# Investigaciones recientes en nanoestructuras magnéticas

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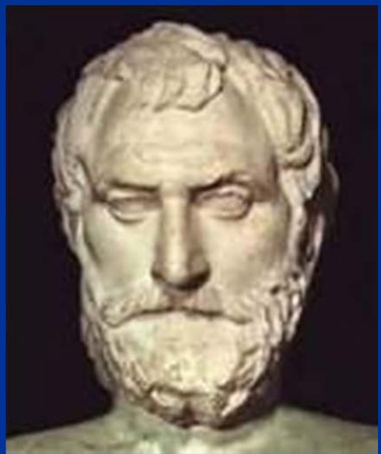
0 500 1000 1500

- Nombre: Magnes (Pastor de Magnesia)
- Plinio el Viejo (Historiador Romano)



**Tales de Mileto**
**(624 – 546 a. De C)**

Magnetita $Fe_3O_4$

**Escuela Animista** ◘, imán “tiene alma”

~100 AD Primer brújula en China


**Describe una brújula flotadora y con un punto como pivote**

*(Actum in castris, in obsidione Luceriæ)*

**?**

**(1269)**

**Pierre de Maricourt**

**(Petrus Peregrinus de Maricourt)**

Epistola de Magnete

Propuso dispositivos de levitación


William
Gilbert
(1544 – 1603)

- **Médico de la Reina Isabel (De Magnete)**
- **Muchas substancias son eléctricas, se crea una fuerza**
- **La tierra es un grán magneto (“Magnus magnes ipse est globus terrestris”)**

**<<<<<<<<<tres maneras de magnetizar:**

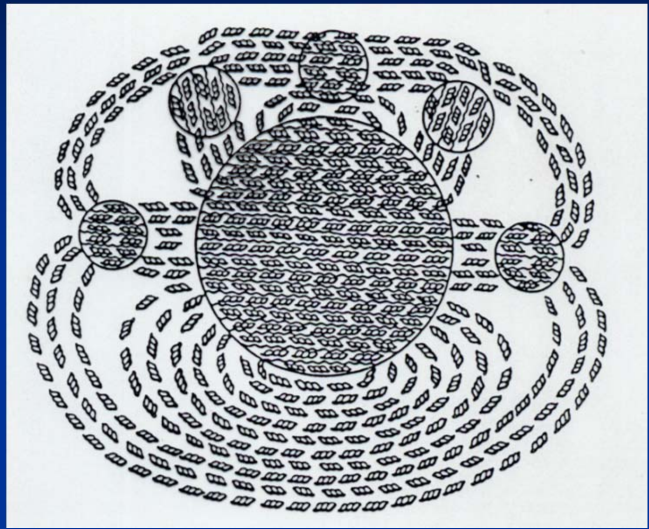
**Tocando un objeto de hierro, niquel o cobalto con un imán,**

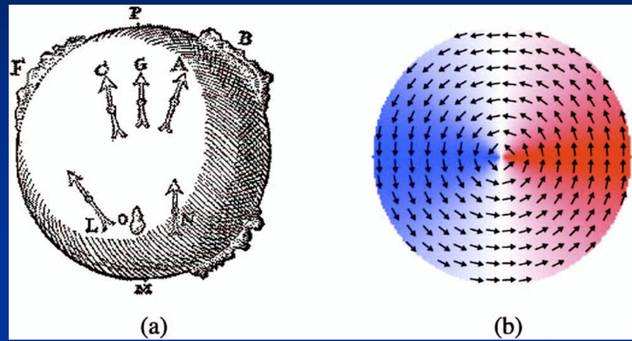
**Enfriando esos objetos orientados en la dirección Norte Sur.**

**Exponer una aguja de esos materiales por un período largo de tiempo con la orientación Norte-Sur**

- **Gilbert inició la era de la Física Moderna y la Astronomía (Kepler, Galileo, Newton)**

*(parties cannelées)*






Gilbert, Descartes 1600 2011

Descartes, Tierra Magneto Gigante (1596-1650)

14 ordenes de magnitud

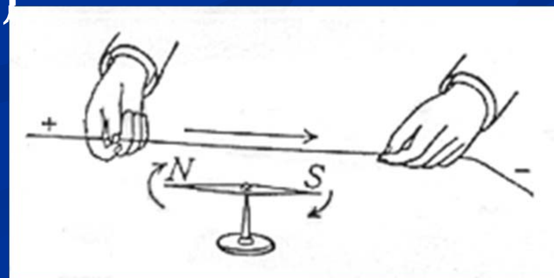
Exorcizó a los imanes del “alma”



**Hans Christian Oersted**

**(1777 – 1851)**

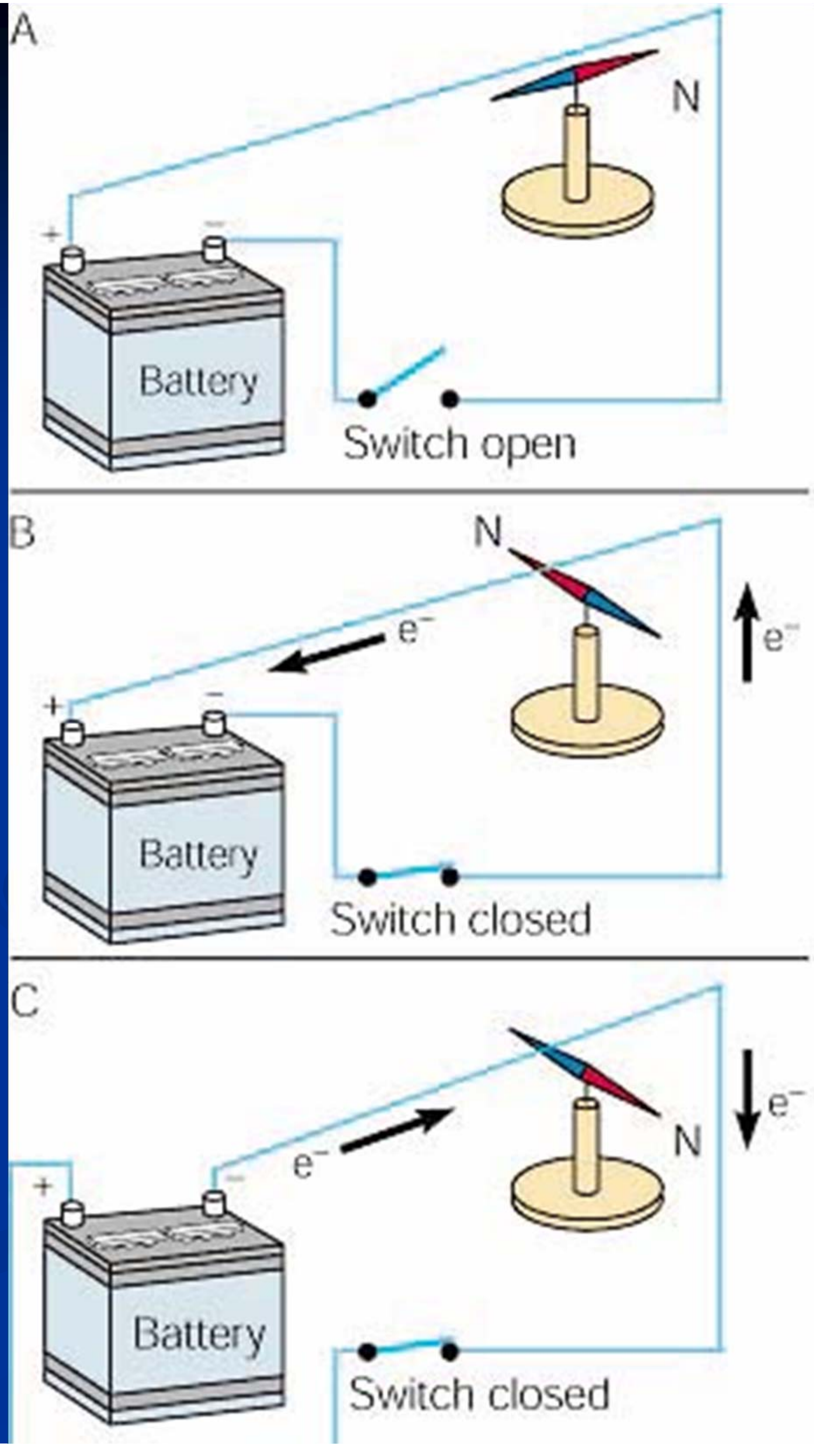
**(1820)**



Oersted descubrió que la aguja de una brújula debajo de un alambre (A) apuntaba al norte cuando no había corriente, (B) se movía a la derecha cuando una corriente fluía en una dada dirección,

y

(C) Se movía en dirección opuesta cuando la corriente se revertía




*"…<<<fracasos son tan importantes como los éxitos..."*

- **1831 Inducción electromagnética, el movimiento de imanes produce electricidad**

**motores/generatores (50-100 años después)**

**Michael Faraday**
**(1791 – 1867)**

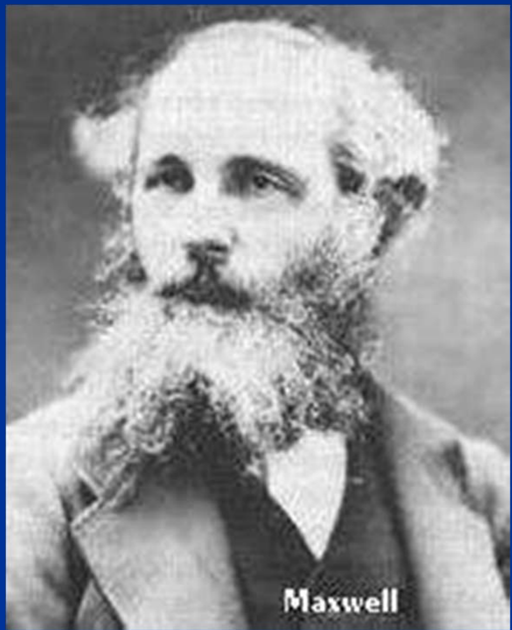
Si electricidad produce magnetismo:
"Porqué no magnetismo produce electricidad??"

