



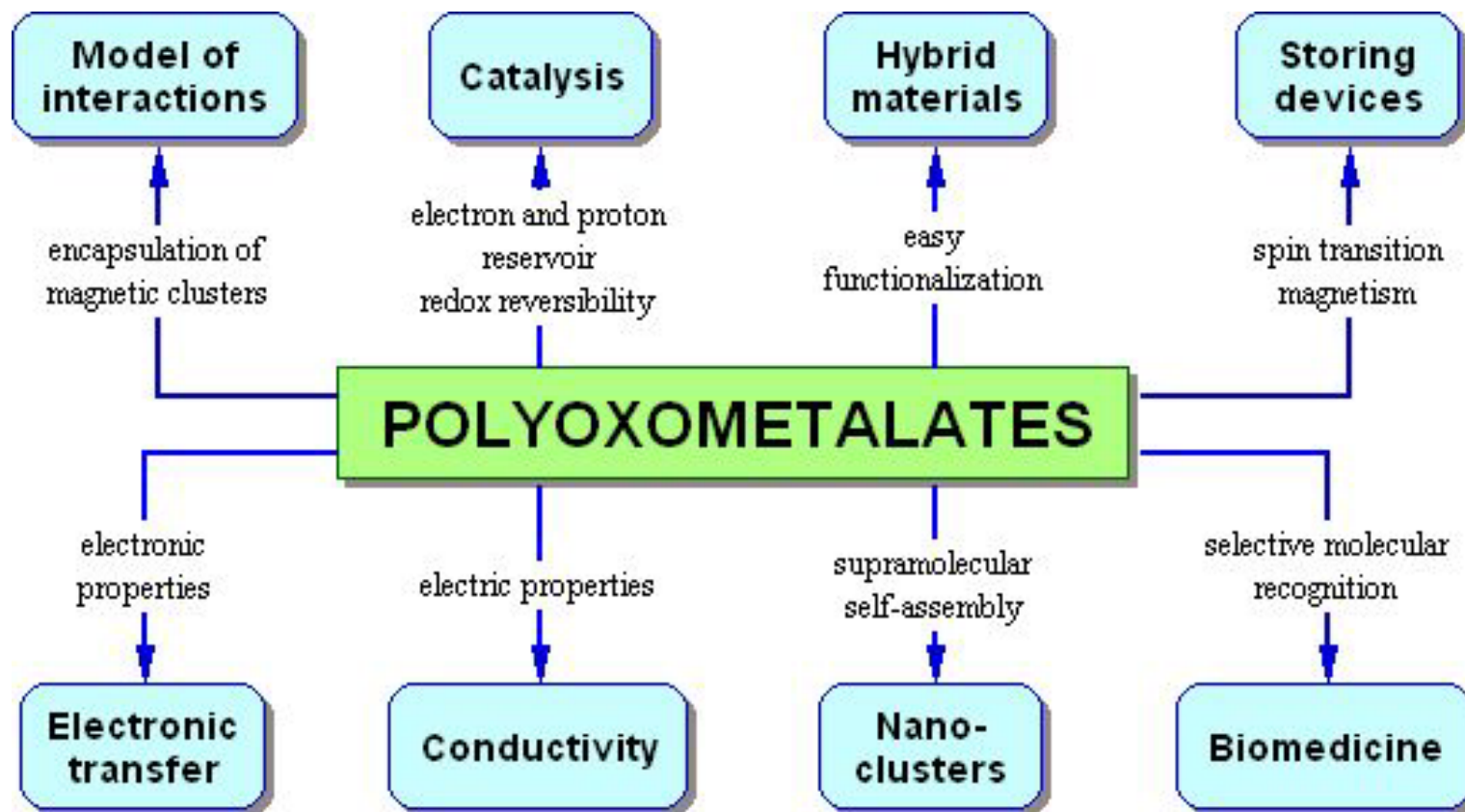
## Programa de Doctorado: “QUIMICA”

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- Departamentos:
    - Química Analítica
    - Química Física
    - Química Inorgánica
  
  - Líneas de investigación del Departamento de Química Inorgánica:
    - Polioxometalatos
    - Química de Coordinación
    - Estado Sólido
-



## Líneas de investigación



Profesor responsable:

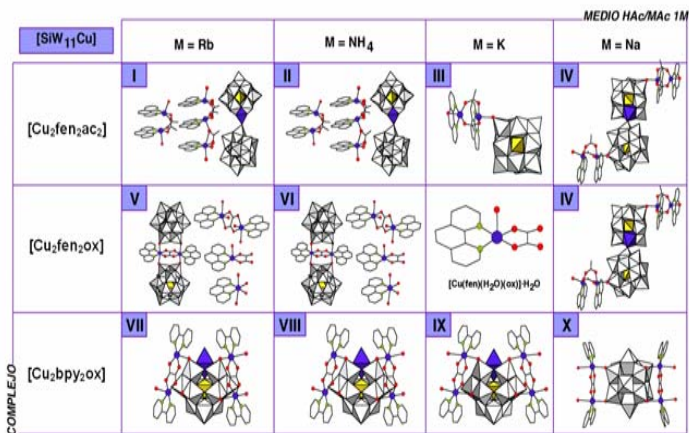
J. M. Gutiérrez Zorrilla (Ext. 5522)



# QUIMICA INORGANICA



**Materiales híbridos con los pollaniones** **SÍNTESIS**  
 $[SiW_{11}O_{39}Cu(H_2O)]^{6-}$  y  $[Si_2W_{22}Cu_2O_{78}(H_2O)]^{12-}$



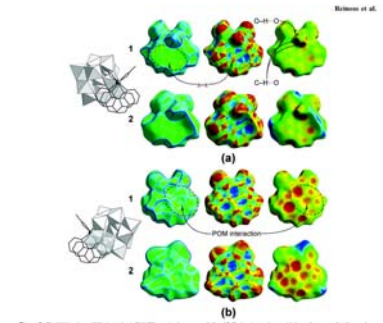
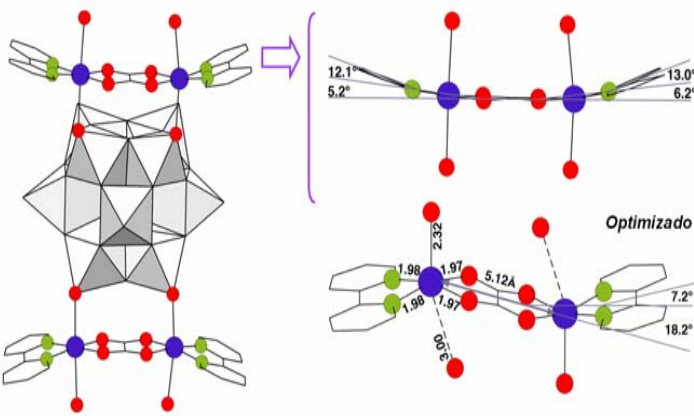
**ORGANIC-INORGANIC HYBRIDS BASED ON NOVEL BINUCLEAR [Si<sub>2</sub>W<sub>22</sub>Cu<sub>2</sub>(H<sub>2</sub>O)]<sup>12-</sup> POLYXOMALATES AND THE POLYNUCLEAR COMPLEX CATIONS [Cat<sub>2</sub>(phen)(H<sub>2</sub>O)]<sup>n+</sup> (n = 2, 3)**

Santiago Reinos, Pablo Vitoria, Leire San Felices, Leticia Lizaraso, and Juan M. Gutiérrez-Zorrilla

**Abstract:** The reaction of a binuclear silicotungstate (Si<sub>2</sub>W<sub>22</sub>)<sup>12-</sup> with copper(II) complex cations in acidic aqueous solution led to the formation of the hybrid metal-organic complex [Cat<sub>2</sub>(phen)(H<sub>2</sub>O)]<sup>n+</sup> [Si<sub>2</sub>W<sub>22</sub>Cu<sub>2</sub>(H<sub>2</sub>O)]<sup>12-</sup> (Cat = NH<sub>4</sub><sup>+</sup>, Rb<sup>+</sup>, K<sup>+</sup>, Na<sup>+</sup>), where the silicotungstate anion and the polynuclear complex cation are covalently bonded to form a novel hybrid material.

**Introduction:** Hybrid inorganic-organic materials have attracted an increasing interest in recent years owing to the possibility of combining the different characteristics of the components to get material properties, or applications (POMs) far out of the ones widely used (organic materials). Individual inorganic or organic moieties<sup>1,2</sup> owing to their intrinsic stability of composition, structure, stoichiometry and synthesis. In this way, the design of new composite materials incorporating POMs and organic moieties (OM) complex structures are emerging.

**POM híbridos con complejos soportados** **CARACTERIZACIÓN ESTRUCTURAL**  
 $X$ . Pollanión  $[SiW_{11}Cu][Cu_2bpy_2ox]_2^{2-}$

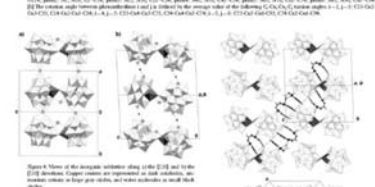


**Figure 6.** Superposition of different views of a dimeric group in compound 1. (a) Cu atoms in green and O atoms in red. (b) Cu atoms in green and O atoms in red. The POM interaction is highlighted.

