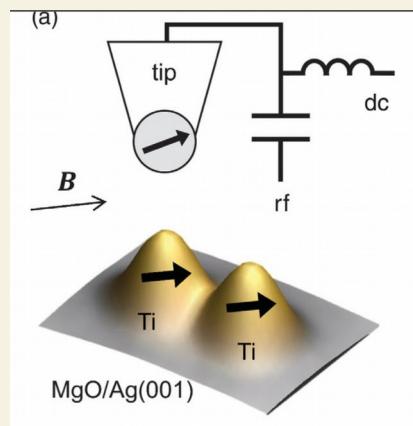
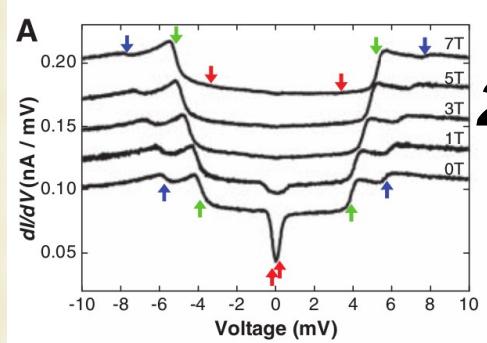
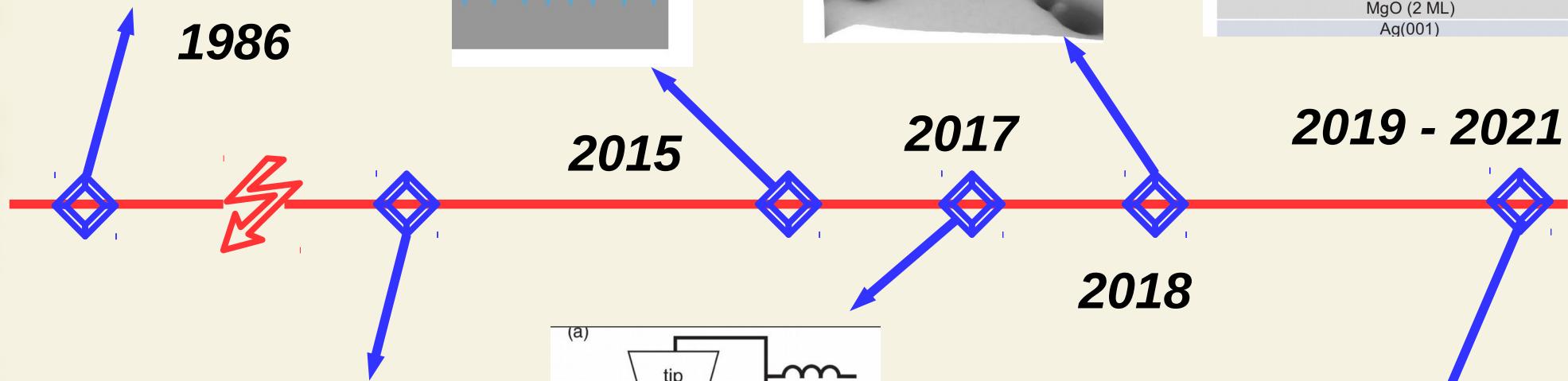
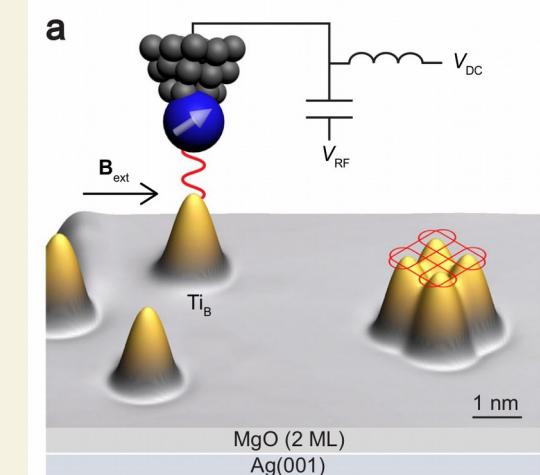
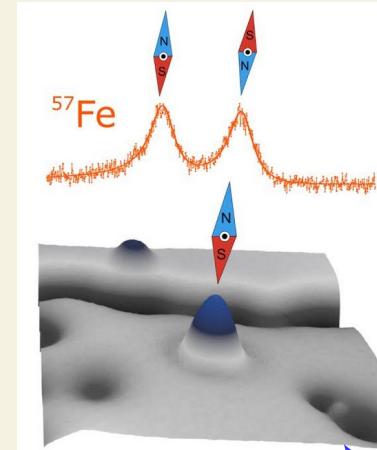
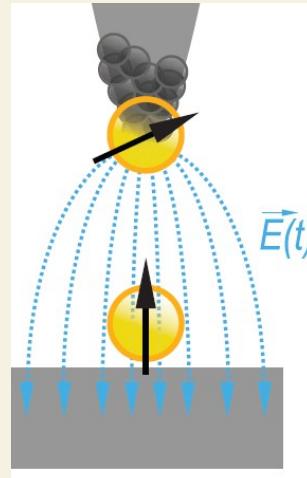
PRL 119, 227206 (2017)

Outline



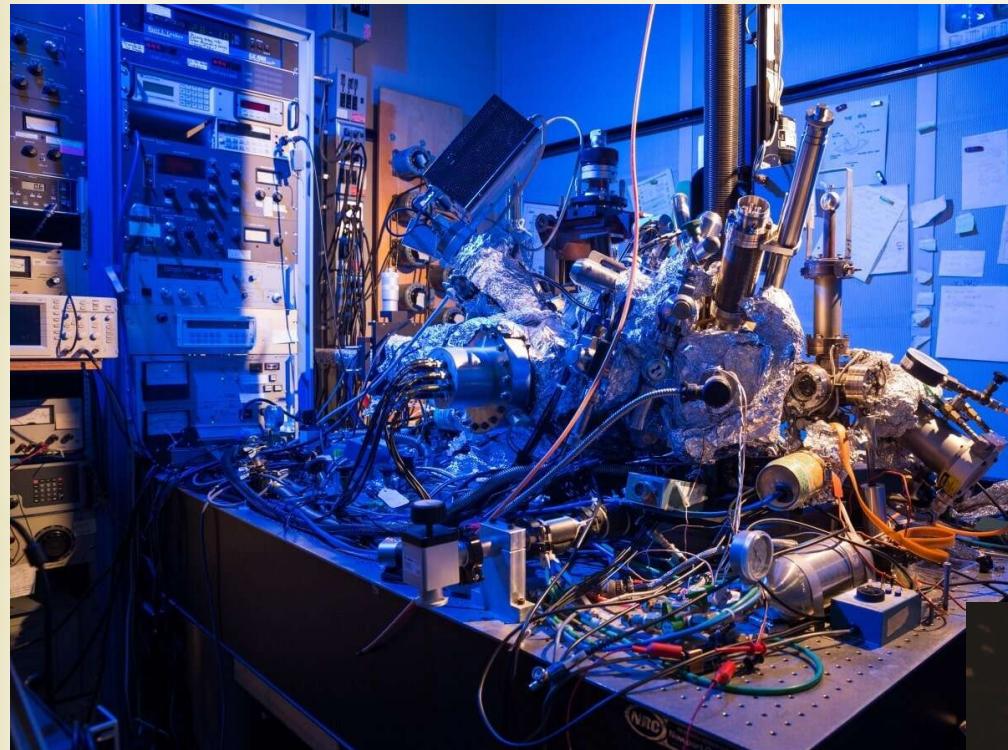
Estructura Hiperfina de un átomo aislado
Science **362**, 336 (2018)
NMR en un átomo aislado
Nature Nano **13**, 1120 (2018)

Outline

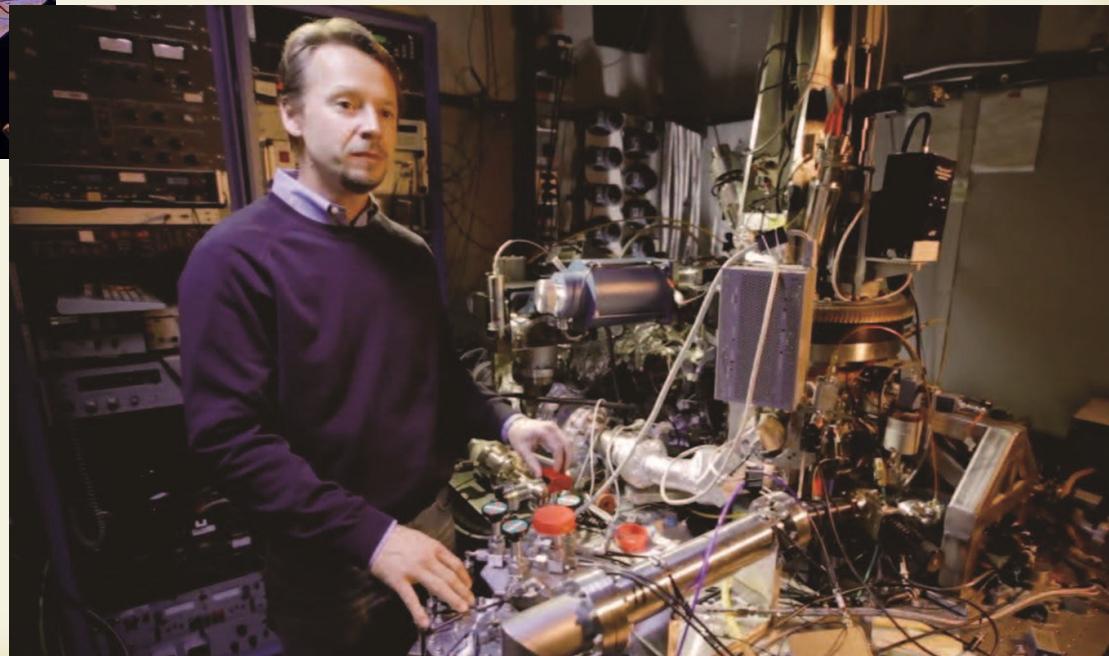


**Control en Cadenas de
átomos Magnéticos**
(Dímeros a Tetrameros)

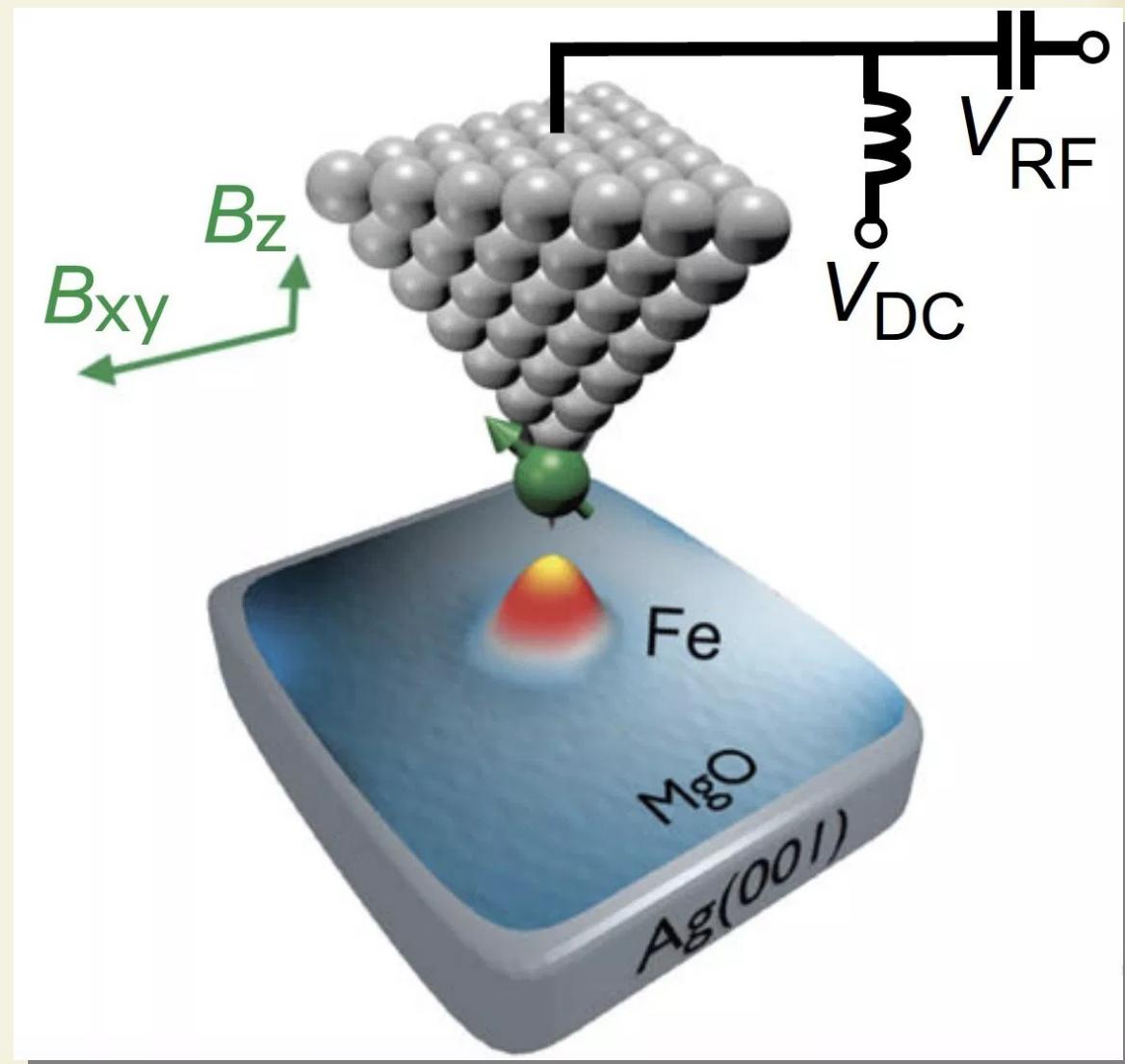
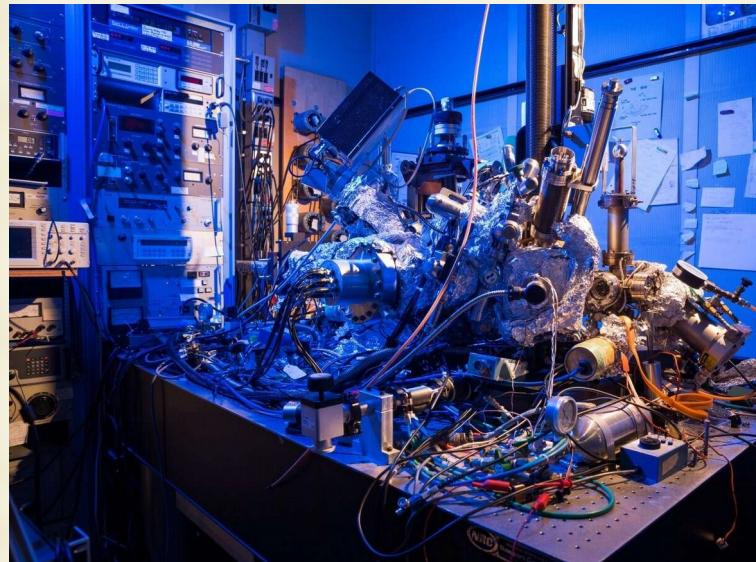
Introducción