**Joseph Henry (1797 – 1878) El Cambio en campos magnéticos puede producir corrientes. Describió la Inductancia**

Bobina rotada

Entre los polos de un magneto

**Heinrich Lenz (1804 – 1865)**


**James Clerk Maxwell**
**(1831 – 1879)**

$$\vec{\nabla}\vec{D} = 4\pi\rho$$

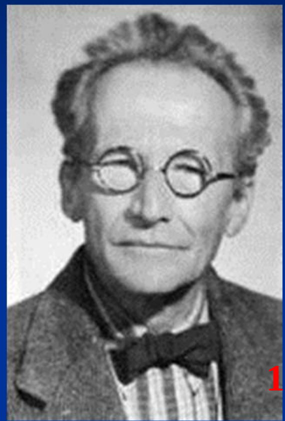
$$\vec{\nabla}x\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t}$$

$$\vec{\nabla}\vec{B} = 0$$

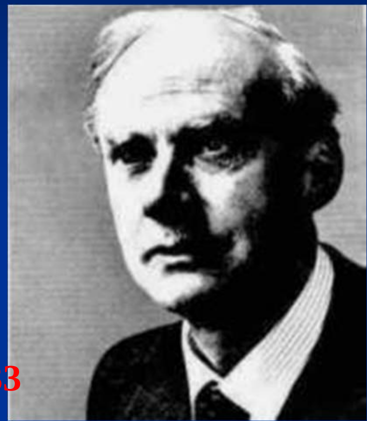
$$\vec{\nabla}x\vec{H} = -\frac{1}{c}\frac{\partial\vec{D}}{\partial t} + \frac{4\pi}{c}\vec{J}$$



**L.de Broglie (1892 – 1987)**



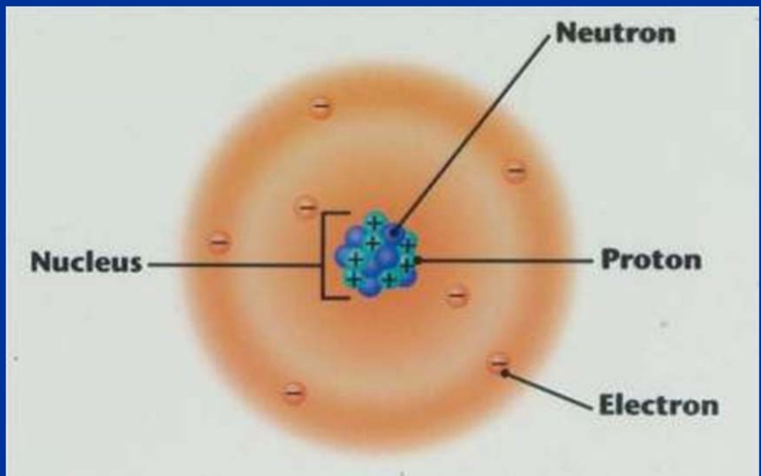

**E. Schrödinger (1887 – 1961)**



**P.A.M. Dirac (1902 – 1984)**


**W. Pauli (1900 – 1958)**


**W. Heisenberg (1901 – 1976)**

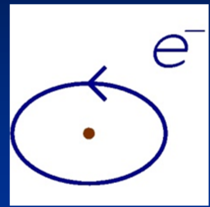



Teoría Cuántica

Espín Uhlenbeck, Goudsmit
Stern-Gerlach

# Fuentes del Magnetismo

1.- Magnetismo Orbital

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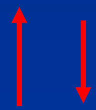
2.- Magnetismo del espín



S

**Naturaleza: Mecánica Cuántica y Relativista**

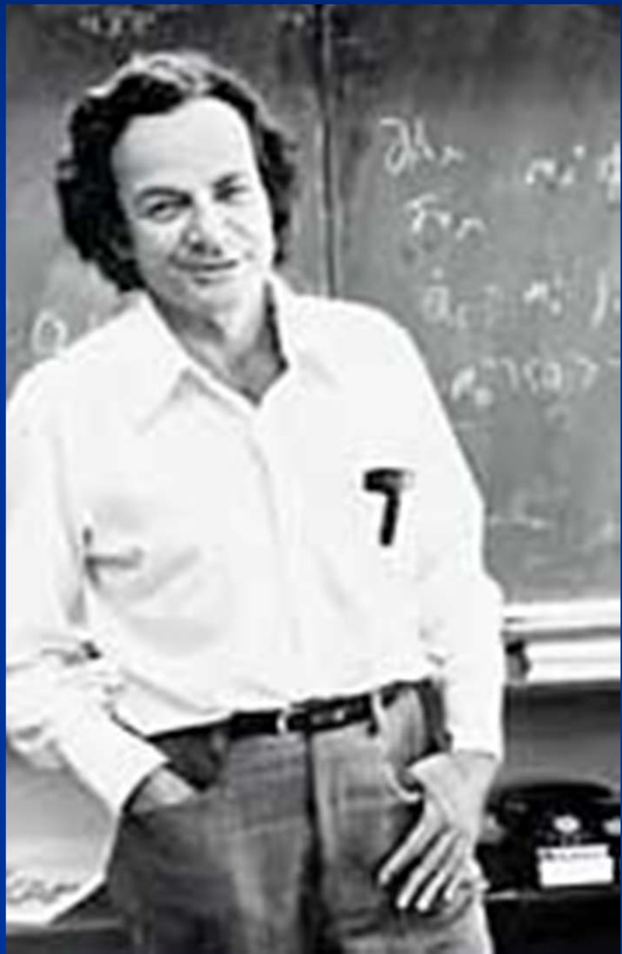
Propiedades Magnéticas: No se produce por la superposición de contribuciones individuales

# Porque es importante estudiar las nanoestructuras?

↓

**En particular, las propiedades magnéticas**

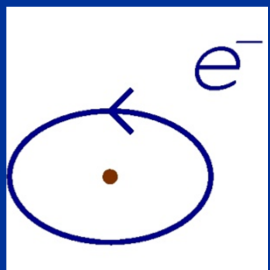
# *There´s plenty of room at the botttom*



- Manipular y controlar a escala atómica
- Información a escala nanoscópica, computadoras, etc.
- Arreglos atómicos?

Propiedades Magnéticas: Sensibles al entorno
(temperatura, estructura, correlaciones electrónicas)

i.e. Fe (fcc) AF
Fe (bcc) FM
(Volumen)




Atomo

Nanostructuras ???

Solido

(Grupo de Fe)