**ORGANIC-INORGANIC HYBRIDS BASED ON NOVEL BINUCLEAR [Si<sub>2</sub>W<sub>22</sub>Cu<sub>2</sub>(H<sub>2</sub>O)]<sup>12-</sup> POLYXOMALATES AND THE POLYNUCLEAR COMPLEX CATIONS [Cat<sub>2</sub>(phen)(H<sub>2</sub>O)]<sup>n+</sup> (n = 2, 3)**

**Table 1.** Crystallographic data for [Cat<sub>2</sub>(phen)(H<sub>2</sub>O)]<sup>n+</sup> [Si<sub>2</sub>W<sub>22</sub>Cu<sub>2</sub>(H<sub>2</sub>O)]<sup>12-</sup> (Cat = NH<sub>4</sub><sup>+</sup>, Rb<sup>+</sup>, K<sup>+</sup>, Na<sup>+</sup>)

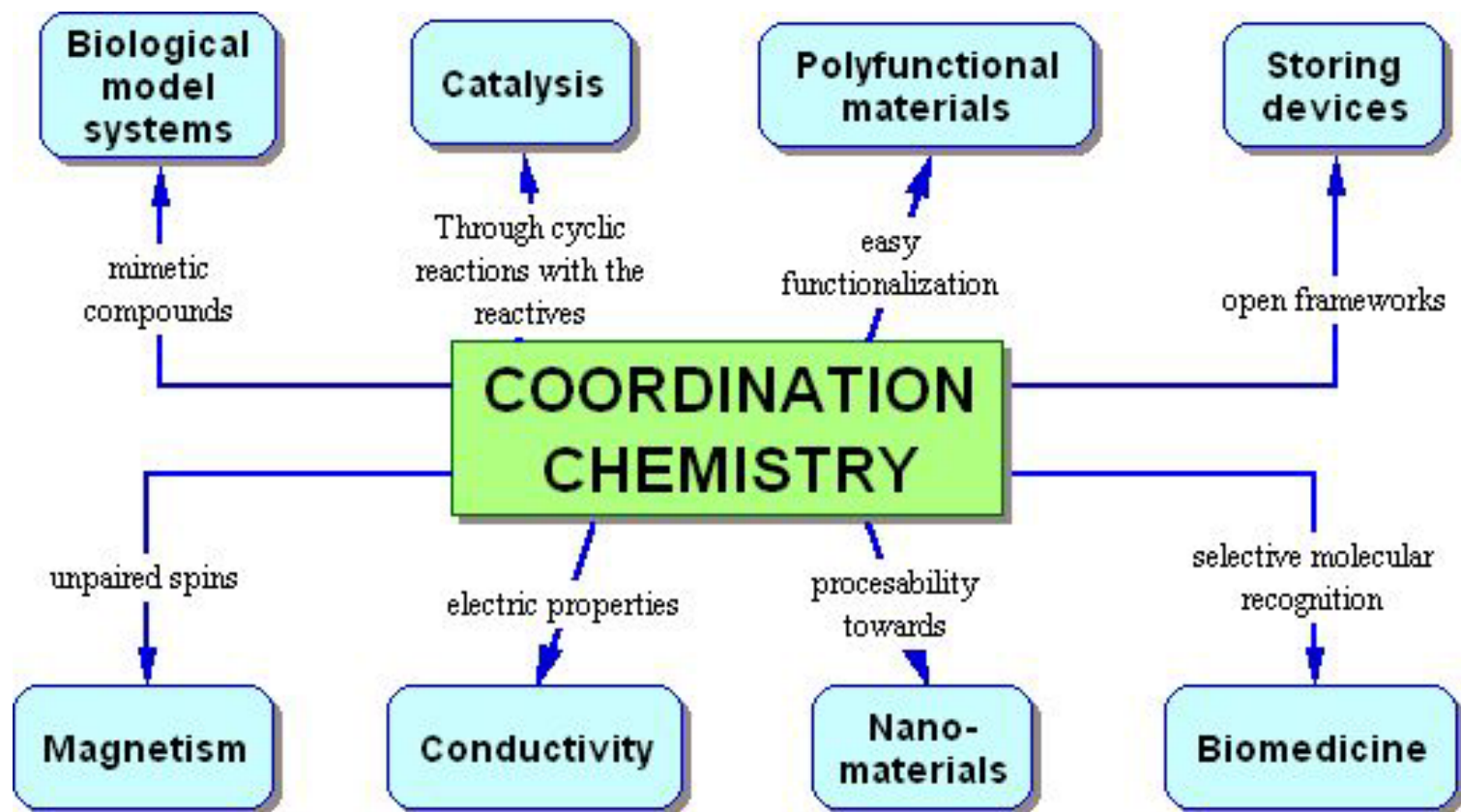
Parameter	[Cat <sub>2</sub> (phen)(H <sub>2</sub> O)] <sup>n+</sup>	[Si <sub>2</sub> W <sub>22</sub> Cu <sub>2</sub> (H <sub>2</sub> O)] <sup>12-</sup>
Formula	C <sub>24</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub>	Si <sub>22</sub> W <sub>22</sub> O <sub>78</sub> Cu <sub>2</sub>
Molar mass	462.46	4622.0
Crystal system	Trigonal	Trigonal
Space group	R-3m	R-3m
Unit cell dimensions (Å)	a = 10.51, c = 10.51	a = 10.51, c = 10.51
Volume (Å <sup>3</sup> )	1148.0	1148.0
Z	1	1