2006-2021



Introducción

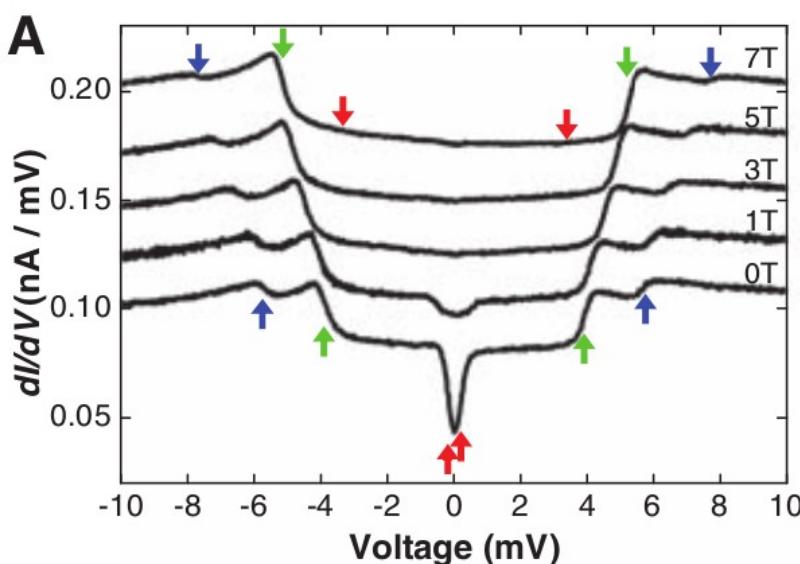


Introducción

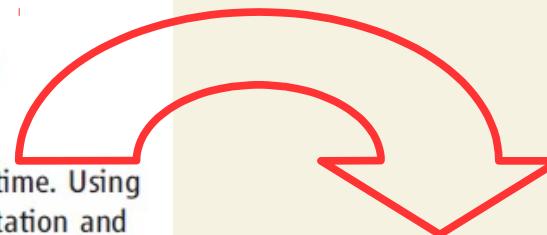
Large Magnetic Anisotropy of a Single Atomic Spin Embedded in a Surface Molecular Network

Cyrus F. Hirjibehedin,¹ Chiung-Yuan Lin,^{1,2} Alexander F. Otte,^{1,3} Markus Ternes,^{1,4} Christopher P. Lutz,¹ Barbara A. Jones,¹ Andreas J. Heinrich¹

Magnetic anisotropy allows magnets to maintain their direction of magnetization over time. Using a scanning tunneling microscope to observe spin excitations, we determined the orientation and strength of the anisotropies of individual iron and manganese atoms on a thin layer of copper nitride. The relative intensities of the inelastic tunneling processes are consistent with dipolar interactions, as seen magnetic atoms become embedded in the copper nitride. These results indicate that the magnetic moments of the atoms in the probes, have a significant effect on the magnetization at low temperatures for a single atomic spin.



Science 31 Aug 2007:
Vol. 317, pp. 1199-1203

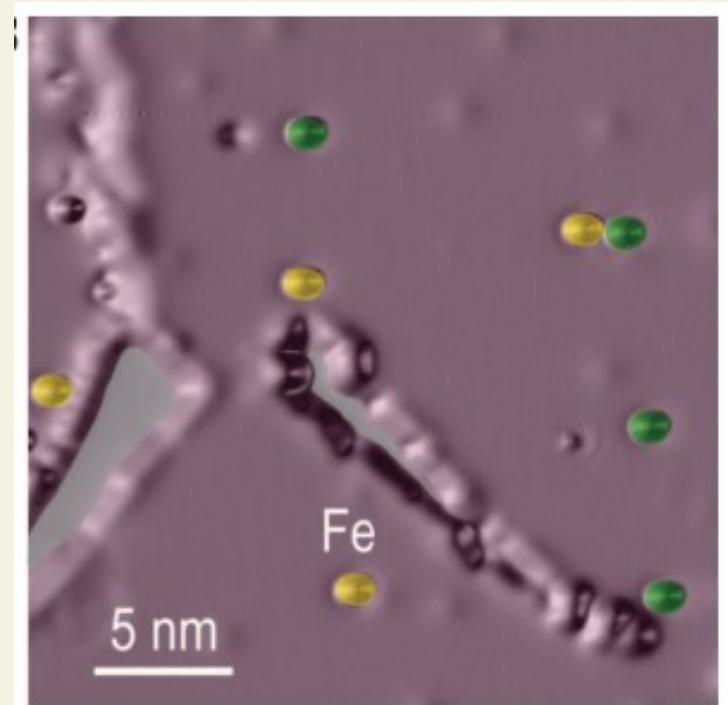
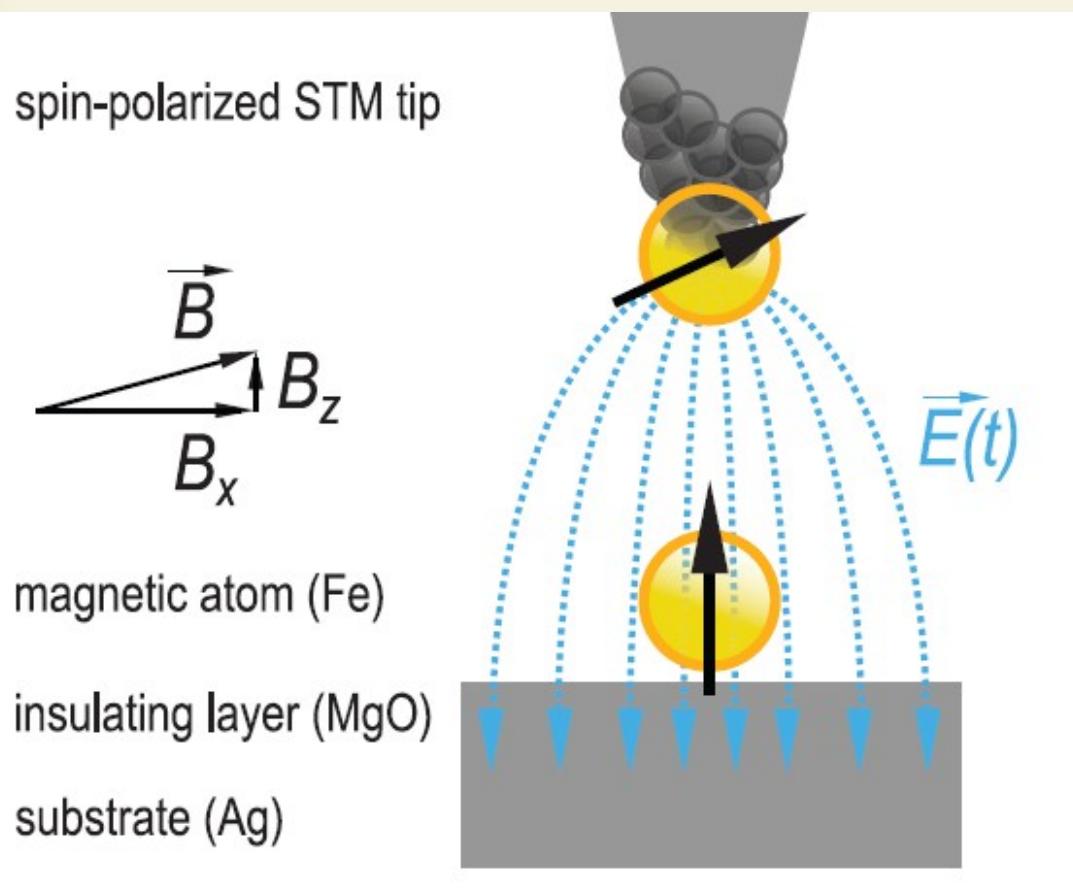


En 2007 miden por primera vez las excitaciones de Spin de un Atomo Aislado. El experimento lo realizó el Grupo de A. Heinrich en IBM

Introducción

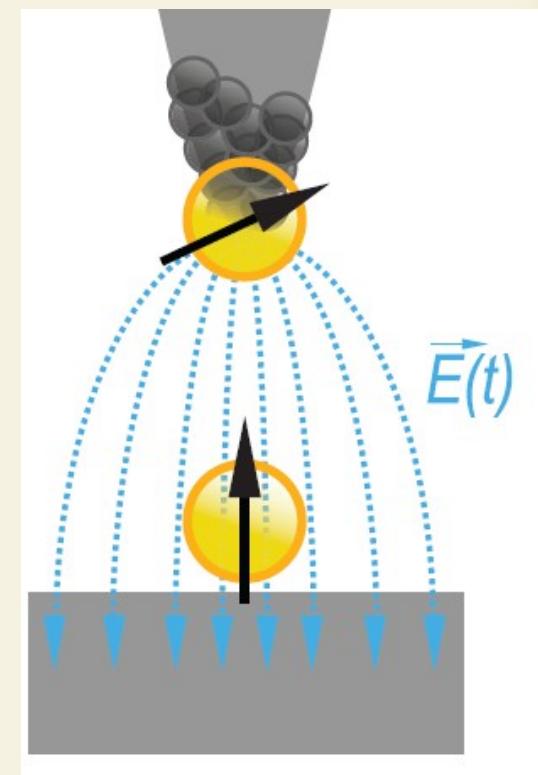
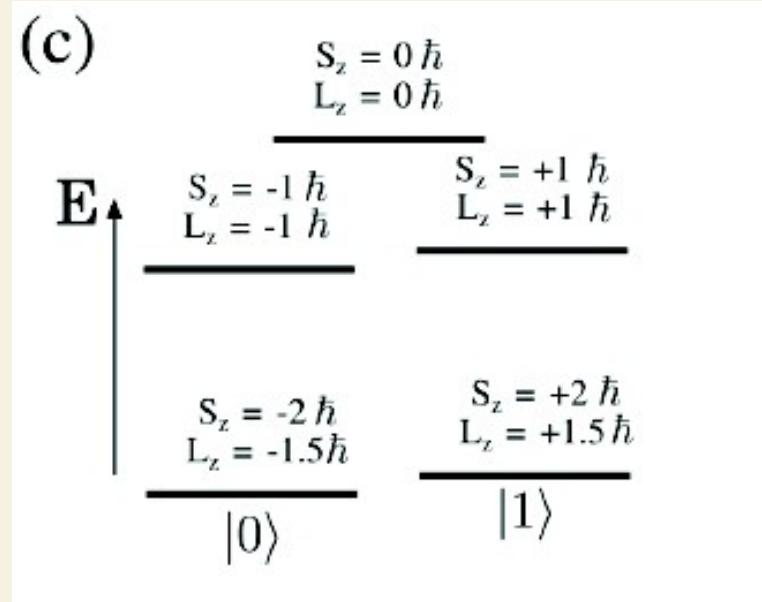
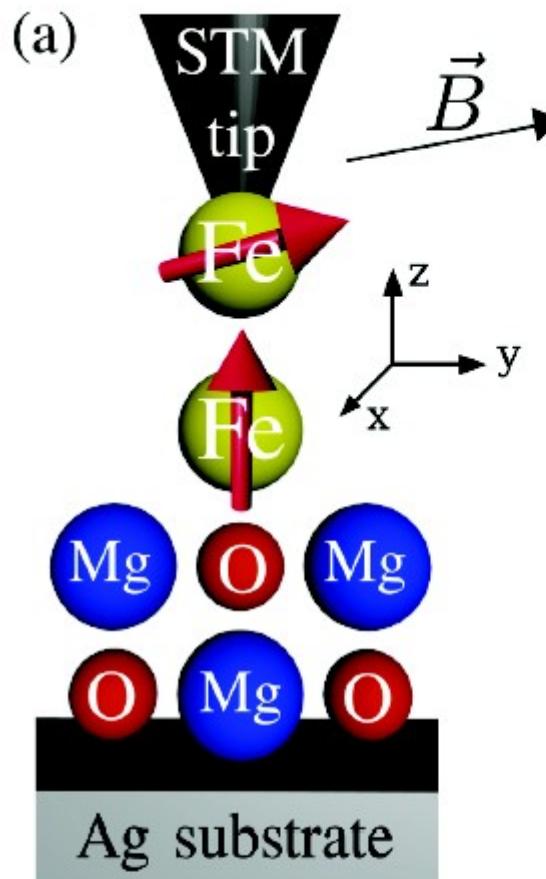
- *Electron Paramagnetic Resonance (ESR) of Individual Atoms on a Surface*

Science (2015) Andreas Heinrich Group (IBM)