Magnetismo Localizado

Mayoría de los átomos son magnéticos

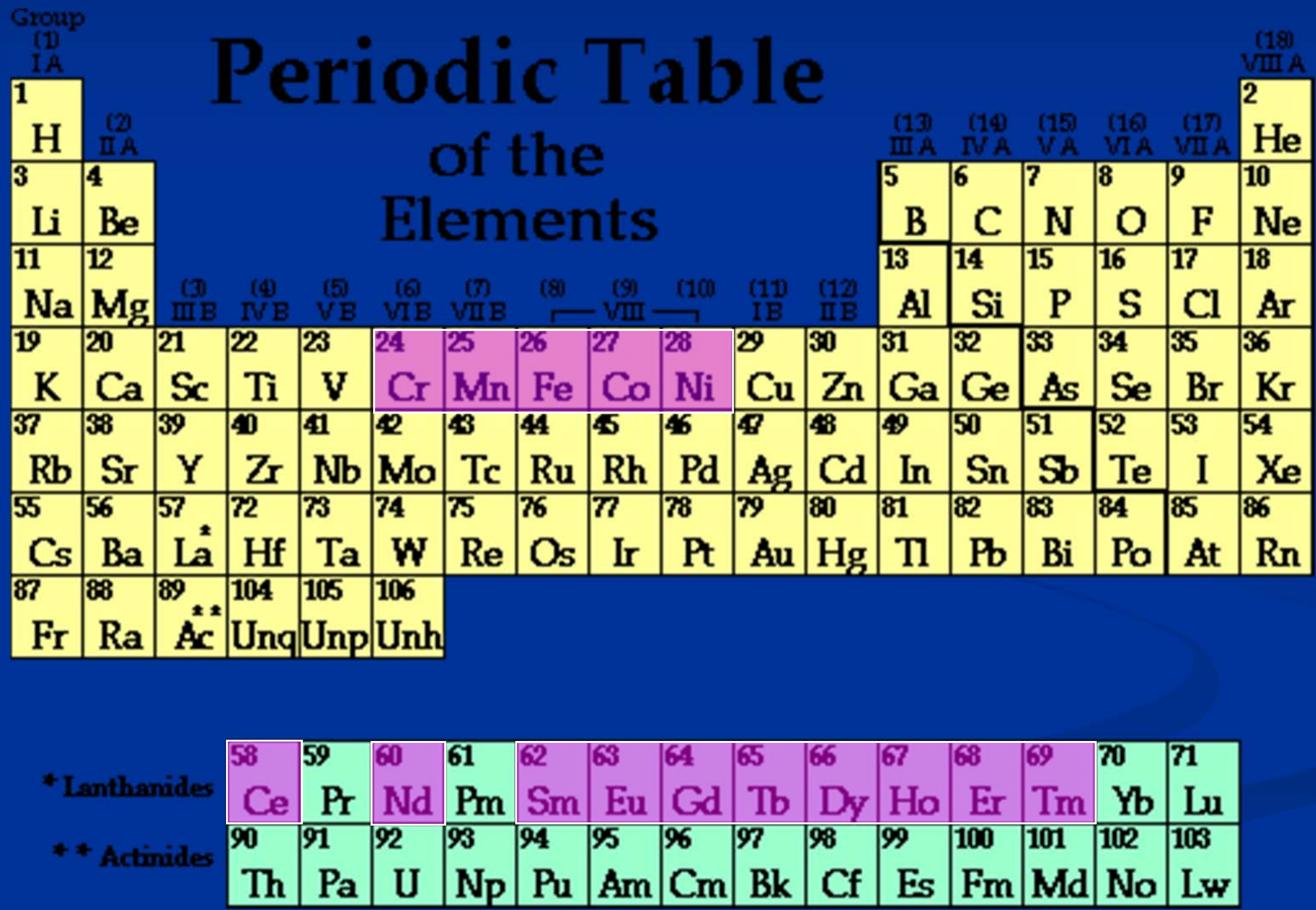
Magnetismo Itinerante

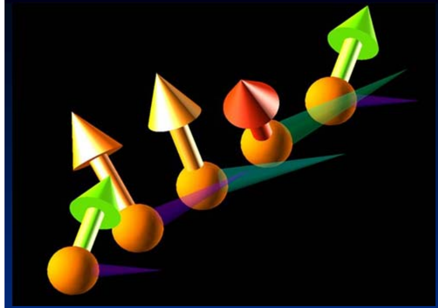
Pocos sólidos son magnéticos

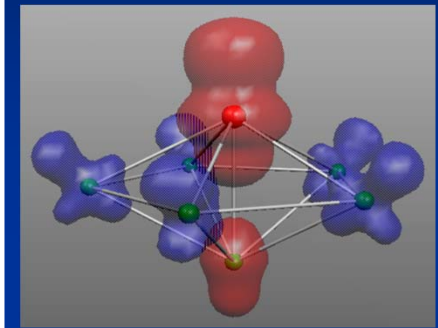
## Elementos con orden magnético

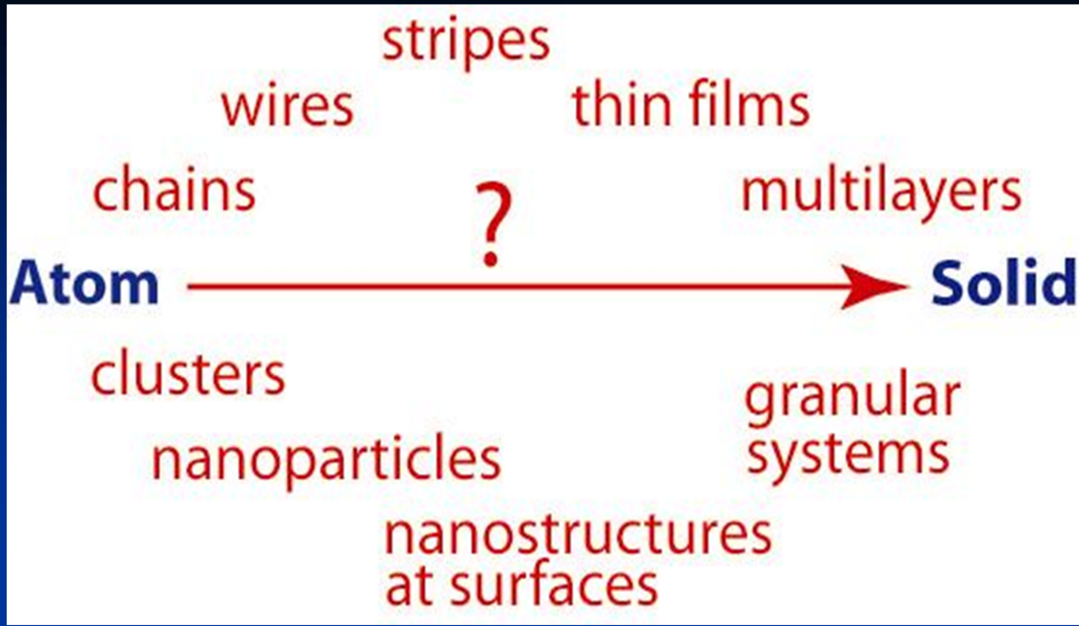
3*d*- metals: Cr, Mn, Fe, Co, Ni

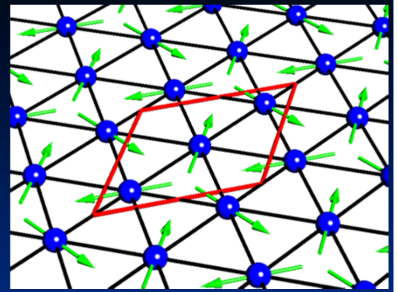
4*f*- metals: Ce, Nd, Sm, Eu, Gd, Th, Dy, Ho, Er, Tm

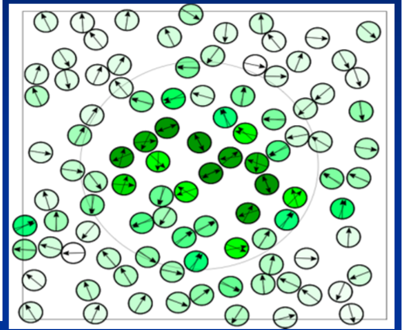










Why magnetism?

* Technological applications → major driving force

High density recording media (→ single particle bit)

New materials with enhanced read/write performance, Spintronic devices (MRAM)

Medicine (hyperthermia cancer therapy)

* Fundamental research

Magnetism is a cooperative many-body phenomenon

Size and dimensionality, number of electrons and correlations, Temperature, Disorder

Atomic magnetism (localized) ≠ Bulk magnetism (itinerant in TM)

Strong local environment dependence (coordination number, chemical environment, etc.)

Proximity effects with nonmagnetic materials (polarization vs screening)

# Importancia Económica

Tecnológica (200,000,000,000.00 USD, en sistemas de grabación)

# Motivación:Dispositivos de almacenamiento

En la actualidad, existe gran interés por fabricar dispositivos de almacenamiento cada vez con mayores densidades de grabación.

1955 (IBM)
capacidad de almacenamiento: 5 Mbits
densidad de grabación: 2 kbits/ $in^2$

Tamaño de las partículas

~ **micrometros**

En 1979 el disco duro era de 5Mb (12" diametro ..30.5 cm!!!)


Creado en los 70's

Discos 5.25"

Doble densidad 360 kB

Alta densidad 720 kb

2002
densidad de grabación: **100 Gbits/ $in^2$**

tamaño de las partículas: **10 nm**


**Hoy alcanzan de 200 TB por pulgada cuadrada (grabación longitudinal)**

- Manganese Nanostructures
  - Manganese dimer and small clusters
  - Two dimensional Heusler Alloys

- Cobalt Nanowires with complex structures
- Chemical and magnetic order in bimetallic nanoclusters

# Mn is a unique transition metal element with fascinating magnetic properties

- The description of Mn has been in general a difficult problem.

- The atomic electronic configuration is $3d^5s^2$ with a $\mu=5\mu_B$

- The unfilled subshell lies 2.14 eV above the occupied and the atomic moment is resilient to minor changes.

- The atomic moment is conserved in doped semiconductors and couple ferromagnetically.

- Dilute solutions of Mn in Cu behave like a spin glass.

- Is $Mn_2$ van der Waals bonded with AF or FM coupling?

# Magnetic properties of small Mn clusters

J. Mejía-López, A.H. Romero, M.E. García, and J.L. Morán-López

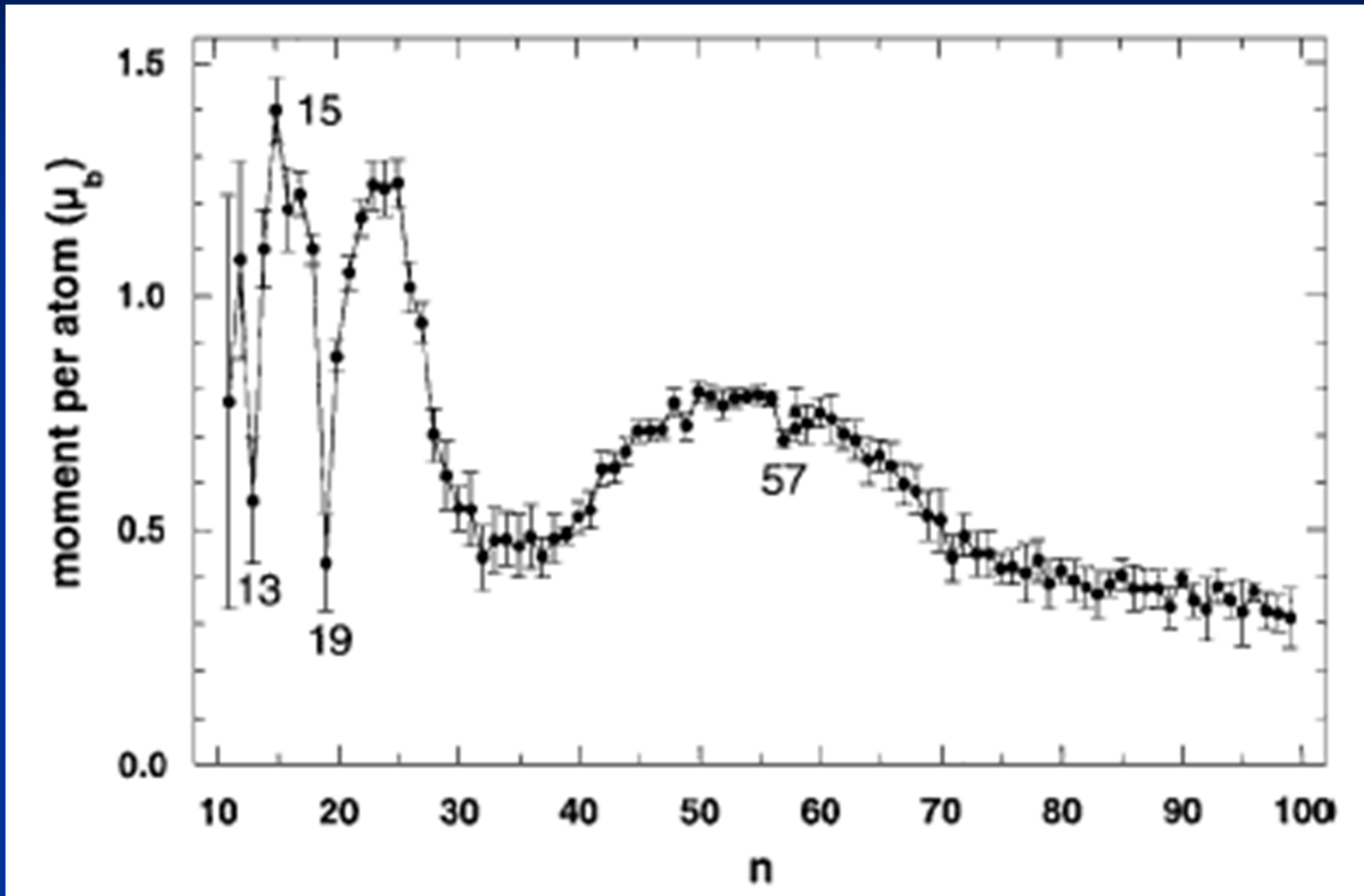
Universidad Católica de Chile

Universidad de Kassel, Alemania

CINVESTAV, Unidad Querétaro

Facultad de Ciencias, UNAM

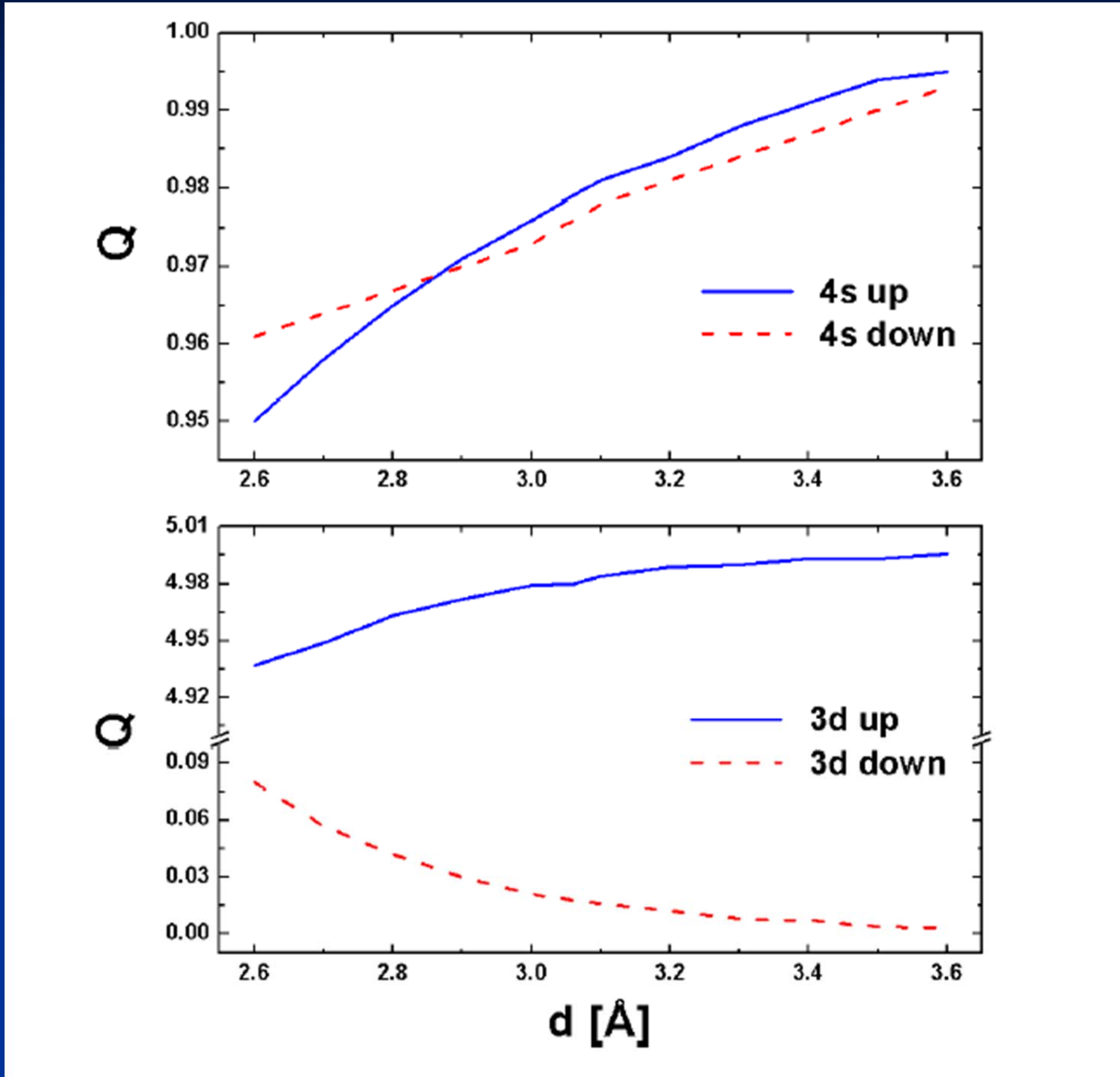
## Magnetic properties of small Mn-clusters