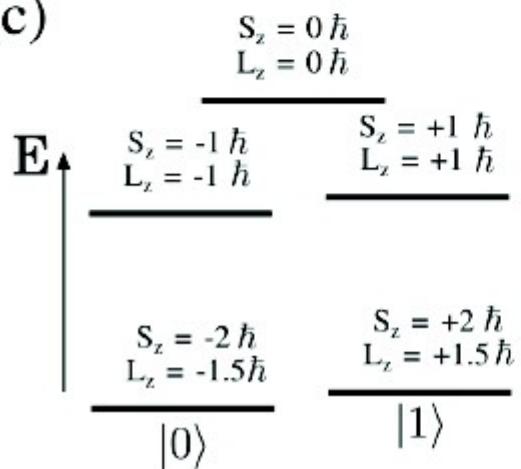
STM - Electron Spin Resonance

Fe@MgO

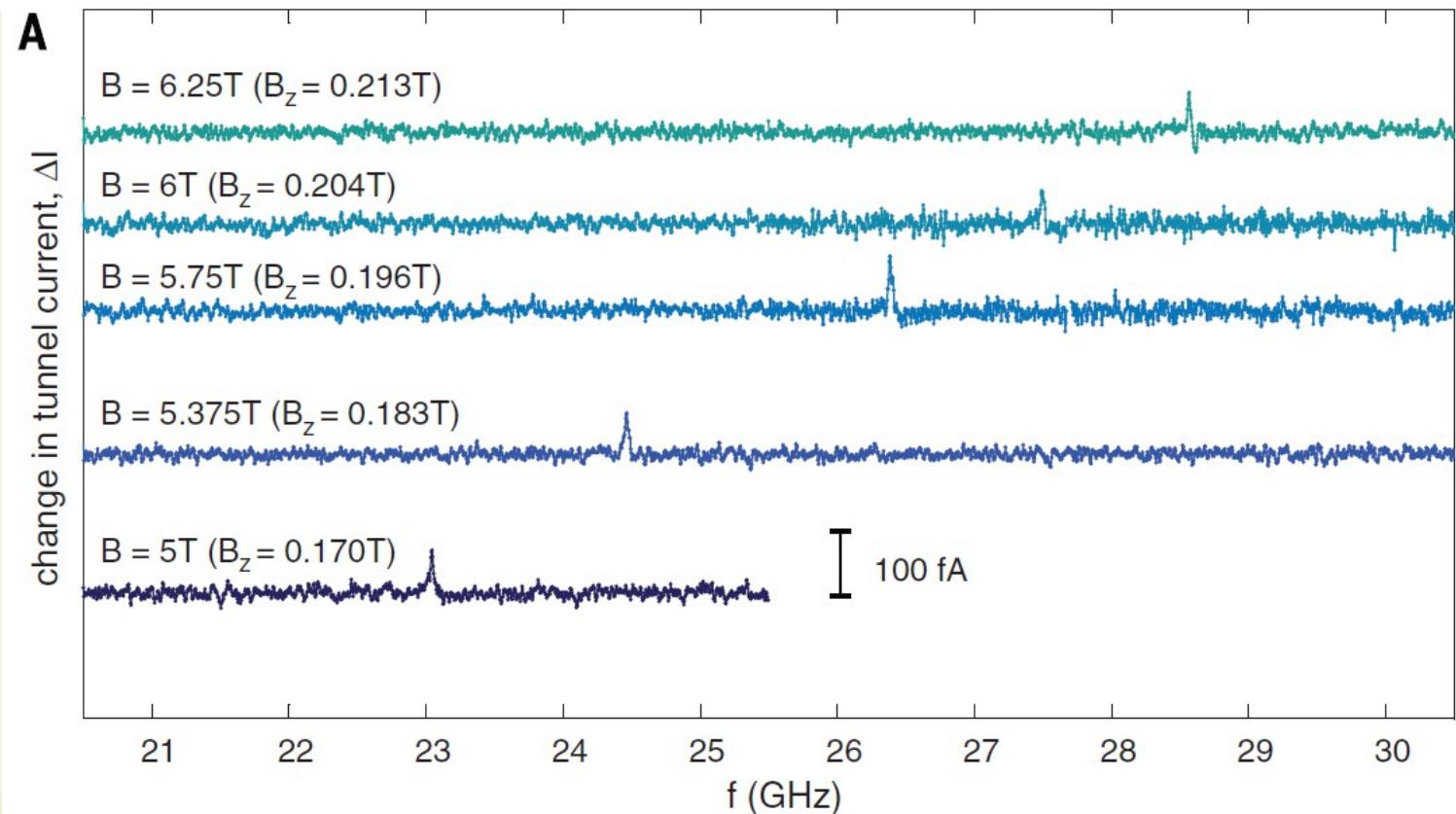


STM - Electron Spin Resonance

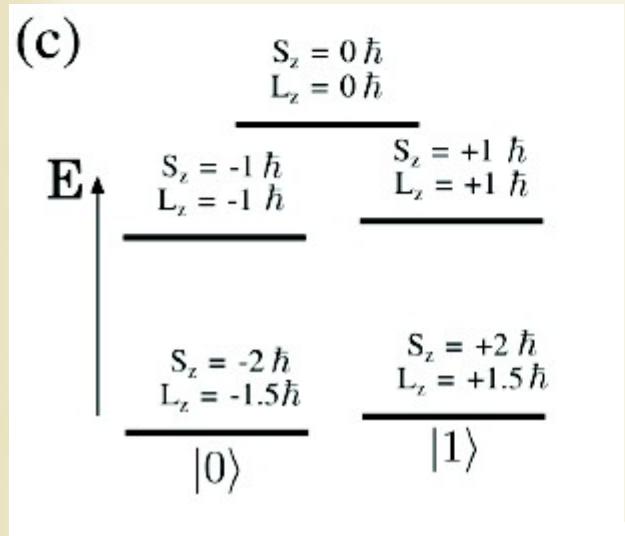
(c)



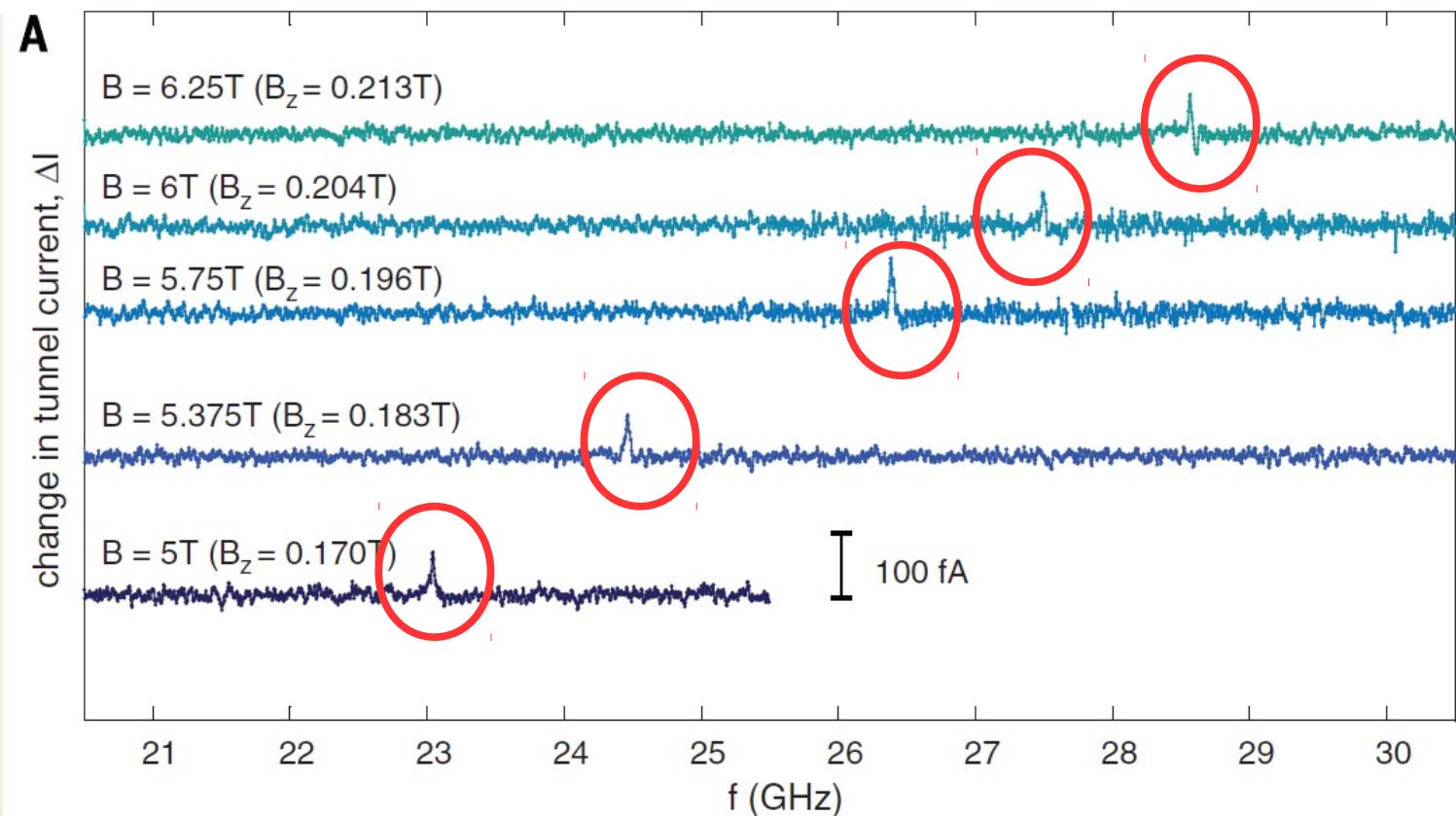
Fe@MgO



STM - Electron Spin Resonance

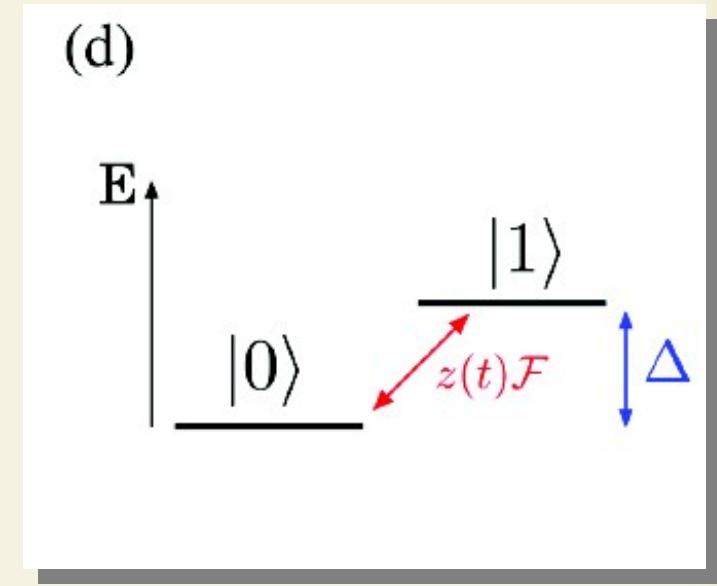
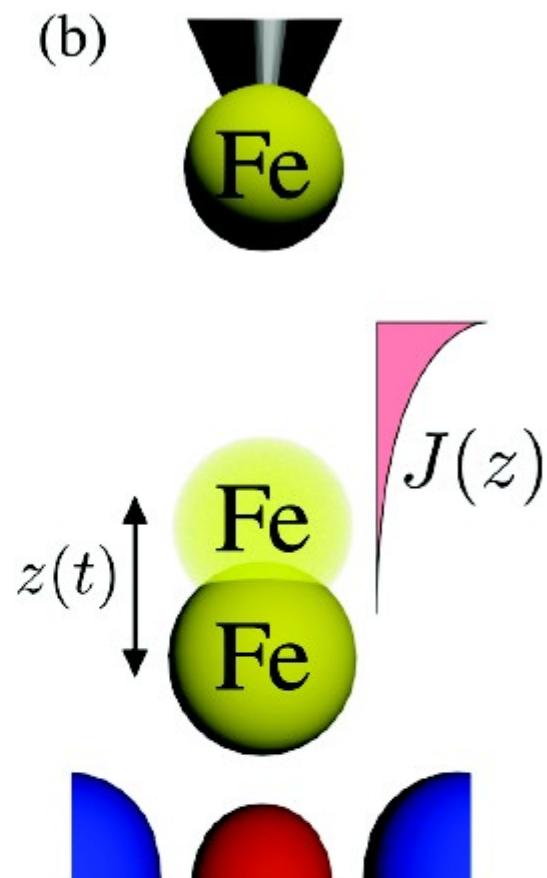


Fe@MgO



STM - Electron Spin Resonance

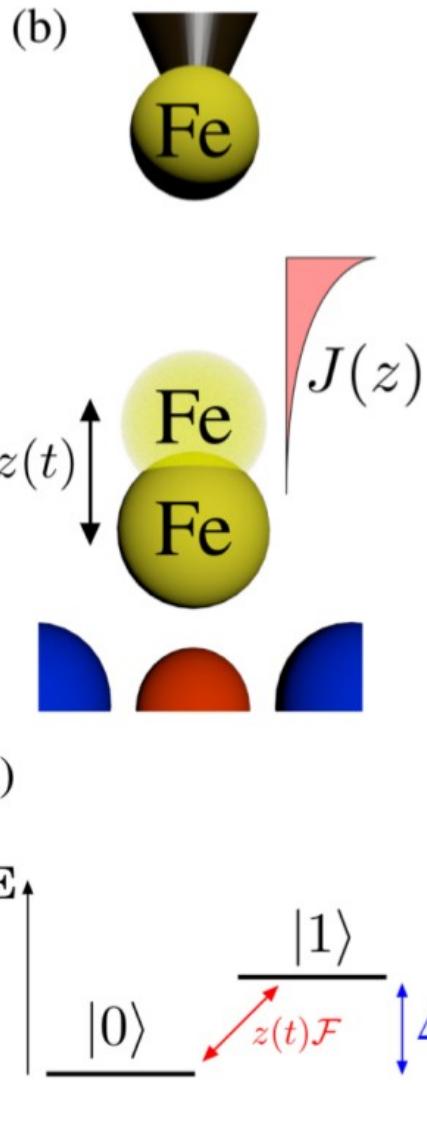
Fe@MgO



$$\mathcal{H} \approx \mathcal{H}_0 + z(t) \frac{\partial \mathcal{H}}{\partial z} \Big|_{z=0}.$$

STM - Electron Spin Resonance

Mecanismos



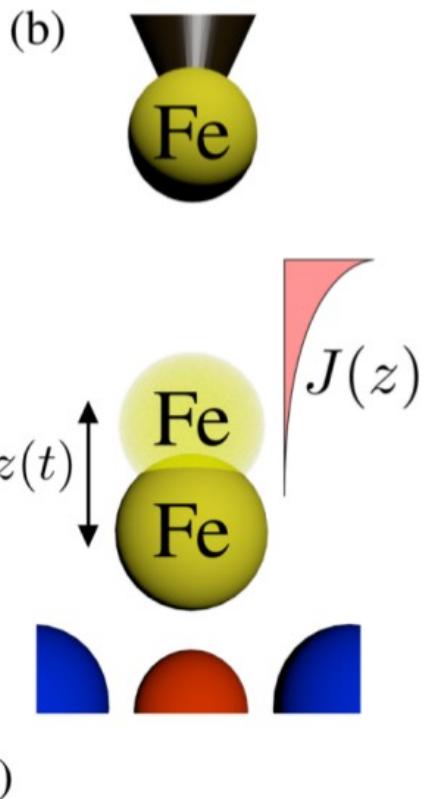
$$\mathcal{H} \approx \mathcal{H}_0 + z(t) \frac{\partial \mathcal{H}}{\partial z} \Big|_{z=0}.$$



$$\mathcal{F}_{\mathcal{N},\mathcal{M}} = \langle N | \frac{\partial \mathcal{H}}{\partial z} | M \rangle \neq 0$$

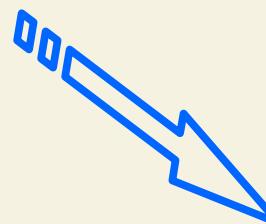
STM - Electron Spin Resonance

Mecanismos



1- Modulación del Crystal Field

$$\mathcal{F}_{CF} = \frac{\partial F_W}{\partial z} \langle 0 | l_x^4 + l_y^4 | 1 \rangle,$$

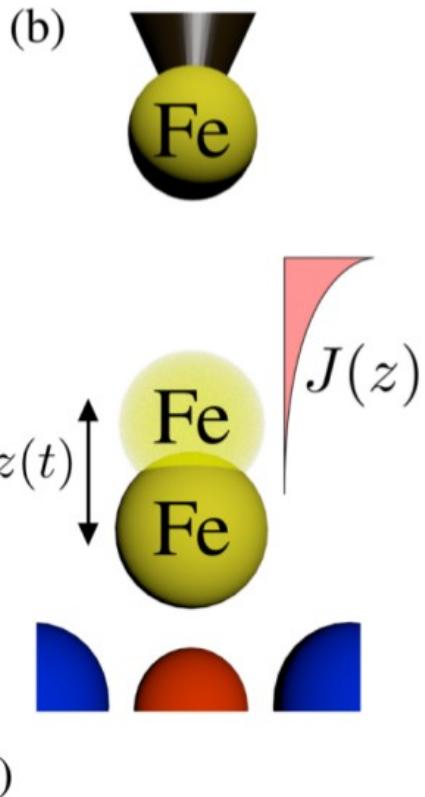


La primera explicación del experimento analizó la distorsión de la superficie durante el proceso y la influencia de la misma en la posibilidad de acoplar el Campo Eléctrico al Spin del Fe.

Science 350, 417 (2015)

STM - Electron Spin Resonance

Mecanismos



2- Mecanismo de Exchange

$$\mathcal{H}_J = J(z(t)) \vec{S}_T \cdot \vec{S}.$$

$$\mathcal{F}_J = \frac{\partial J(z)}{\partial z} \langle \vec{S}_T \rangle \cdot \langle 0 | \vec{S} | 1 \rangle.$$

PHYSICAL REVIEW B 96, 205420 (2017)

Exchange mechanism for electron paramagnetic resonance of individual adatoms

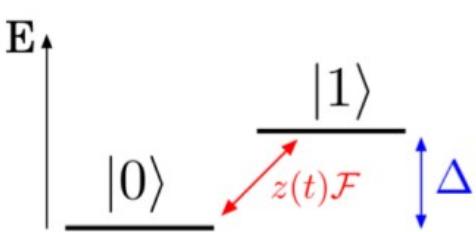
J. L. Lado,¹ A. Ferrón,² and J. Fernández-Rossier^{1,3}

¹QuantaLab, International Iberian Nanotechnology Laboratory (INL), Avenida Mestre Jos Veiga, 4715-330 Braga, Portugal

²Instituto de Modelado e Innovación Tecnológica (CONICET-UNNE) and Facultad de Ciencias Exactas, Naturales y Agrimensura, Universidad Nacional del Nordeste, Avenida Libertad 5400, W3404AAS Corrientes, Argentina

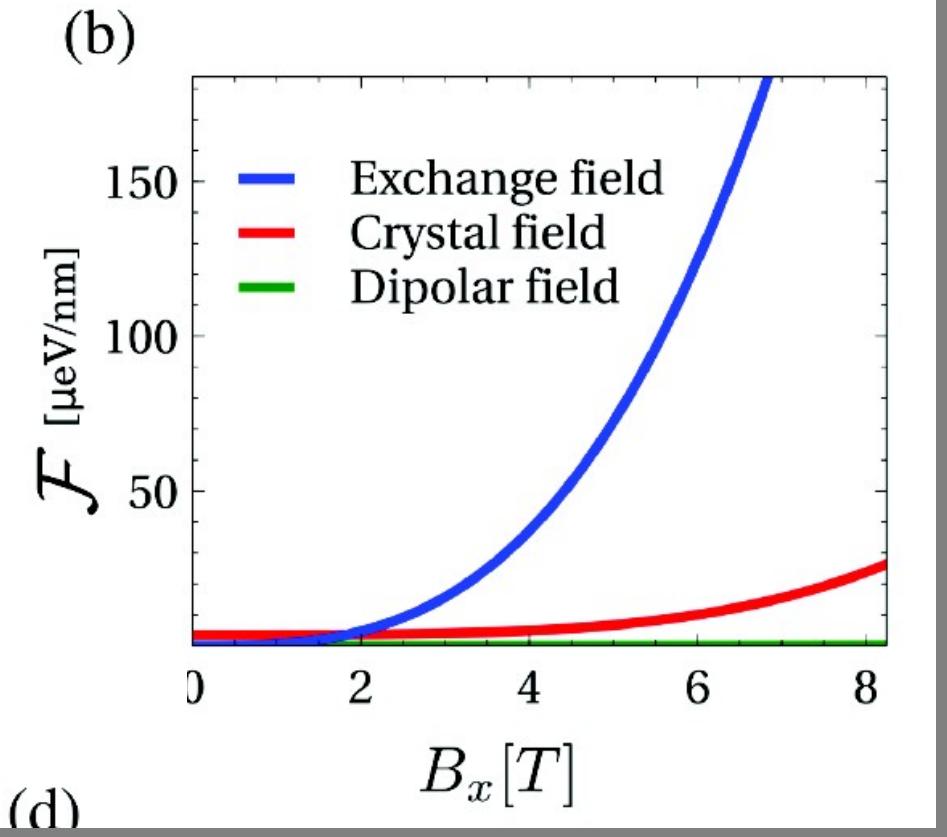
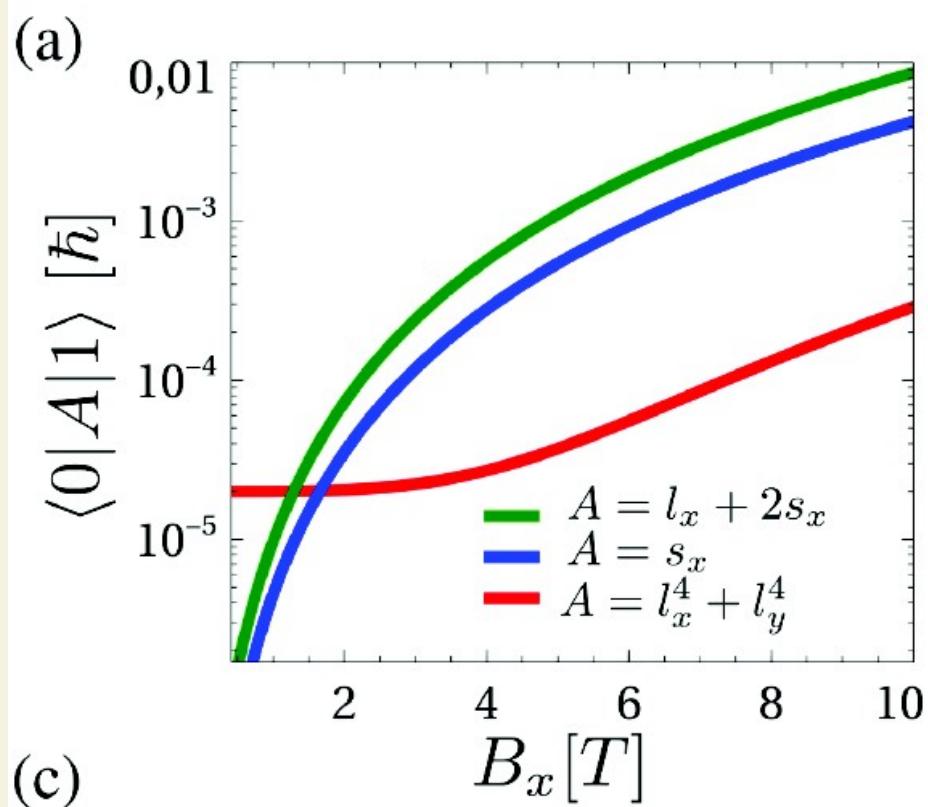
³Departamento de Física Aplicada, Universidad de Alicante, 03690 Spain

(Received 10 November 2016; revised manuscript received 31 August 2017; published 13 November 2017)



STM - Electron Spin Resonance

Fe@MgO

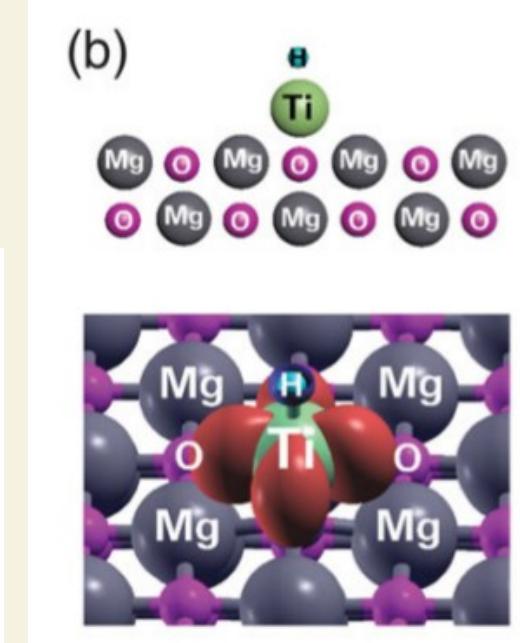
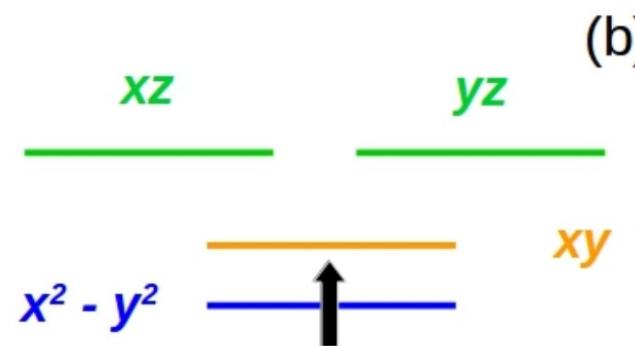
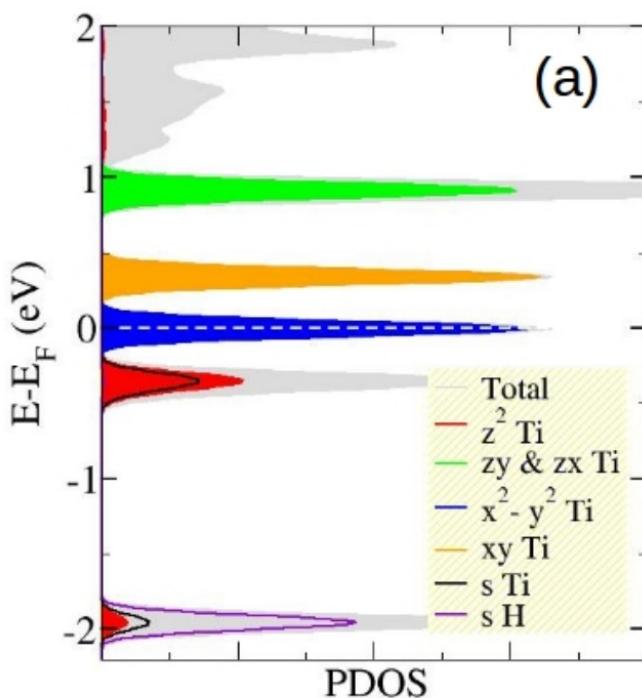


STM-ESR: Ti atoms at MgO

STM-ESR: Ti atoms at MgO

Mediciones de Excitaciones de spin con STM sugieren:

Ti $S=1/2$

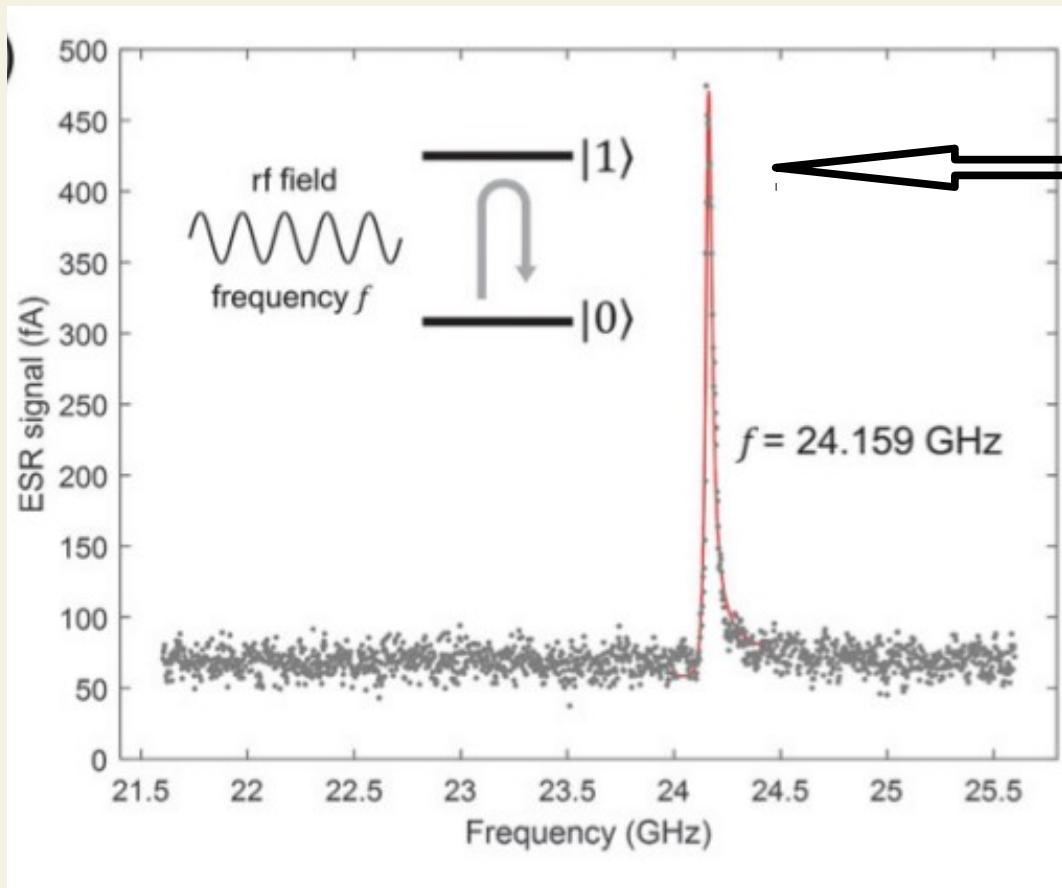


Cálculos DFT del magnetismo
del **Ti+H** confirman

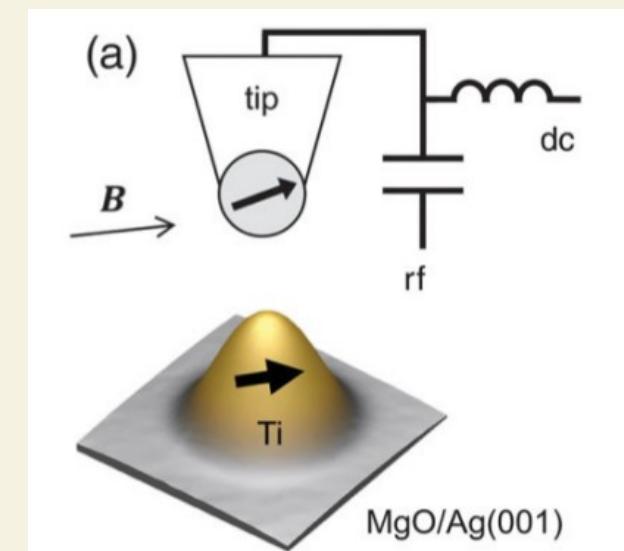
$S=1/2$

STM-ESR: Ti atoms at MgO

Experimento de Electron Spin Resonance para un solo Ti aislado:



Pico STM-ESR
Para el Ti



STM-ESR: Ti atoms at MgO

PHYSICAL REVIEW RESEARCH 1, 033185 (2019)

Single spin resonance driven by electric modulation of the g-factor anisotropy

A. Ferrón^{1,*}, S. A. Rodríguez¹, S. S. Gómez¹, J. L. Lado², and J. Fernández-Rossier^{3,†}

¹*Instituto de Modelado e Innovación Tecnológica (CONICET-UNNE) and Facultad de Ciencias Exactas, Naturales y Agrimensura, Universidad Nacional del Nordeste, Avenida Libertad 5400, W3404AAS Corrientes, Argentina*

²*Department of Applied Physics, Aalto University, Espoo, Finland*

³*QuantaLab, International Iberian Nanotechnology Laboratory (INL), Avenida Mestre José Veiga, 4715-330 Braga, Portugal*



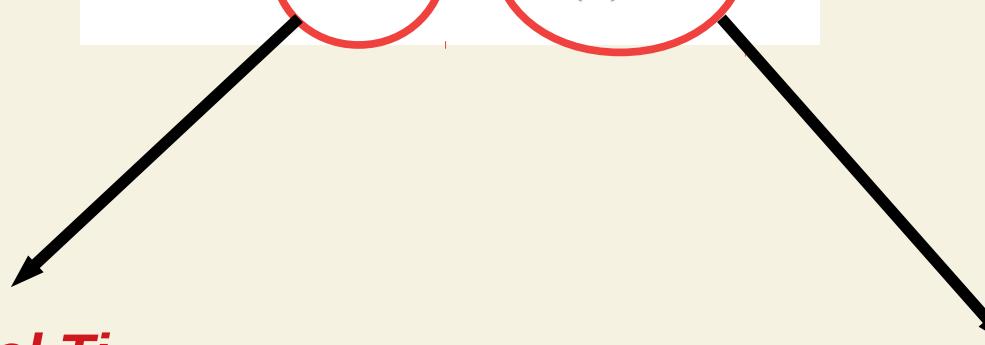
(Received 20 September 2019; revised manuscript received 12 November 2019; published 18 December 2019)

We address the problem of electronic and nuclear spin resonance of an individual atom on a surface driven by a scanning tunneling microscope. Several mechanisms have been proposed so far, some of them based on the modulation of exchange and crystal field associated with a piezoelectric displacement of the adatom driven by the radio frequency (RF) tip electric field. Here we consider another mechanism, where the piezoelectric displacement modulates the g-factor anisotropy, leading both to electronic and nuclear spin flip transitions. We discuss thoroughly the cases of hydrogenated Ti ($S = 1/2$) and Fe ($S = 2$) on MgO, relevant for recent experiments. We model the system using two approaches. First, an analytical model that includes crystal field, spin orbit coupling, and hyperfine interactions. Second, we carry out density-functional-based calculations. We find that the modulation of the anisotropy of the g tensor due to the piezoelectric displacement of the atom is

$$\mathcal{H} = \vec{b}_0 \cdot \vec{S} + \vec{b}_1(t) \cdot \vec{S}$$

STM-ESR: Ti atoms at MgO

$$\mathcal{H} = \vec{b}_0 \cdot \vec{S} + \vec{b}_1(t) \cdot \vec{S}$$



Hamiltoniano para el Ti depositado en MgO. En caso de ser necesario tambien incluye el efecto de la punta.