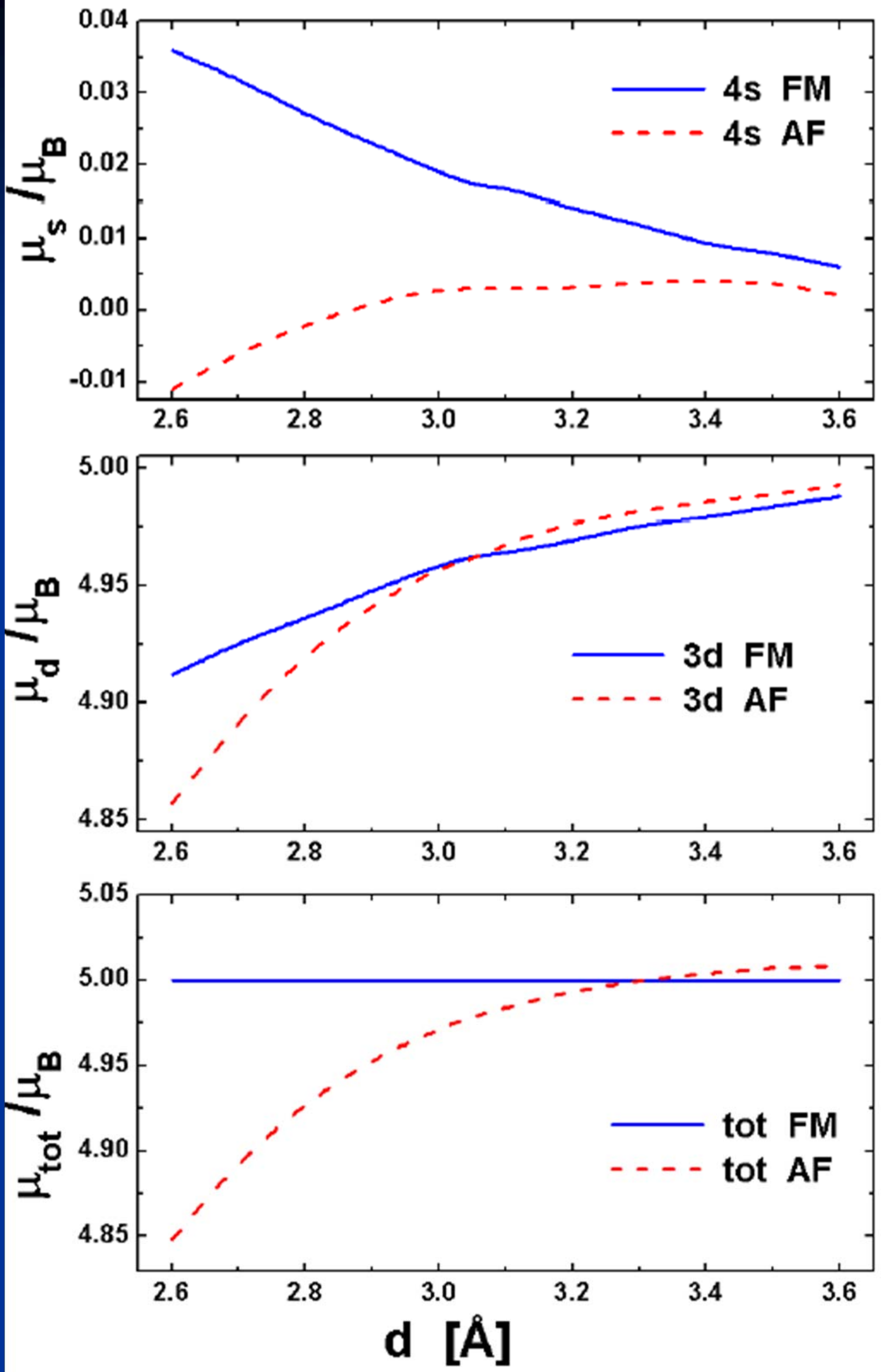



Experiment:
Knickelbein, PRL **86**, 5255 (2001)

Phys. Rev. B 70, 014424 (2004)]