Hamiltoniano de driving

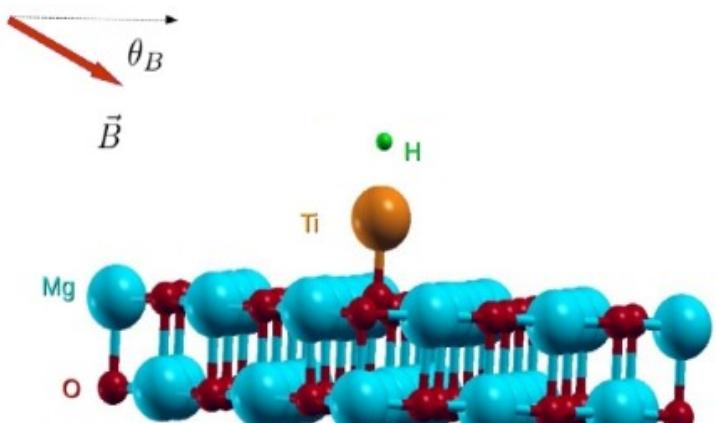
$$\mathcal{H} \approx \mathcal{H}_0 + z(t) \frac{\partial \mathcal{H}}{\partial z} \Big|_{z=0}.$$

STM-ESR: Ti atoms at MgO

$$\mathcal{H} = \vec{b}_0 \cdot \vec{S} + \vec{b}_1(t) \cdot \vec{S}$$



$$\vec{b}_0 = |\vec{b}_0|(\sin \theta_0, 0, \cos \theta_0)$$



Donde, en el caso de que solo haya campo externo, los ángulos se pueden calcular:

$$\sin \theta_0 = \frac{g_x B_x}{\sqrt{(g_x B_x)^2 + (g_z B_z)^2}}$$

$$\cos \theta_0 = \frac{g_z B_z}{\sqrt{(g_x B_x)^2 + (g_z B_z)^2}}$$

$$\boxed{\vec{b}_0 = \mu_B (g_x B_x, 0, g_z B_z)}$$

STM-ESR: Ti atoms at MgO

Trabajar con un spin $\frac{1}{2}$ es esencialmente un ejercicio de Cuántica I y podemos hacer todo (o casi todo) analítico:

$$\mathcal{H} = \vec{b}_0 \cdot \vec{S}$$

$$\vec{b}_0 = \mu_B (g_x B_x, 0, g_z B_z)$$

Podemos (y debemos) diagonalizar el Hamiltoniano sin “perturbar”.

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$
$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$

$$\sin \theta_0 = \frac{g_x B_x}{\sqrt{(g_x B_x)^2 + (g_z B_z)^2}}$$

$$\cos \theta_0 = \frac{g_z B_z}{\sqrt{(g_x B_x)^2 + (g_z B_z)^2}}$$

STM-ESR: Ti atoms at MgO

Ahora miremos el Hamiltoniano completo:

$$\mathcal{H} = \vec{b}_0 \cdot \vec{S} + \vec{b}_1(t) \cdot \vec{S}$$

Para analizar la posibilidad de que nuestro driving genere transiciones debemos calcular “Rabi”:



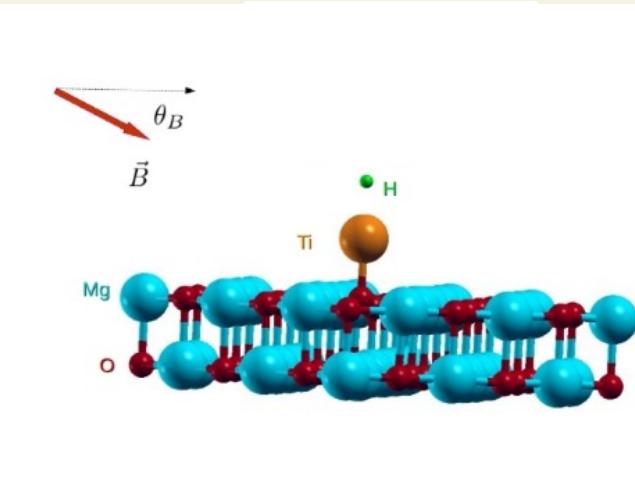
$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

Usando

$$\vec{b}_0 = \mu_B (g_x B_x, 0, g_z B_z)$$

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$

$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$



STM-ESR: Ti atoms at MgO

Ahora miremos el Hamiltoniano completo:

$$\mathcal{H} = \vec{b}_0 \cdot \vec{S} + \vec{b}_1(t) \cdot \vec{S}$$

Para analizar la posibilidad de que nuestro driving genere transiciones debemos calcular “Rabi”:



$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

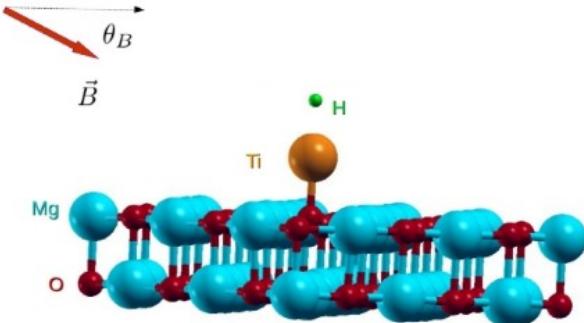
Usando

$$\vec{b}_0 = \mu_B (g_x B_x, 0, g_z B_z)$$

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$

$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$

Para empezar, y solo para empezar

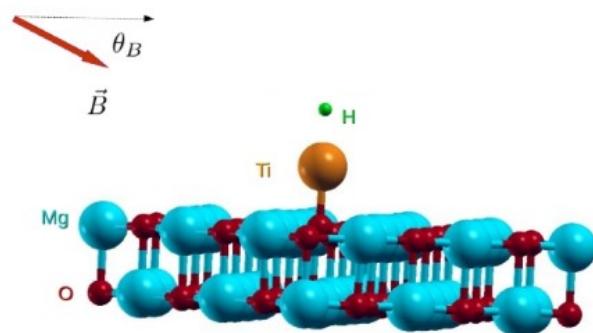


$$\vec{b}_1 = \mu_B (\delta g_x B_x, 0, \delta g_z B_z)$$

STM-ESR: Ti atoms at MgO

$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

Hagamos las cuentas!



$$\vec{b}_1 = \mu_B (\delta g_x B_x, 0, \delta g_z B_z)$$

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$

$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$

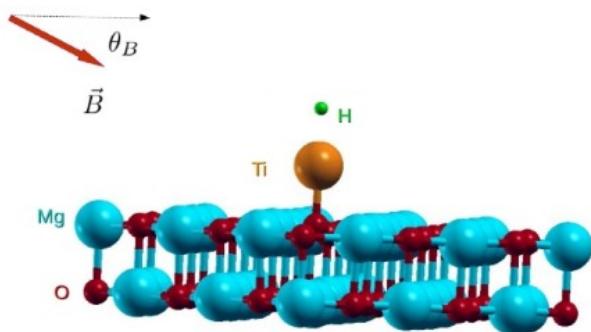
$$\langle + | S_x | - \rangle = \frac{1}{2} \left(\sin^2 \frac{\theta_0}{2} - \cos^2 \frac{\theta_0}{2} \right) = -\frac{1}{2} \cos \theta_0$$

$$\langle + | S_z | - \rangle = \sin \frac{\theta_0}{2} \cos \frac{\theta_0}{2} = \frac{1}{2} \sin \theta_0$$

STM-ESR: Ti atoms at MgO

$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

Hagamos las cuentas!



$$\vec{b}_1 = \mu_B (\delta g_x B_x, 0, \delta g_z B_z)$$

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$

$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$

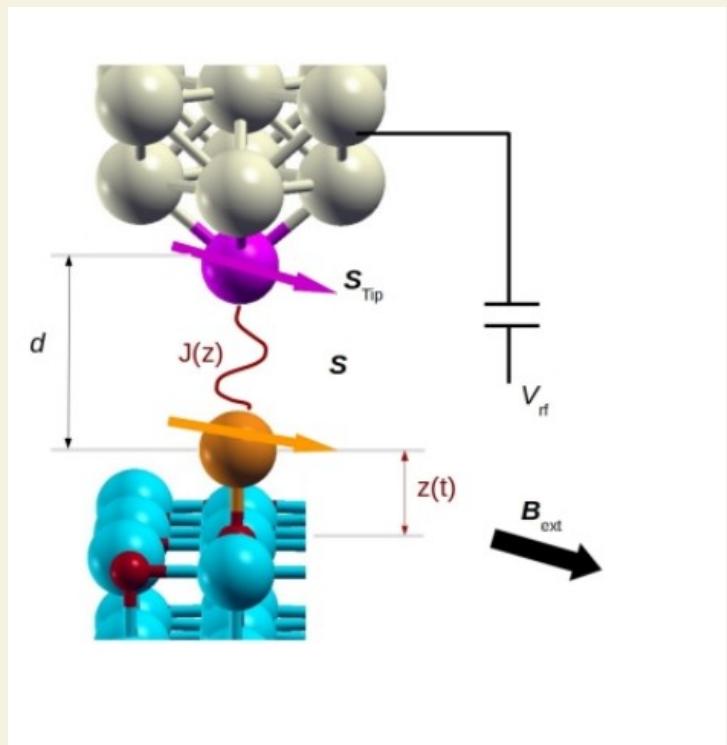
$$\langle + | S_x | - \rangle = \frac{1}{2} \left(\sin^2 \frac{\theta_0}{2} - \cos^2 \frac{\theta_0}{2} \right) = -\frac{1}{2} \cos \theta_0$$

$$\langle + | S_z | - \rangle = \sin \frac{\theta_0}{2} \cos \frac{\theta_0}{2} = \frac{1}{2} \sin \theta_0$$

$$\Omega = \frac{\mu_B}{4} |\vec{b}_0| \sin 2\theta_0 \left(\frac{\delta g_z}{g_z} - \frac{\delta g_x}{g_x} \right)$$

STM-ESR: Ti atoms at MgO

$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$



Ahora vamos a considerar, como en nuestro primer trabajo, la interacción del Ti con el Fe que está en la punta del STM:

$$\mathcal{V}_{\text{exch}} = J(z) \vec{n}_T \cdot \vec{S}$$

$$\vec{n}_T = (\cos(\theta_B + \delta), 0, \sin(\theta_B + \delta))$$



Agregamos este término al Hamiltoniano anterior

STM-ESR: Ti atoms at MgO

$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

Hagamos las cuentas otra vez!

$$\mathcal{V}_{\text{exch}} = J(z) \vec{n}_T \cdot \vec{S}$$

$$\vec{n}_T = (\cos(\theta_B + \delta), 0, \sin(\theta_B + \delta))$$

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$
$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$

$$\sin \theta_0 = \frac{g_x B_x + J n_x}{\Delta_Z^*}$$

$$\cos \theta_0 = \frac{g_z B_z + J n_z}{\Delta_Z^*}$$

$$\Delta_Z^* \equiv \sqrt{(g_x \mu_B B_x + J n_x)^2 + (g_z \mu_B B_z + J n_z)^2}$$

STM-ESR: Ti atoms at MgO

$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

$$|+\rangle = \cos \frac{\theta_0}{2} | \uparrow \rangle + \sin \frac{\theta_0}{2} | \downarrow \rangle$$
$$|-\rangle = \sin \frac{\theta_0}{2} | \uparrow \rangle - \cos \frac{\theta_0}{2} | \downarrow \rangle$$

Ahora nuestro driving proviente de la modulacion del Exchange entre la punta y el átomo:

$$\vec{b}_1(t) = \delta J(n_x, 0, n_z)$$

STM-ESR: Ti atoms at MgO

$$\Omega = \langle + | \vec{b}_1 \cdot \vec{S} | - \rangle$$

$$|+\rangle = \cos \frac{\theta_0}{2} |\uparrow\rangle + \sin \frac{\theta_0}{2} |\downarrow\rangle$$
$$|-\rangle = \sin \frac{\theta_0}{2} |\uparrow\rangle - \cos \frac{\theta_0}{2} |\downarrow\rangle$$

Ahora nuestro driving proviente de la modulacion del Exchange entre la punta y el átomo:

$$\vec{b}_1(t) = \delta J(n_x, 0, n_z)$$

Haciendo las cuentas
obtenemos “Rabi”

$$\Omega_J = \frac{\delta J}{2\Delta_z^*} (g_x \mu_B \cdot B_x n_z - g_z \mu_B B_z n_x)$$

STM-ESR: Ti atoms at MgO

$$\vec{b}_1(t) = \delta J(n_x, 0, n_z)$$

$$\Omega_J = \frac{\delta J}{2\Delta_z^*} (g_x \mu_B B_x n_z - g_z \mu_B B_z n_x)$$

Pero!



$$g_x = g + \Delta g_x$$
$$g_z = g + \Delta g_z$$

STM-ESR: Ti atoms at MgO

$$\vec{b}_1(t) = \delta J(n_x, 0, n_z)$$

$$\Omega_J = \frac{\delta J}{2\Delta_z^*} (g_x \mu_B B_x n_z - g_z \mu_B B_z n_x)$$

$$g_x = g + \Delta g_x$$
$$g_z = g + \Delta g_z$$

Reemplazando y jugando con algunos términos:



donde

$$\mathcal{E}_J \equiv \frac{\delta J}{2\Delta_z^*} g \mu_B B$$

$$\begin{aligned}\Omega_J &= \mathcal{E}_J \sin \delta + \\ &\mathcal{E}_J \left(\frac{\Delta g_x}{g} - \frac{\Delta g_z}{g} \right) \cos \theta_B \sin \theta_B \cos \delta + \\ &+ \mathcal{E}_J \left(\frac{\Delta g_x}{g} \cos^2 \theta_B + \frac{\Delta g_z}{g} \sin^2 \theta_B \right) \sin \delta\end{aligned}$$

STM-ESR: Ti dimers at MgO

PRL 119, 227206 (2017)

PHYSICAL REVIEW LETTERS

week ending
1 DECEMBER 2017

Engineering the Eigenstates of Coupled Spin-1/2 Atoms on a Surface

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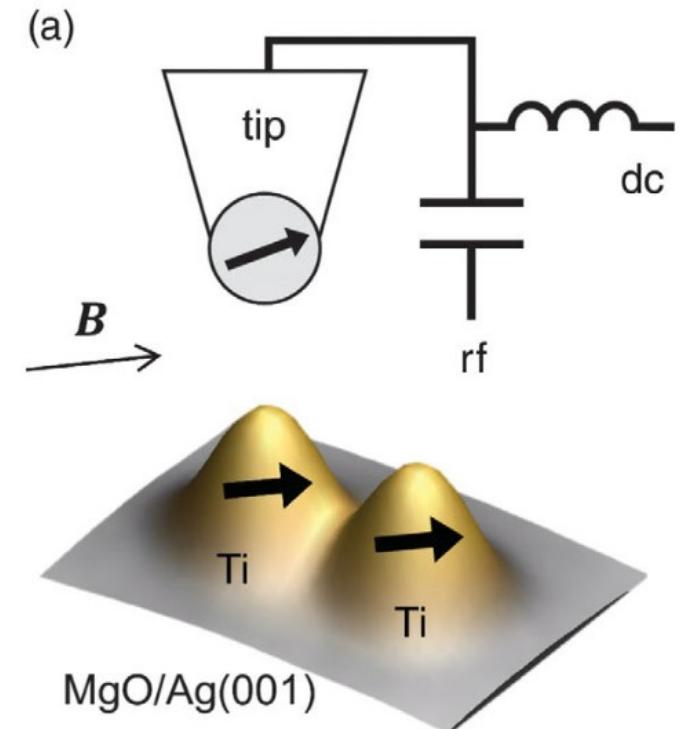
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Quantum spin networks having engineered geometries and interactions are eagerly pursued for quantum simulation and access to emergent quantum phenomena such as spin liquids. Spin-1/2 centers are particularly desirable, because they readily manifest coherent quantum fluctuations. Here we introduce a controllable spin-1/2 architecture consisting of titanium atoms on a magnesium oxide surface. We tailor the spin interactions by atomic-precision positioning using a scanning tunneling microscope (STM) and subsequently perform electron spin resonance on individual atoms to drive transitions into and out of quantum eigenstates of the coupled-spin system. Interactions between the atoms are mapped over a range of distances extending from highly anisotropic dipole coupling to strong exchange coupling. The local magnetic field of the magnetic STM tip serves to precisely tune the superposition states of a pair of spins. The precise control of the spin-spin interactions and ability to probe the states of the coupled-spin network by addressing individual spins will enable the exploration of quantum many-body systems based on networks of spin-1/2 atoms on surfaces.

DOI: 10.1103/PhysRevLett.119.227206



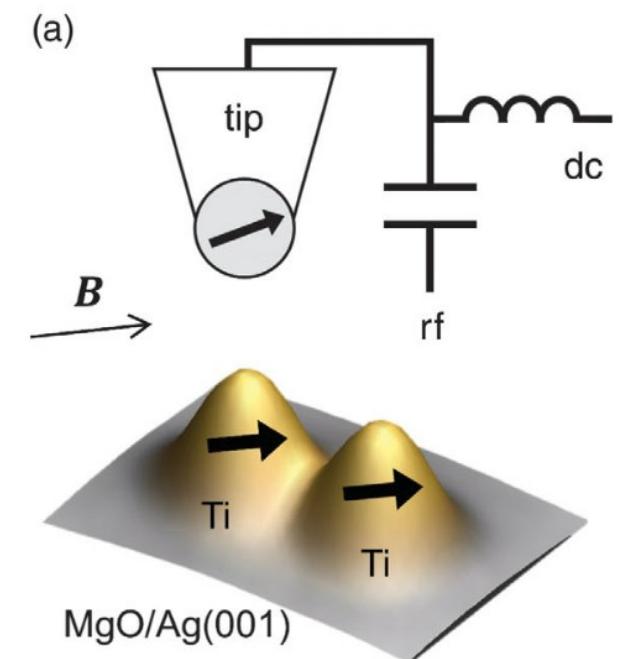
STM-ESR: Ti dimers at MgO

Escribamos el Hamiltoniano más general que se nos ocurra para dos spins $\frac{1}{2}$ teniendo en cuenta la presencia de la Punta del STM:

$$H = \gamma_1 \hbar \mathbf{S}_1 \cdot (\mathbf{B} + \mathbf{B}_{tip}) + \gamma_2 \hbar \mathbf{S}_2 \cdot \mathbf{B} \\ + D_0 (\mathbf{S}_1 \cdot \mathbf{S}_2 - 3(\mathbf{S}_1 \cdot \hat{\mathbf{r}})(\mathbf{S}_2 \cdot \hat{\mathbf{r}})) + J \mathbf{S}_1 \cdot \mathbf{S}_2$$

$$D_0 = \frac{\mu_0 \gamma^2 \hbar^2}{4\pi r^3}$$

$$J = J_0 \cdot \exp(-(r - r_0)/d_{ex})$$



STM-ESR: Ti dimers at MgO

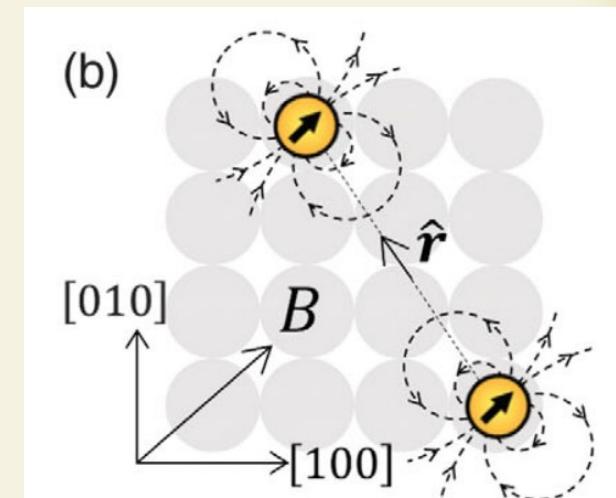
$$H = \gamma_1 \hbar \mathbf{S}_1 \cdot (\mathbf{B} + \mathbf{B}_{tip}) + \gamma_2 \hbar \mathbf{S}_2 \cdot \mathbf{B} \\ + D_0 (\mathbf{S}_1 \cdot \mathbf{S}_2 - 3(\mathbf{S}_1 \cdot \hat{\mathbf{r}})(\mathbf{S}_2 \cdot \hat{\mathbf{r}})) + J \mathbf{S}_1 \cdot \mathbf{S}_2$$

$$D_0 = \frac{\mu_0 \gamma^2 \hbar^2}{4\pi r^3}$$

$$J = J_0 \cdot \exp(-(r - r_0)/d_{ex})$$

Supongamos que los spines están alineados con el campo magnético (bajo protesta):

$$H \approx \gamma \hbar S_{1z}(B + B_{tip}) + \gamma \hbar S_{2z}B + J \mathbf{S}_1 \cdot \mathbf{S}_2 + D (3S_{1z}S_{2z} - \mathbf{S}_1 \cdot \mathbf{S}_2) \\ = \gamma \hbar S_{1z}(B + B_{tip}) + \gamma \hbar S_{2z}B + (J + 2D)S_{1z}S_{2z} + (J - D)(S_{1x}S_{2x} + S_{1y}S_{2y})$$



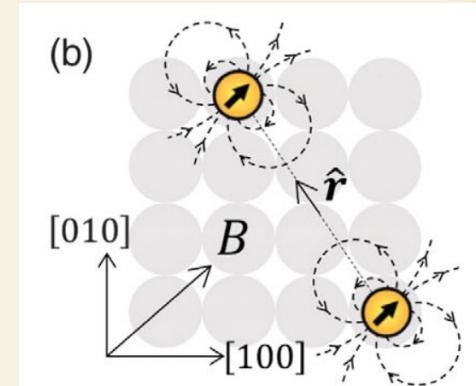
$$D = \frac{D_0}{2} (1 - 3\cos^2\theta) = \frac{\mu_0 \mu_{Ti}^2}{2\pi r^3} (1 - 3\cos^2\theta)$$

STM-ESR: Ti dimers at MgO

$$H \approx \gamma \hbar S_{1z}(B + B_{\text{tip}}) + \gamma \hbar S_{2z}B + J \mathbf{S}_1 \cdot \mathbf{S}_2 + D (3S_{1z}S_{2z} - \mathbf{S}_1 \cdot \mathbf{S}_2)$$
$$= \gamma \hbar S_{1z}(B + B_{\text{tip}}) + \gamma \hbar S_{2z}B + (J + 2D)S_{1z}S_{2z} + (J - D)(S_{1x}S_{2x} + S_{1y}S_{2y})$$

$$J = J_0 \cdot \exp(-(r - r_0)/d_{\text{ex}})$$

$$D = \frac{D_0}{2} (1 - 3\cos^2\theta) = \frac{\mu_0 \mu_{Ti}^2}{2\pi r^3} (1 - 3\cos^2\theta)$$



Elegimos para trabajar la base producto $|00\rangle$, $|01\rangle$, $|10\rangle$ y $|11\rangle$, donde $|0\rangle$ y $|1\rangle$ son autostados de S_{1z} o S_{2z} . $|00\rangle$ y $|11\rangle$ son autoestados de nuestro Hamiltoniano pero $|10\rangle$ y $|01\rangle$ son superposiciones de estados up y down por culpa de los términos flip-flop del Hamiltoniano.

STM-ESR: Ti dimers at MgO

$$H \approx \gamma \hbar S_{1z}(B + B_{\text{tip}}) + \gamma \hbar S_{2z}B + J \mathbf{S}_1 \cdot \mathbf{S}_2 + D (3S_{1z}S_{2z} - \mathbf{S}_1 \cdot \mathbf{S}_2)$$

$$= \gamma \hbar S_{1z}(B + B_{\text{tip}}) + \gamma \hbar S_{2z}B + (J + 2D)S_{1z}S_{2z} + (J - D)(S_{1x}S_{2x} + S_{1y}S_{2y})$$

$$J = J_0 \cdot \exp(-(r - r_0)/d_{\text{ex}})$$

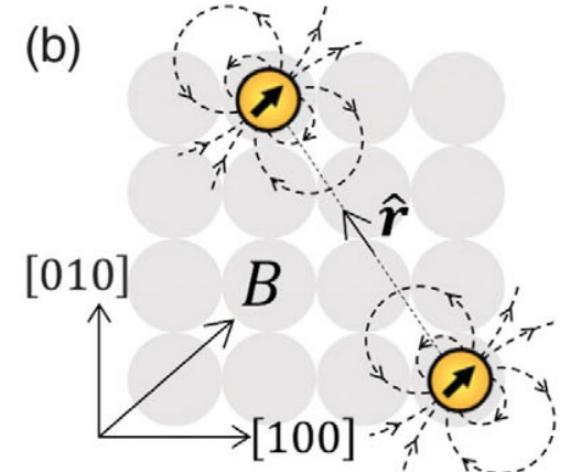
$$D = \frac{D_0}{2} (1 - 3\cos^2\theta) = \frac{\mu_0 \mu_{Ti}^2}{2\pi r^3} (1 - 3\cos^2\theta)$$

$$E_{11} = \frac{1}{4}(J + 2D) + \frac{1}{2}\gamma \hbar(2B + B_{\text{tip}})$$

$$E_+ = -\frac{1}{4}(J + 2D) + \frac{1}{2}\sqrt{(J - D)^2 + (\gamma \hbar B_{\text{tip}})^2}$$

$$E_- = -\frac{1}{4}(J + 2D) - \frac{1}{2}\sqrt{(J - D)^2 + (\gamma \hbar B_{\text{tip}})^2}$$

$$E_{00} = \frac{1}{4}(J + 2D) - \frac{1}{2}\gamma \hbar(2B + B_{\text{tip}})$$



STM-ESR: Ti dimers at MgO

$$H \approx \gamma\hbar S_{1z}(B + B_{tip}) + \gamma\hbar S_{2z}B + J \mathbf{S}_1 \cdot \mathbf{S}_2 + D(3S_{1z}S_{2z} - \mathbf{S}_1 \cdot \mathbf{S}_2)$$
$$= \gamma\hbar S_{1z}(B + B_{tip}) + \gamma\hbar S_{2z}B + (J + 2D)S_{1z}S_{2z} + (J - D)(S_{1x}S_{2x} + S_{1y}S_{2y})$$

$$E_{11} = \frac{1}{4}(J + 2D) + \frac{1}{2}\gamma\hbar(2B + B_{tip})$$

$$E_+ = -\frac{1}{4}(J + 2D) + \frac{1}{2}\sqrt{(J - D)^2 + (\gamma\hbar B_{tip})^2}$$

$$E_- = -\frac{1}{4}(J + 2D) - \frac{1}{2}\sqrt{(J - D)^2 + (\gamma\hbar B_{tip})^2}$$

$$E_{00} = \frac{1}{4}(J + 2D) - \frac{1}{2}\gamma\hbar(2B + B_{tip})$$

Ahora tenemos que pensar como es posible realizar transiciones entre los distintos estados durante una experimento ESR.

Esto se podría hacer bien o hacer como lo vamos a hacer acá.

STM-ESR: Ti dimers at MgO

$$H \approx \gamma\hbar S_{1z}(B + B_{tip}) + \gamma\hbar S_{2z}B + J \mathbf{S}_1 \cdot \mathbf{S}_2 + D(3S_{1z}S_{2z} - \mathbf{S}_1 \cdot \mathbf{S}_2)$$
$$= \gamma\hbar S_{1z}(B + B_{tip}) + \gamma\hbar S_{2z}B + (J + 2D)S_{1z}S_{2z} + (J - D)(S_{1x}S_{2x} + S_{1y}S_{2y})$$

$$E_{11} = \frac{1}{4}(J + 2D) + \frac{1}{2}\gamma\hbar(2B + B_{tip})$$

$$E_+ = -\frac{1}{4}(J + 2D) + \frac{1}{2}\sqrt{(J - D)^2 + (\gamma\hbar B_{tip})^2}$$

$$E_- = -\frac{1}{4}(J + 2D) - \frac{1}{2}\sqrt{(J - D)^2 + (\gamma\hbar B_{tip})^2}$$

$$E_{00} = \frac{1}{4}(J + 2D) - \frac{1}{2}\gamma\hbar(2B + B_{tip})$$

El Ti bajo la punta se desplaza (PEC) y las modulaciones que esto produce podría (o no) darnos un driving proporcional a S_{1x}

Ahora tenemos que pensar como es posible realizar transiciones entre los distintos estados durante una experimento ESR.