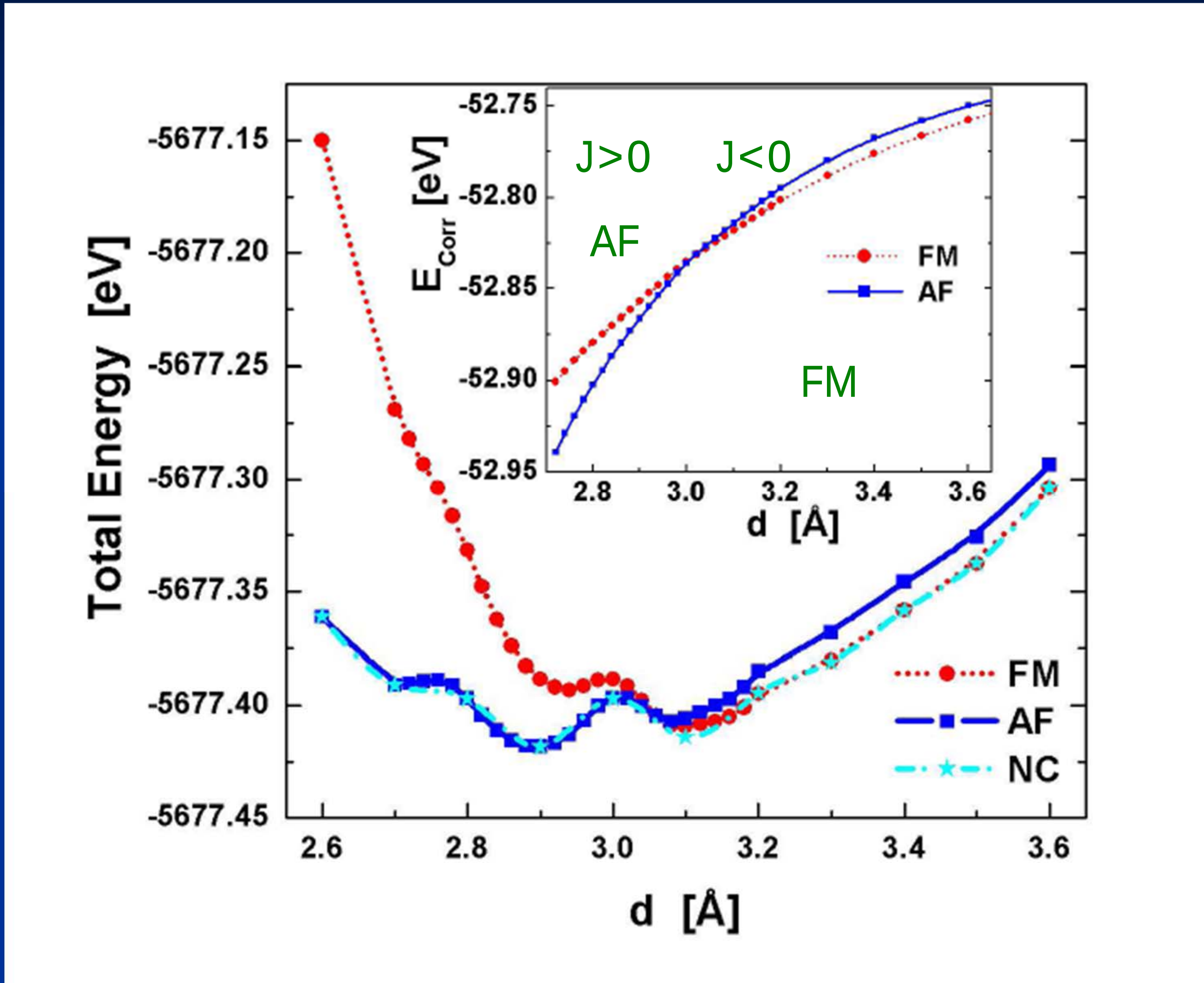
# Antifferomagnetic arrangement






Magnetic moments as a function of the distance

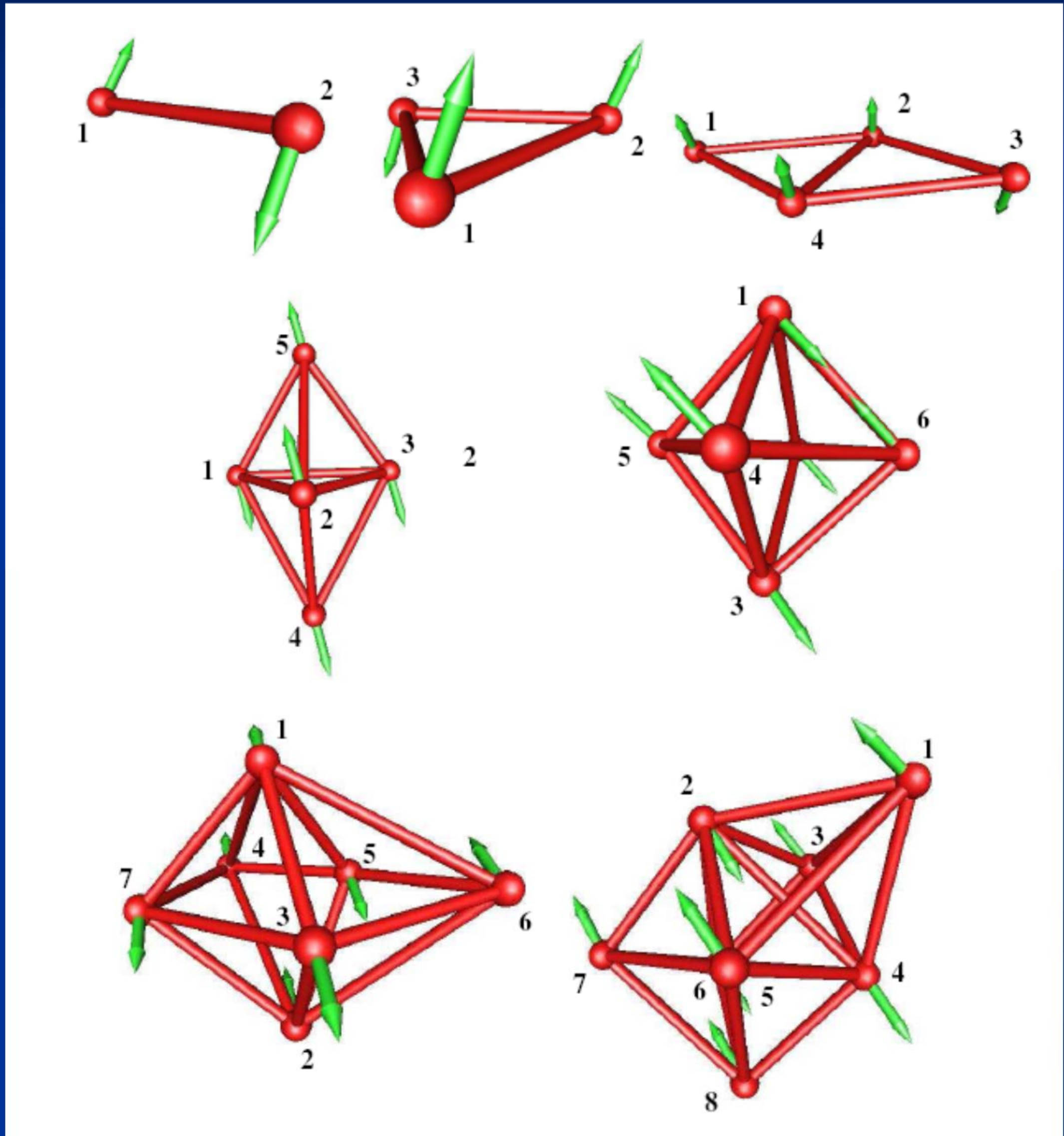
Correlation energy as a function of distance

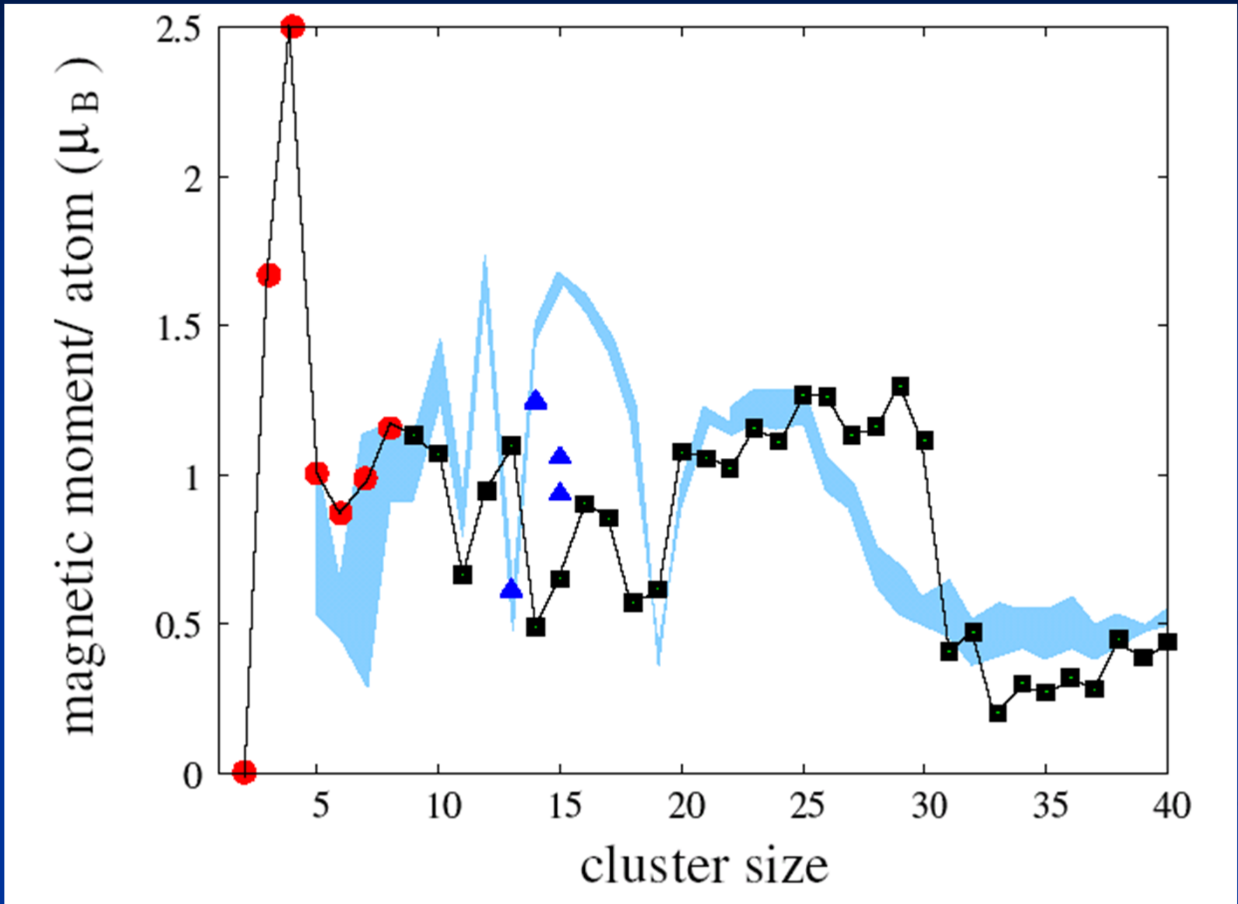



~ 3.06 Å

Total electronic energy of Mn2 as a function of interatomic distance for Non-collinear, ferromagnetic and antiferromagnetic arrangements

# **Results:** small clusters






Red circles: ab-initio results

Black squares: effective Spin Hamiltonian

Blue triangles: isomers with Lower cohesive energy

Lightblue shadow: Experimental Results including error bars

Good agreement with experiment
(order of magnitude and size dependence)

# Conclusions

- Mn clusters exhibit a delicate balance between kinetic, exchange and correlation energies
- At short distances the electron transfer between 4s and 3d stabilizes the antiferromagnetic coupling.
- The properties are dominated by spin frustration due to the presence of different spin-spin coupling constants , which leads to noncollinear magnetism.
- This leads to the formation of magnetic nanodomains
- The change in magnetic behavior at atomic distances close to those of equilibrium leads to complex magnetic structures, which may explain the **multifarious** behavior of Mn systems

- Noncollinear magnetism, spin frustration and magnetic nanodomains
- in small $Mn_n$ clusters

J. Mejía-López, A.H. Romero, M.E. García, and J.L. Morán-López
Physical Review B, Rapid Communications, 74, 140405 (2006)

# Monoatomic and Dimer Mn Adsorption on Au(111)

Francisco Muñoz,, A.H. Romero, J. Mejía-López, and
J.L. Morán-López
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CINVESTAV, Unidad Querétaro
Facultad de Ciencias, UNAM

# Caracterización de la superficie (111) de Oro

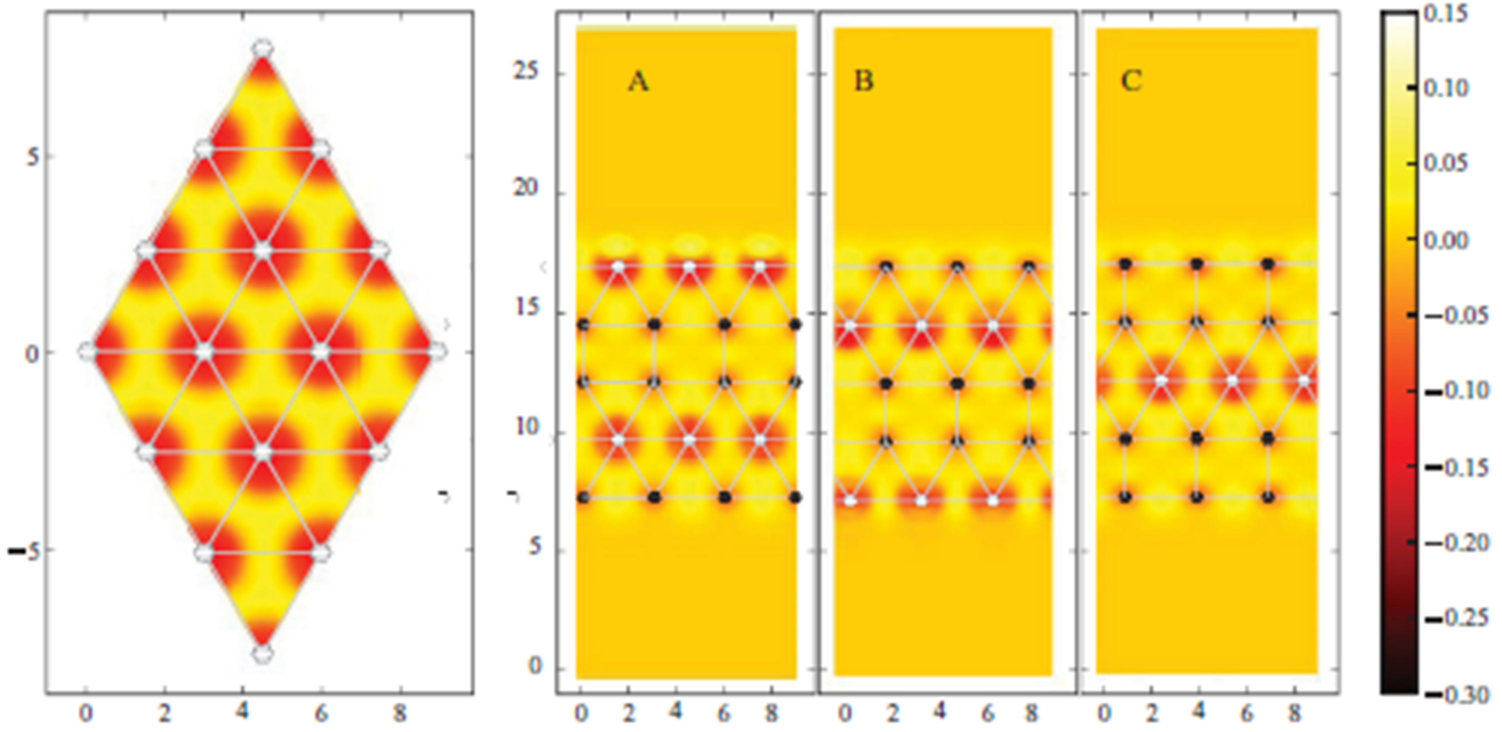



FIG. 1. (Color online) Charge redistribution $\delta\rho$ of a Au(111) relaxed surface. The left-hand image shows the topmost surface plane passing through the relaxed surface atoms. The images A, B, C show the electronic redistribution at planes perpendicular to the surface and passing through the atoms of the three different layers (ABC fcc stacking). The distances are in Å, and the color bar in $e/Å^3$.