Esto se podría hacer bien o hacer como lo vamos a hacer acá.

$$\langle a | S_{1x} | b \rangle \neq 0$$



$$\Delta m_s = \pm 1$$

$$f_I = \frac{1}{\hbar}(E_- - E_{00})$$

$$f_{II} = \frac{1}{\hbar}(E_{11} - E_+)$$

$$f_{III} = \frac{1}{\hbar}(E_+ - E_{00})$$

$$f_{IV} = \frac{1}{\hbar}(E_{11} - E_-)$$

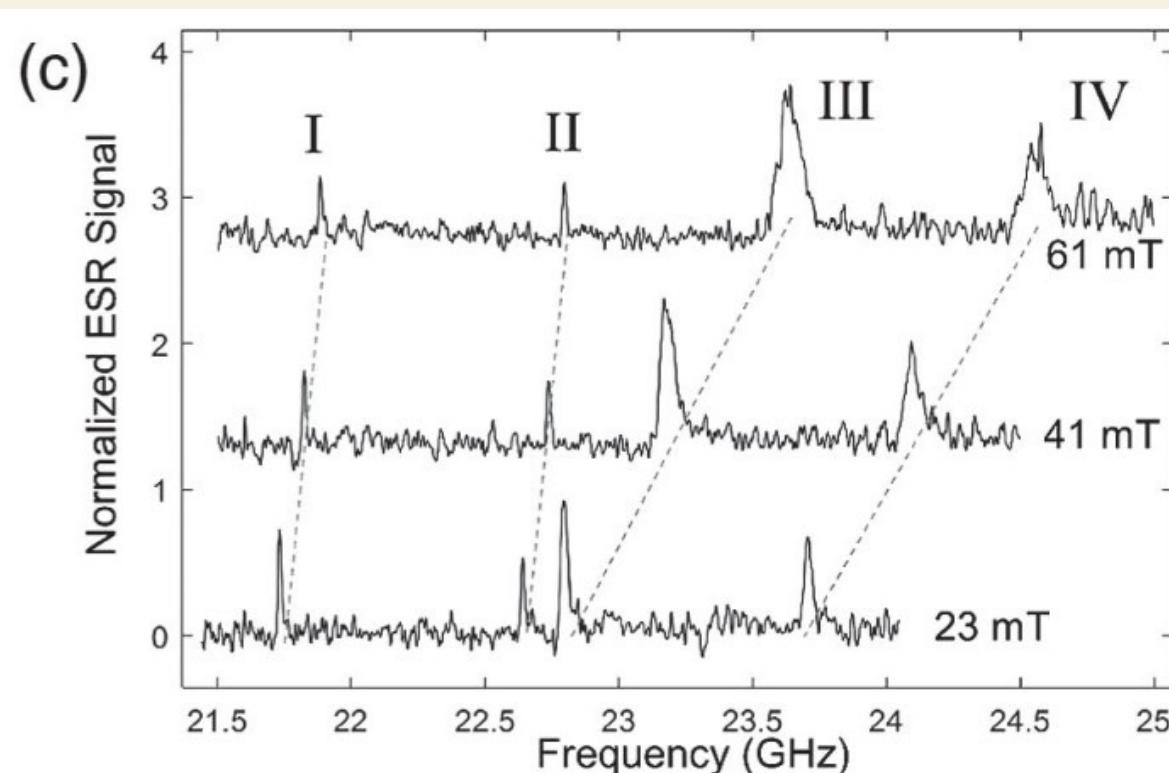
STM-ESR: Ti dimers at MgO

$$f_I = \frac{1}{\hbar} (E_- - E_{00})$$

$$f_{II} = \frac{1}{\hbar} (E_{11} - E_+)$$

$$f_{III} = \frac{1}{\hbar} (E_+ - E_{00})$$

$$f_{IV} = \frac{1}{\hbar} (E_{11} - E_-)$$



El experimento muestra, como era de esperar (?), 4 picos en frecuencia!

STM-ESR: Ti dimers at MgO

$$f_I = \frac{1}{\hbar} (E_- - E_{00})$$

$$f_{II} = \frac{1}{\hbar} (E_{11} - E_+)$$

$$f_{III} = \frac{1}{\hbar} (E_+ - E_{00})$$

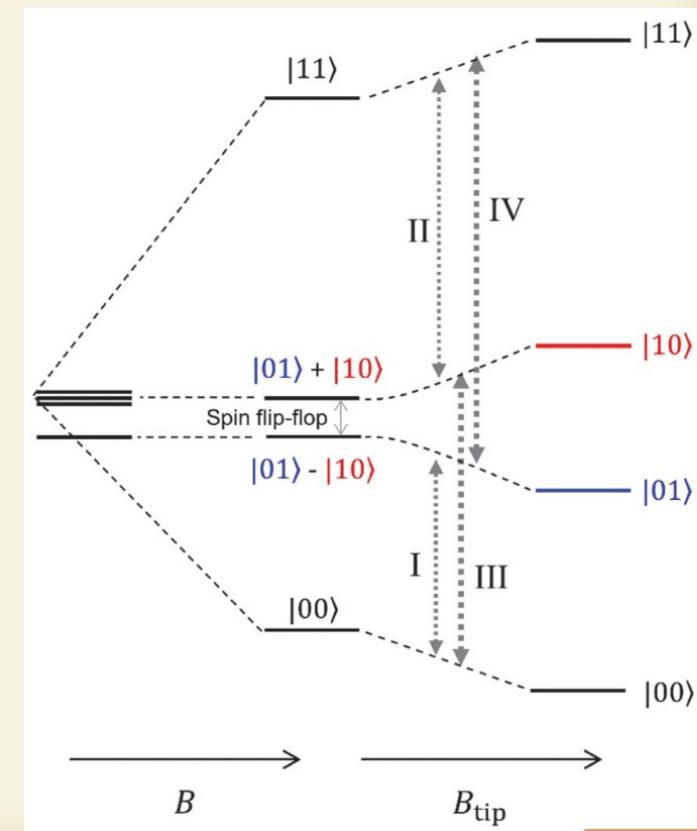
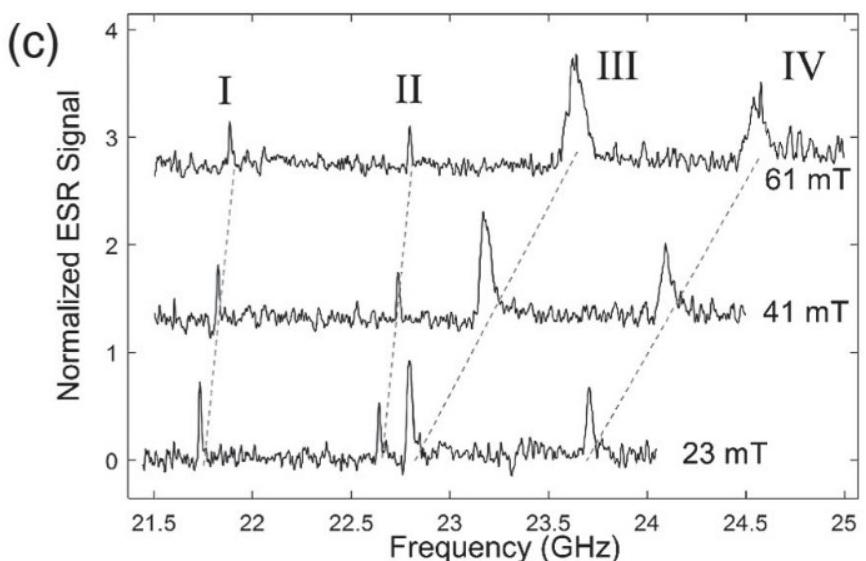
$$f_{IV} = \frac{1}{\hbar} (E_{11} - E_-)$$



Veamos las diferencias entre las distintas frecuencias o distancias entre picos

$$\Delta f_1 = f_{IV} - f_{III} = f_{II} - f_I = \frac{1}{\hbar} (J + 2D)$$

$$\Delta f_2 = f_{III} - f_I = \frac{1}{\hbar} \sqrt{(J - D)^2 + (\gamma \hbar B_{tip})^2}$$



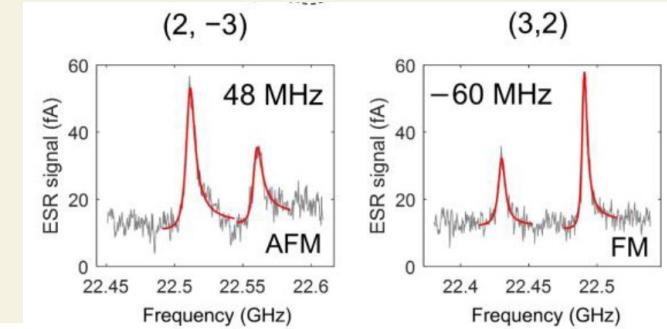
STM-ESR: Ti dimers at MgO

$$\Delta f_1 = f_{\text{IV}} - f_{\text{III}} = f_{\text{II}} - f_{\text{I}} = \frac{1}{\hbar} (J + 2D)$$

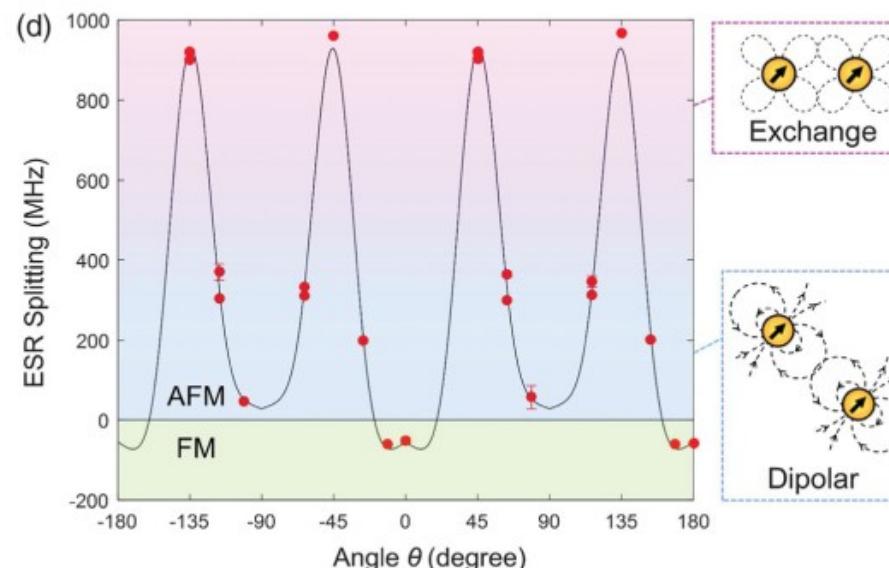
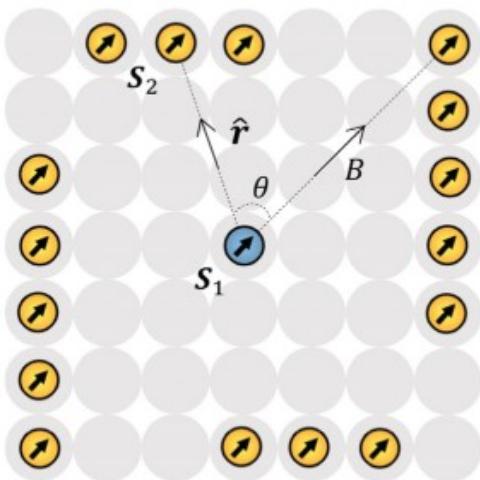
$$\Delta f_2 = f_{\text{III}} - f_{\text{I}} = \frac{1}{\hbar} \sqrt{(J - D)^2 + (\gamma \hbar B_{tip})^2}$$

$$J = J_0 \cdot \exp(-(r - r_0)/d_{\text{ex}})$$

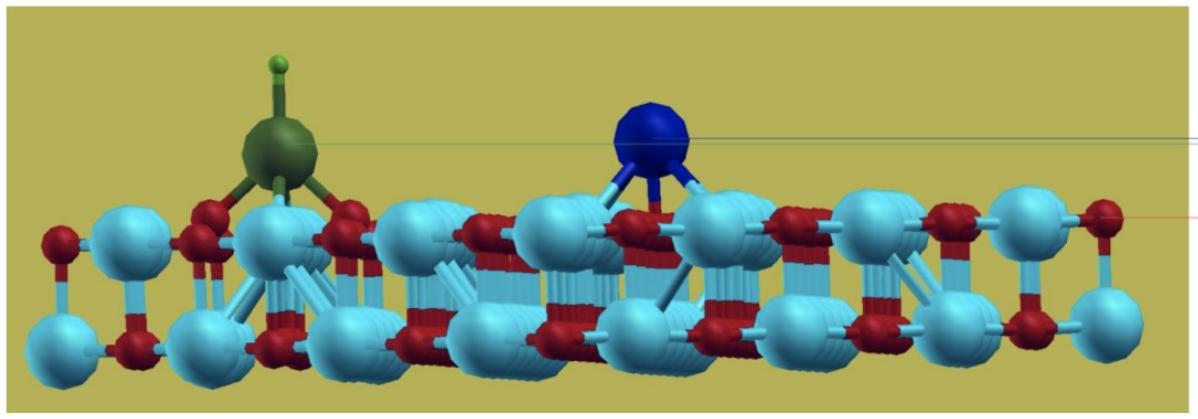
$$D = \frac{D_0}{2} (1 - 3 \cos^2 \theta) = \frac{\mu_0 \mu_{Ti}^2}{2\pi r^3} (1 - 3 \cos^2 \theta)$$



(c)



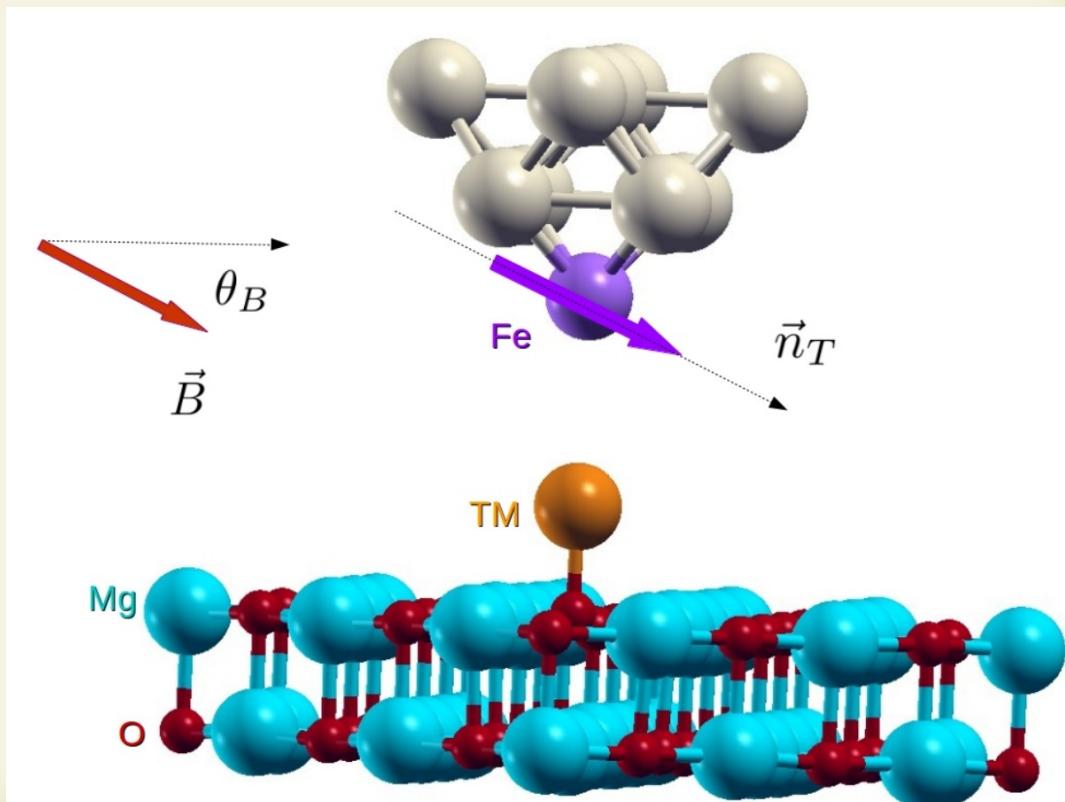
STM-ESR: TiFe dimers at MgO



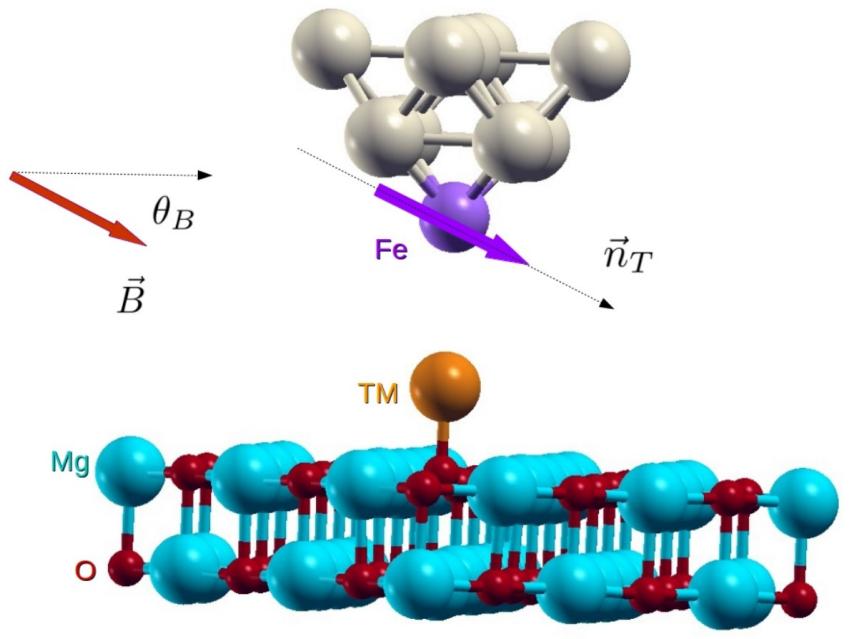
*Experimentos (muy) recientes
muestran dos picos
(barriendo en frecuencia).*

*Curiosamente uno de los
picos desaparece al alejar la
punta y el otro no.*

Ueeeeeee!!!!



STM-ESR: TiFe dimers at MgO



Partamos (nuevamente) desde acá:

$$\mathcal{H} = (\vec{b}_0 + \vec{b}_1)\vec{S}$$

Consideraremos al Fe como un spin Ising (TLS):

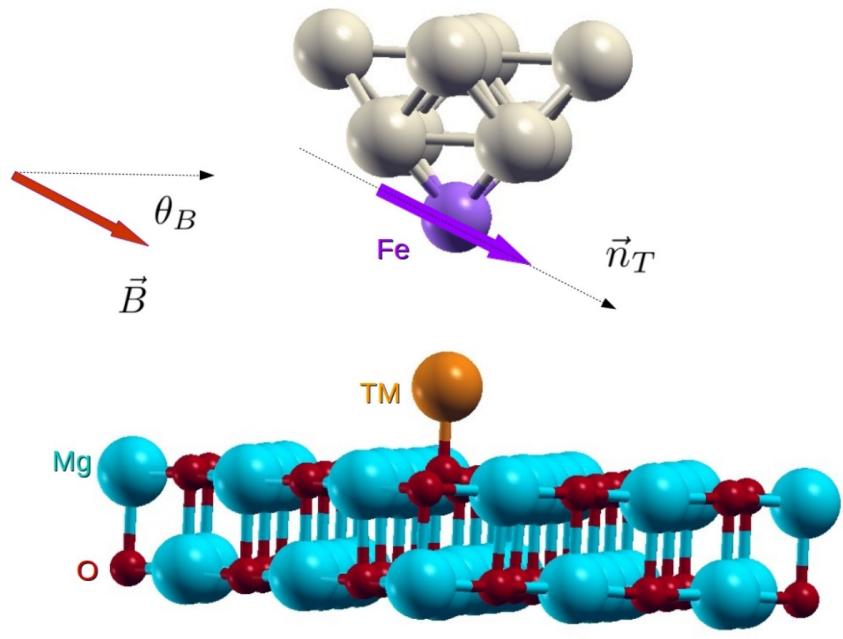
$$\vec{b}_0^\pm = (\mu_B g_x B_x + b_{Tx}, 0, \mu_B g_z B_z + b_{Tz} \pm J_{Fe})$$

donde

$$\begin{aligned}\vec{b}_T(z) &= b_T(z) \left(\sin(\theta + \delta) \hat{i} + \cos(\theta + \delta) \hat{k} \right) \\ b_T(z) &= 2\hbar J_0 e^{-(z-z_{pc})/d_{ex}}\end{aligned}$$

$$J_{Fe}(r) = J_0^{Fe} e^{-r/d_{exp}}$$

STM-ESR: TiFe dimers at MgO



Partamos desde acá:

$$\mathcal{H} = (\vec{b}_0 + \vec{b}_1) \vec{S}$$

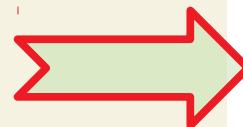
Consideremos al Fe como un spin Ising (TLS):

$$\vec{b}_0^\pm = (\mu_B g_x B_x + b_{Tx}, 0, \mu_B g_z B_z + b_{Tz} \pm J_{Fe})$$

Igual que para el Ti:

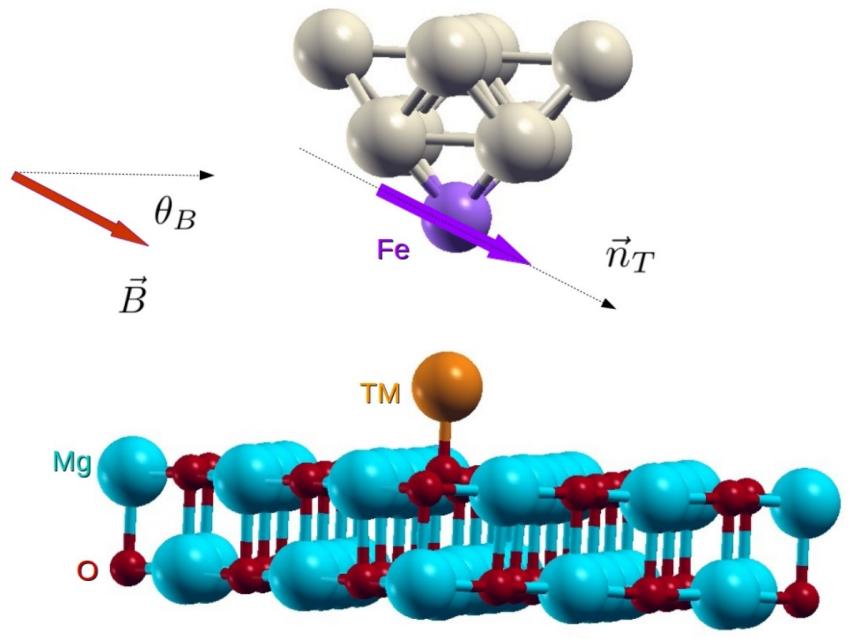
$$\vec{b}_0^\pm = b_0^\pm (\sin \theta_0^\pm, 0, \cos \theta_0^\pm)$$

$$b_0^\pm = \sqrt{(g_x \mu_B B_x + b_{Tx})^2 + (g_z \mu_B B_z + b_{Tz} \pm J_{Fe})^2}$$



$$|+\rangle = \cos \frac{\theta_0^\pm}{2} |\uparrow\rangle + \sin \frac{\theta_0^\pm}{2} |\downarrow\rangle$$
$$|-\rangle = \sin \frac{\theta_0^\pm}{2} |\uparrow\rangle - \cos \frac{\theta_0^\pm}{2} |\downarrow\rangle$$

STM-ESR: TiFe dimers at MgO



Ahora lo hacemos “mejor” que antes.

El campo electrico de la punta mueve ambos átomos. Los átomos no se mueven de la misma forma.

Se modula el exchange Ti-Tip y el exchange Ti-Fe.

Partamos desde acá:

$$\mathcal{H} = (\vec{b}_0 + \vec{b}_1) \vec{S}$$

Ahora el término de driving!

$$\mathcal{H} \approx \mathcal{H}_0 + z(t) \frac{\partial \mathcal{H}}{\partial z} \Big|_{z=0}.$$



$$\vec{b}_1 = \pm \vec{b}_{1Fe} + \vec{b}_{1tip}$$

$$\vec{b}_{1tip} = \frac{\partial \vec{b}_{tip}}{\partial z} g_0$$

$$\vec{b}_{1Fe} = \frac{\partial J_{Fe}}{\partial z} f_0 \hat{k}$$

STM-ESR: TiFe dimers at MgO

Volvamos a Calcular Rabi:

$$\Omega_{\pm} = \langle +|\vec{b}_1 \vec{S}|-\rangle$$

STM-ESR: TiFe dimers at MgO

Volvamos a Calcular Rabi:

$$\Omega_{\pm} = \langle + | \vec{b}_1 \vec{S} | - \rangle$$

Usando

$$|+\rangle = \cos \frac{\theta_0^{\pm}}{2} |\uparrow\rangle + \sin \frac{\theta_0^{\pm}}{2} |\downarrow\rangle$$
$$|-\rangle = \sin \frac{\theta_0^{\pm}}{2} |\uparrow\rangle - \cos \frac{\theta_0^{\pm}}{2} |\downarrow\rangle$$

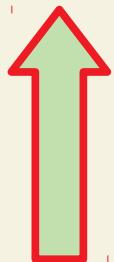
$$\langle + | S_z | - \rangle = \frac{1}{2} \sin \theta_0^{\pm}$$

$$\langle + | S_x | - \rangle = -\frac{1}{2} \cos \theta_0^{\pm}$$

$$\Omega_{\pm} = -\frac{\partial b_{Tx}}{\partial z} g_0 \cos \theta_0^{\pm} + \left(\frac{\partial b_{Tz}}{\partial z} g_0 \pm \frac{\partial J_{Fe}}{\partial z} f_0 \right) \sin \theta_0^{\pm}$$

STM-ESR: TiFe dimers at MgO

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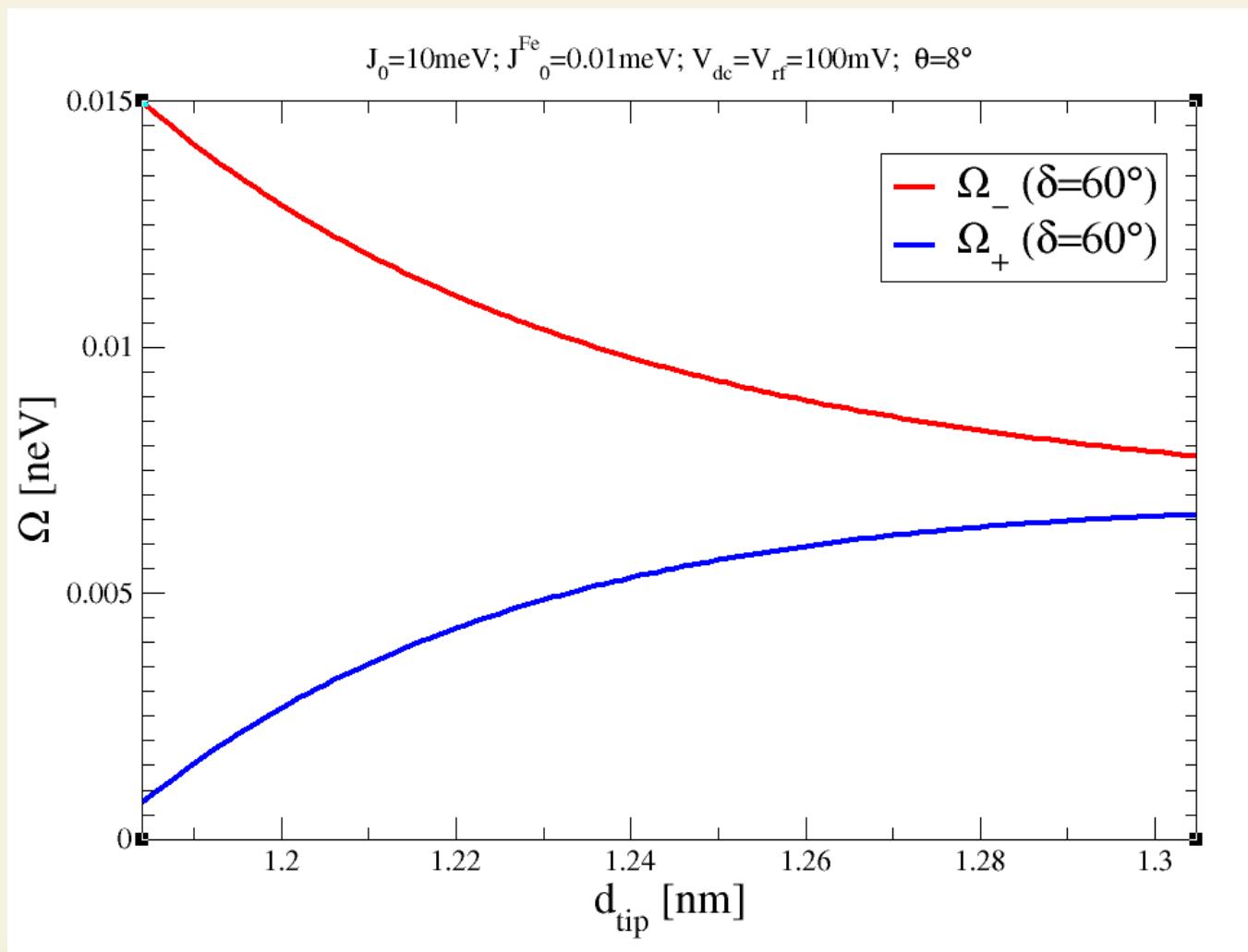


$$\sin \theta_0^{\pm} = \frac{g_x \mu_b B_x + b_{Tx}}{\sqrt{(g_x \mu_b B_x + b_{Tx})^2 + (g_z \mu_B B_z + b_{Tz} \pm J_{Fe})^2}}$$

$$\cos \theta_0^{\pm} = \frac{g_z \mu_B B_z + b_{Tz} \pm J_{Fe}}{\sqrt{(g_x \mu_b B_x + b_{Tx})^2 + (g_z \mu_B B_z + b_{Tz} \pm J_{Fe})^2}}$$

STM-ESR: TiFe dimers at MgO

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Concluding Remarks

- Podemos (lo hemos hecho) estudiar diferentes mecanismos en los experimentos ESR. Santiago nos va a mostrar, en su seminario, los detalles “oscuros” en un experimento de ESR en Fe.
- Entendemos el rol de diversos factores como, por ejemplo, las diferentes anisotropías (punta o g). Existen varias cosas que aún se escapan a nuestro entendimiento. La influencia del Spin Orbita es algo poco analizado hasta el momento. Alba se encuentra jugando con otros átomos depositados en MgO esperando que un mayor SO cambie cualitativamente las cosas.
- Trabajos en cadenas hay pocos (además de nuestro prl):

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Probing resonating valence bond states in artificial quantum magnets

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Free coherent evolution of a coupled atomic spin system initialized by electron scattering

Lukas M. Veldman, Laëtitia Farinacci, Rasa Rejali, Rik Broekhoven, Jérémie Gobéil, David Coffey, Markus Ternes, Alexander F. Otte

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- Trabajos en cadenas hay pocos.

Nosotros estamos trabajando (con Omar, Pablo (Serra), Sergio y Diego) en control en cadenas infinitas. Es tiempo de prestar atención a cadenas más chicas que se puedan realizar experimentalmente!

Ademas continuamos colaborando en cadenas (Dimeros y Trimeros) con la gente de IBM.

GRACIAS!!

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