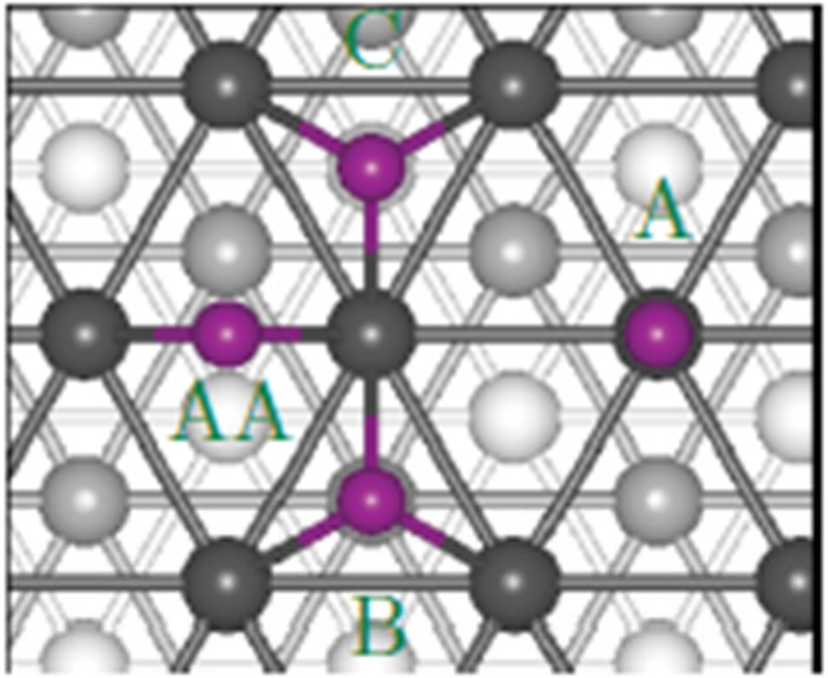



FIG. 2. (Color online) Adsorption sites on a fcc (111) surface. The site of type A is on the top of a surface atom, B and C, are above the surface and coordinated to three surface atoms, and AA is bonded to two surface atoms. The difference between B and C is that B has a Au neighbor in the second layer while C does not.

TABLE II. Adsorption energy in eV, the Mn magnetic moment in $\mu_B$, and the distance between the Mn atom and the surface plane ($d_{Mn\text{-}surf}$) in Å.

| Site | $E_A$ | $\mu$ | $d_{Mn\text{-}surf}$ |
|---|---|---|---|
| A | −1.95 | 5.07 | 2.44 |
| AA | −2.73 | 4.83 | 2.52 |
| B | −2.80 | 4.83 | 2.58 |
| C | −2.81 | 4.82 | 2.58 |

# Distribución electrónica

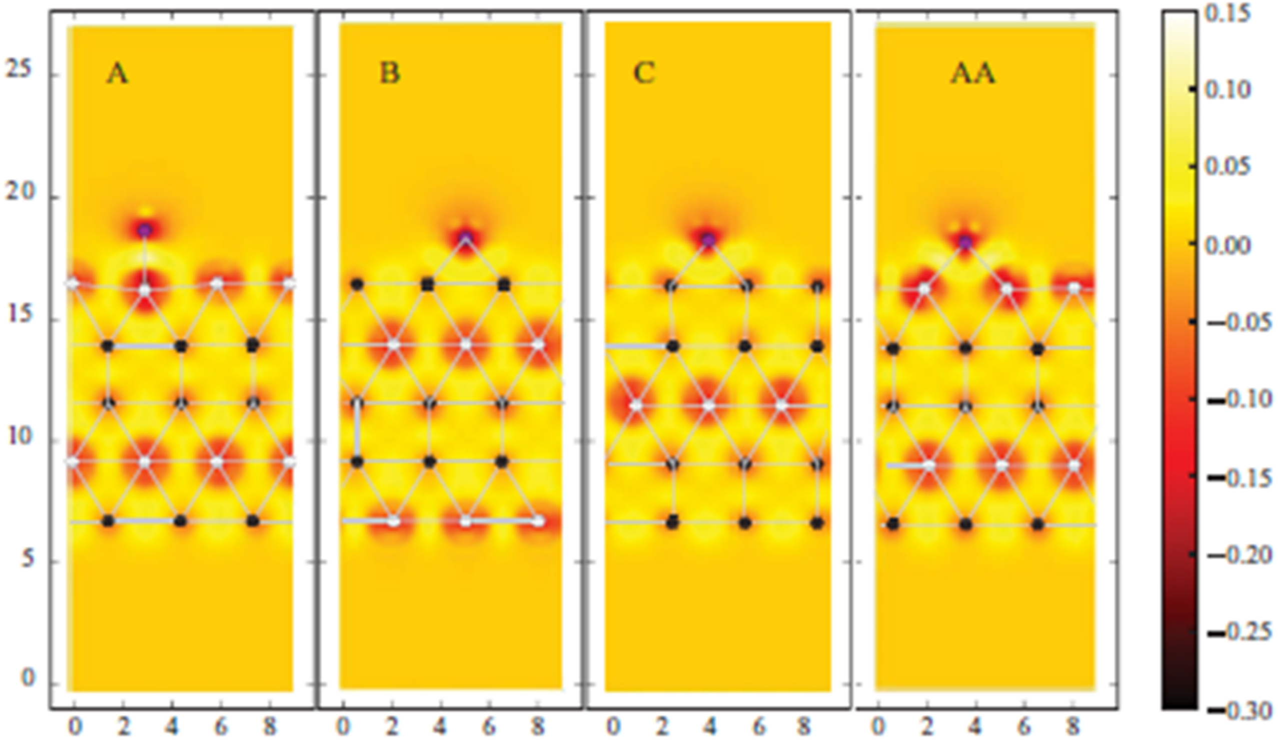



FIG. 3. (Color online) Charge redistribution $\delta\rho$ for each adsorption site of a (111) Au surface. The red circles denote the Mn and the substrate atoms located at the same plane. The distances are in Å, and the color bar in $e/\text{Å}^3$.

# Geometrías de adsorbción del dímero

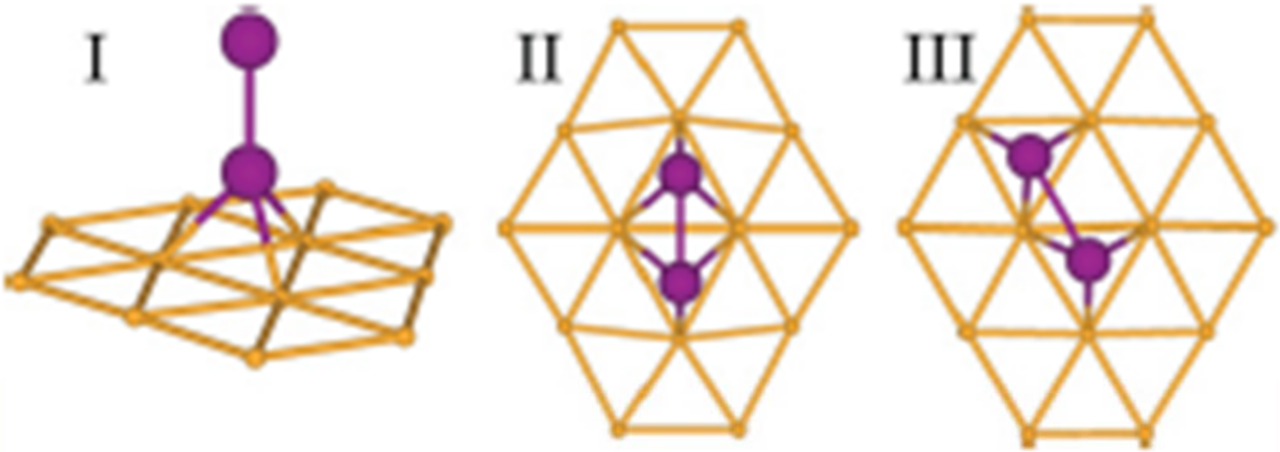



FIG. 5. (Color online) Adsorption geometries considered for $Mn_2$ on a Au (111) surface. Site I correspond to the dimer chemisorbed, perpendicular to the surface, on a threefold coordinated site. In cases II and III the dimer is chemisorbed parallel to the surface, on nonequivalent and equivalent triangles, respectively.

TABLE III. $Mn_2$ adsorption on (111) Au: The adsorption energy is in eV, the magnetic moment is in $\mu_B$, the Mn-Mn bond length ($d_{Mn\text{-}Mn}$), and Mn-surface ($d_{Mn\text{-}surf}$) distances are given in Å.

| | $E_A$ | | $\mu$ | | $d_{Mn\text{-}Mn}$ | | $d_{Mn\text{-}surf}$ | |
|---|---|---|---|---|---|---|---|---|
| Site\Mag | FM | AFM | FM | AFM | FM | AFM | FM | AFM |
| I | −3.67 | −3.93 | 9.45 | 0.25 | 2.71 | 2.48 | 2.61 | 2.59 |
| II | −5.35 | −5.40 | 9.22 | 0.00 | 2.67 | 2.56 | 2.52 | 2.53 |
| III | −5.45 | −5.51 | 9.28 | 0.00 | 2.84 | 2.74 | 2.60 | 2.59 |

# Conclusiones

# Conclusiones

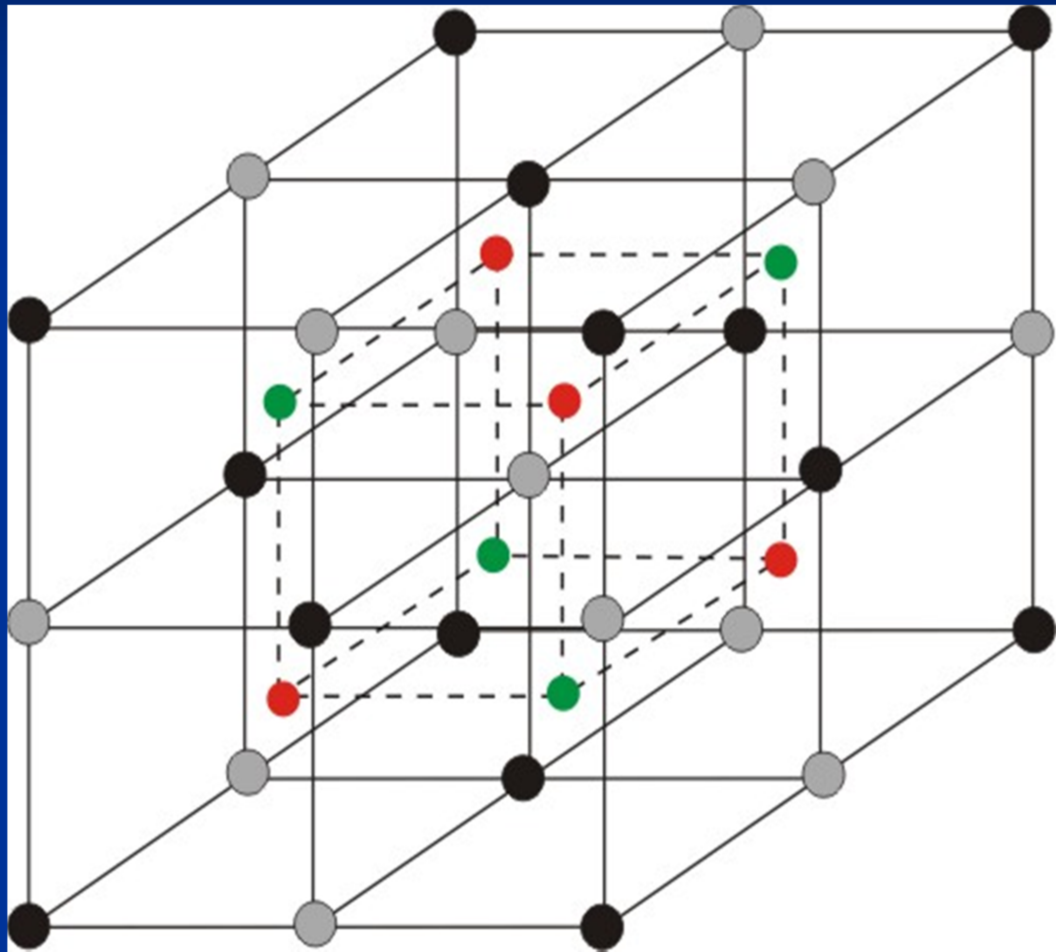
- El átomo de Mn se adorbe primordialmente en sitios del tipo C (con coordinación 3)
- En momento magnético obtenido es de 4.82 $\mu_{B.}$
- El dímero se absorbe paralelo a la superficie con sus átomos en sitios de coordinación 3.
- La orientación de los momentos magnéticos es antiparalela (acoplamiento antiferromagnético)
- En momento magnético de cada átomo es de 4.6 $\mu_{B.}$
- Energéticamente es mas favorable que el dímero se disocie.

# Two Dimensional Heusler Alloys

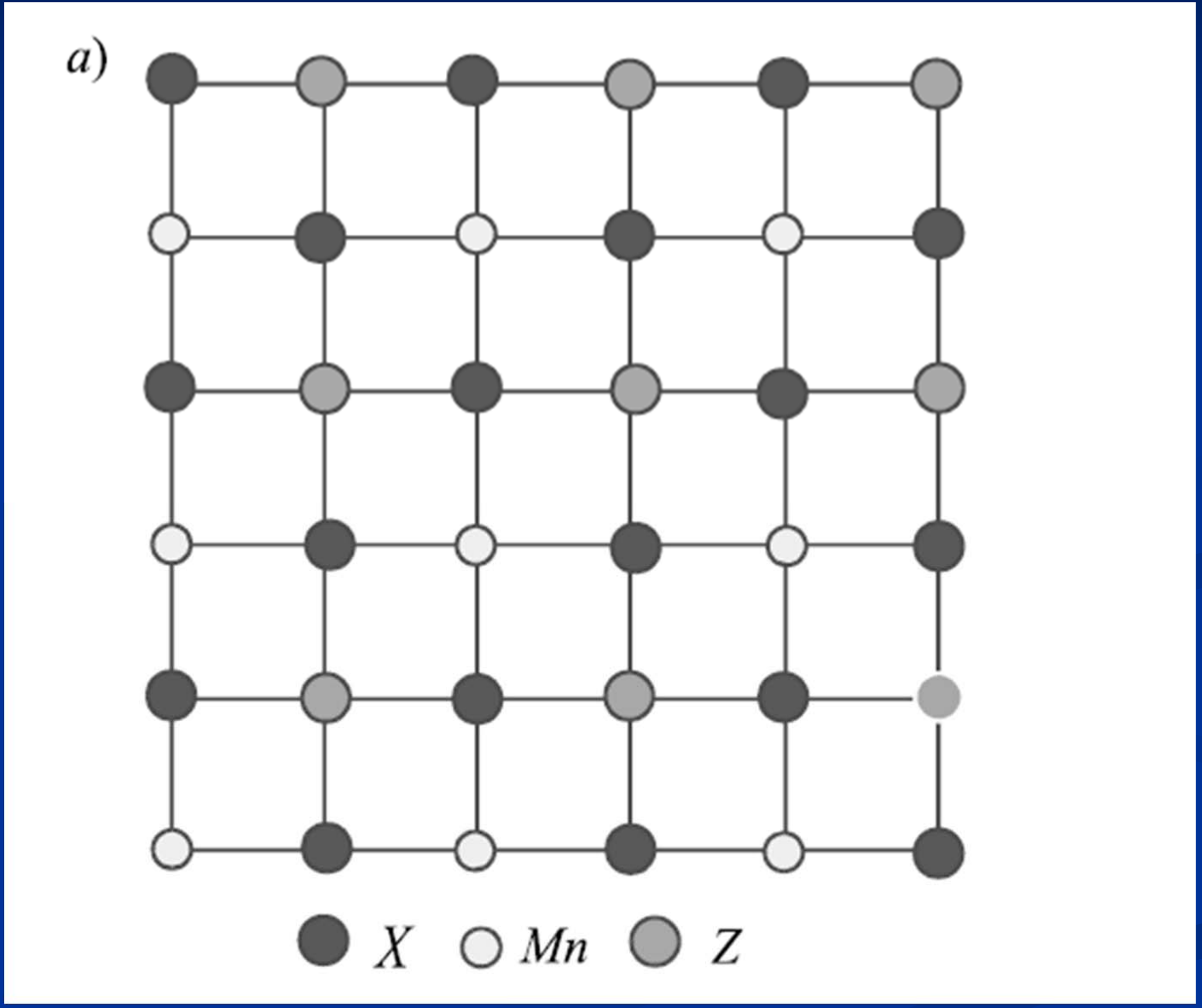
R. Rodríguez-Alba, F. Aguilera-Granja and J.L. Morán-López
Instituto de Física, Universidad Autónoma de San Luis Potosí
Facultad de Ciencias, Universidad Nacional Autónoma de México

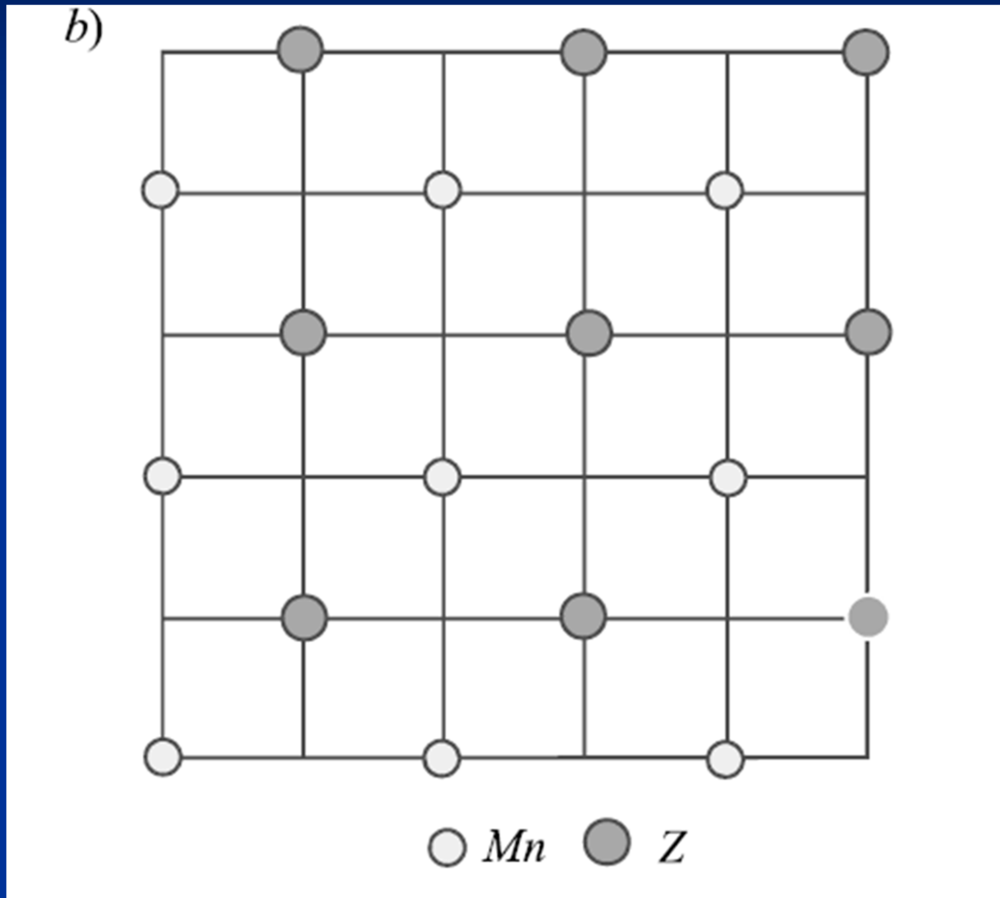
- Heusler alloys, are ternary systems X2MnZ that have been know since 1903. These systems have Mn as one of the main components and show a rich variety of magnetic phases, depending on the two other chemical components and on the temperature.
- These alloys looked very promising for applications since Mn has a magnetic moment close to 4 μB. According to a previous calculations the role of the X atoms is to determine the lattice constant and the Z atoms mediate the interactions between Mn atoms.

This structure can be described by four interpenetrating fcc Sublattices.
Two of them occupied by X transition metal atoms, Y by Mn and Z by atoms of the B subgroups 3,4, or 5

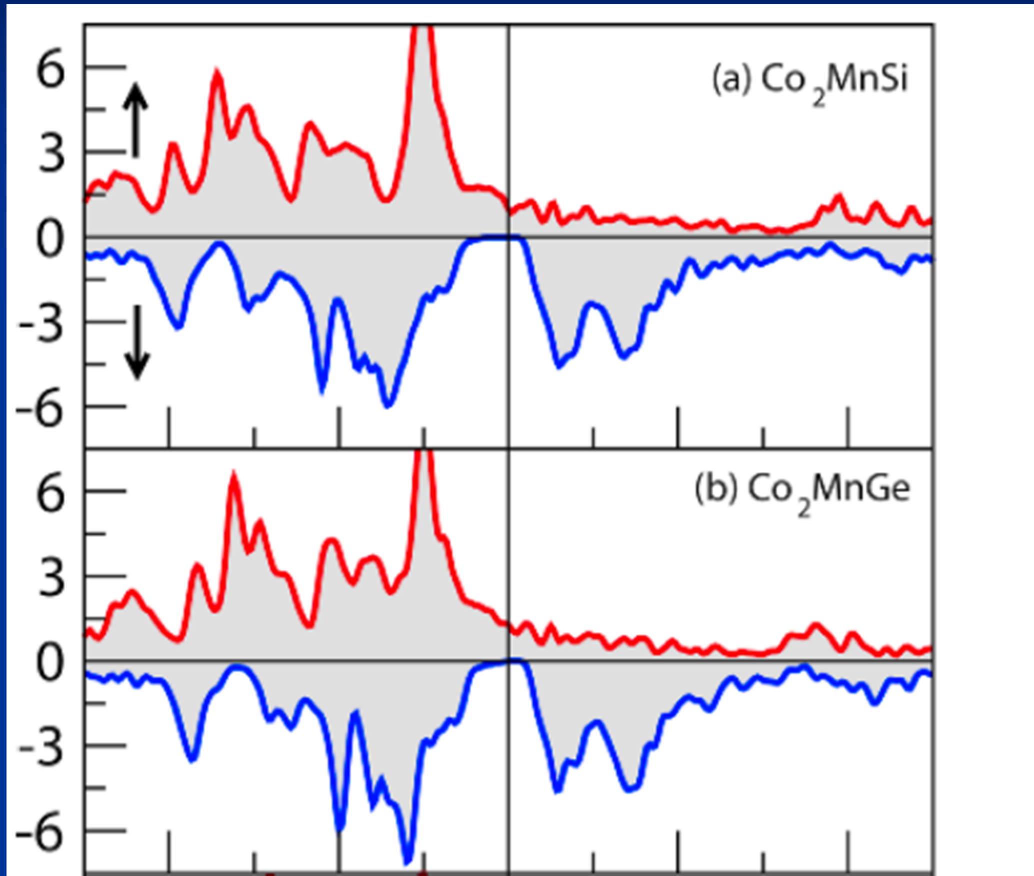


# Two dimensional Version

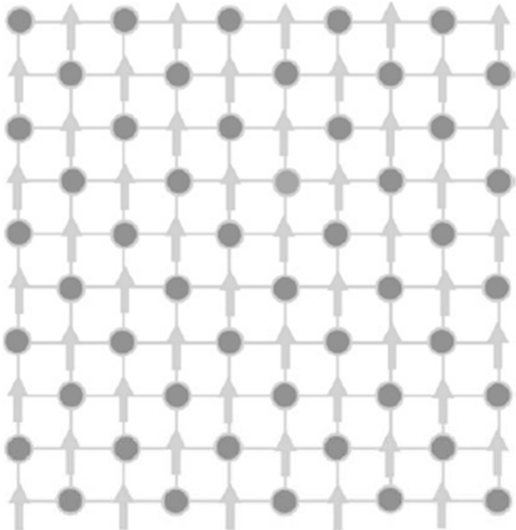



b)
Mn
Z

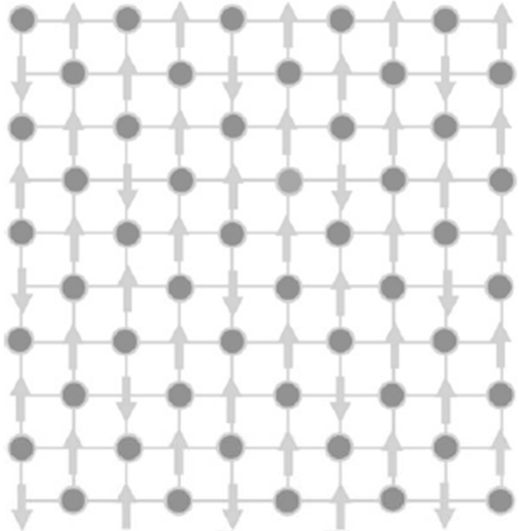
- There are more complex Heusler alloys in which the element X is also magnetic. Recently these kind of systems have been intensively studied owing to great potential for spintronics, magnetically driven actuators and shape memory materials.
- Examples: $Co_2MnGa$ and $Ni_2MnGe$. In particular, the Co alloys has a density of states that show half-metallicity. i.e. the majority and minority spin bands show a metallic and semiconductor character. This makes this alloys attractive for applications in spintronics where the capability to inject electrically spin-polarized carriers into unpolarized semiconductors is the key element. On the other hand, the Ni alloys are important as magnetic shape memory materials.



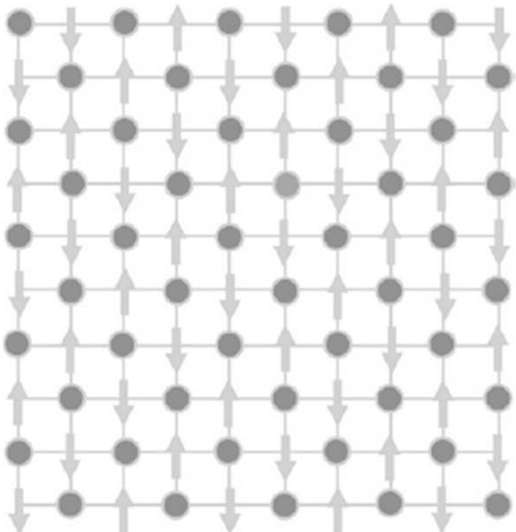
(a) Co2MnSi
(b) Co2MnGe
6
3
0
-3
-6
6
3
0
-3
-6



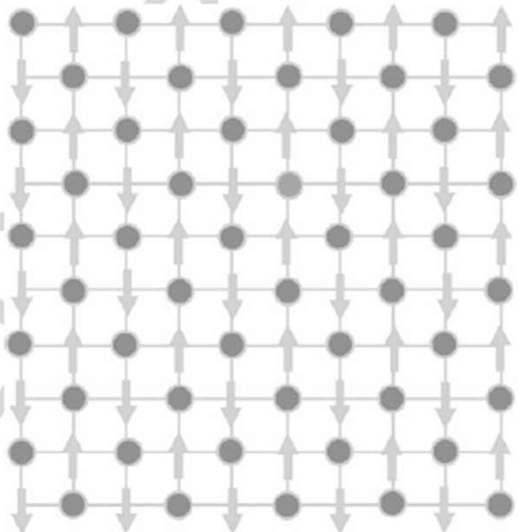
(a) Ferromagnet.



(b) Ferro–antiferromagnet.

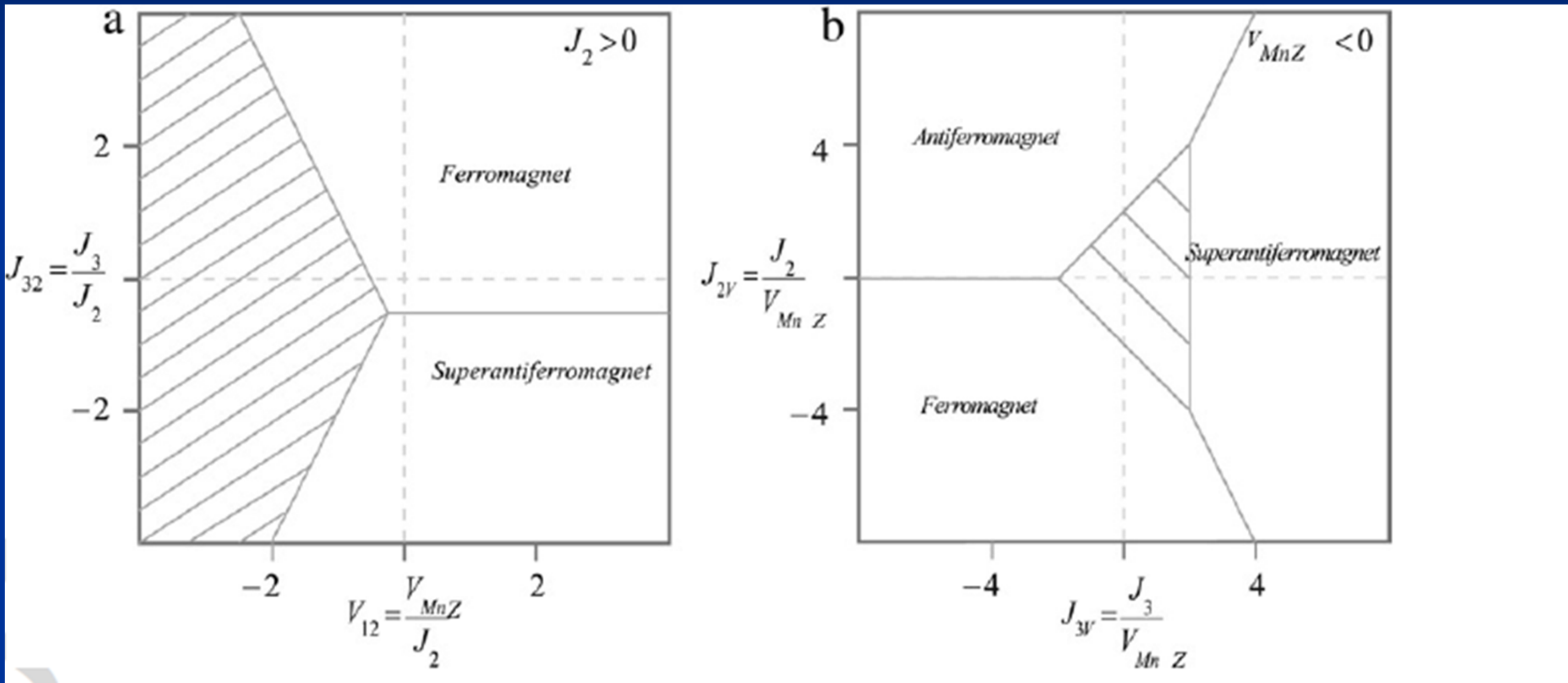


(c) Superantiferromagnet.



(d) Antiferromagnet.

**Fig. 2.** The various magnetic phases of a Heusler alloy with $c = 1/2$.



a
$J_2 > 0$
Ferromagnet
Superantiferromagnet
2
−2
$J_{32} = \frac{J_3}{J_2}$
−2
2
$V_{12} = \frac{V_{MnZ}}{J_2}$
b
$V_{MnZ} < 0$
Antiferromagnet
Superantiferromagnet
Ferromagnet
4
−4
$J_{2V} = \frac{J_2}{V_{Mn\ Z}}$
−4
4
$J_{3V} = \frac{J_3}{V_{Mn\ Z}}$

# Magnetic Properties of Co Nanowires with Complex Geometries

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- Motivated by the technological interest involving the miniaturization of sensors and the continuous increase of the magnetic storage density, techniques for fabrication and characterization have been developed.
- Molecular beam epitaxy or laser ablation followed by nanolithography represent the state of the art for producing nanomagnets.

# Ordenamiento Químico y Magnético en nanestructuras bimetálicas

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- Elements that do not show magnetic phases in bulk samples, like rhodium or palladium, display magnetic moments in small clusters.
- The 4*d* transition metal macroscopic systems do not fulfill the Stoner criterion to develop permanent magnetic moments.
- Since the reduction in dimensionality brings a natural narrowing in the width of the electronic bands, it is expected that, at least in some elements of that row, the electronic density of states at the Fermi energy or its equivalent, increases to the extent that the criterion is fulfilled.