**Figure 7.** Three views of the organic support along the [110], [110], and [110] directions. The views show the arrangement of the organic support in the hybrid material.



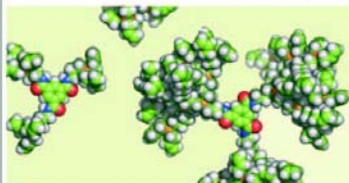
## Líneas de investigación



Profesor responsable: O. Castillo (Ext. 5991) y A. Luque (Ext.2701)



## New dendrimer detects amino acids



A novel carbosilane dendrimer that can tell the difference between the enantiomers of an amino acid analogue may lead to new organocatalysts and resolving agents.

Dendrimers are of interest as potential drug delivery agents because they can be bound to other molecules or guests, offering stability in conditions where the guest would otherwise deteriorate. Carbosilane dendrimers, so-called because they are composed mainly

**Carbosilane dendrimer could lead to new drug delivery agents**

**Reference**  
P van Heerbeek et al, *Org. Biomol. Chem.*, 2006, 4, 271

of carbon and silicon, form a versatile range of these polymers.

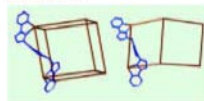
Joost Reek and co-workers at the University of Amsterdam, the Netherlands, used a technique called convergent dendrimer synthesis to prepare the branches of a carbosilane dendrimer before joining them to its core. Reek's approach led to dendrimers previously difficult to obtain that were capable of recognizing guest molecules.

The physical properties of carbosilane dendrimers can be tuned by varying the monomers used or by attaching different groups to the outer surface, but until now very little research has focused on modifications to the core of these dendrimers. This new line of enquiry has already led to the synthesis of important new dendrimers and may be of interest for the fields of organocatalysis and resolution chemistry, says Reek. *Celia Clarke*

## Controlling self-assembly

Two different molecular cages, made from the same metal salt and bridging ligand, could aid the development of controlled self-assembly.

Self-assembly of simple building-blocks into complex, highly symmetrical structures is commonly found in nature for example in virus formation. Self-assembly of a metal salt and ligand can occur by different pathways, leading to a mixture of two distinct architectures.



**Simple building blocks spontaneously assemble into a cube and an open book**

Michael Ward at the University of Sheffield, UK, and colleagues at the University of Huddersfield, UK, have shown how two different structures, one resembling a cube and one an open book, can be made from the same basic chemical components.

Eight metal ions and 12 bridging ligands made a cubic cage, a structure capable of acting as a molecular container into which other small molecules can be placed. The same six metal ions and nine ligands also made an open book structure.

There is 'an almost magical fascination in seeing these structures appear without any major effort', said Ward. He also said that the complexity of these structures is surprising because he would expect much simpler architecture to be formed instead.

Understanding the reasons for this might allow researchers to regain control of the structures produced by self-assembly. A longer-term challenge will be to use computational techniques to predict the outcome of these self-assembly processes, he said. *Suzanne Abbott*

**Reference**  
P Argenti et al, *Dalton Trans.*, 2006, 542

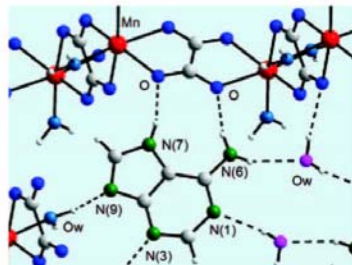
## Basic route to new biomimetics

Research into non-covalent interactions of nucleobases might hold the key to the development of materials for medical and molecular science applications.

Nucleobases, such as adenine, guanine and cytosine, bind to ribose derivatives and then pair up to form DNA. The interaction of these bases and their derivatives with metals plays a crucial role in the structure and function of nucleic acids. These interactions are also important in genetic information transfer and for the rational design and elaboration of biomimetic systems.

Oscar Castillo and co-workers at the Universidad del País Vasco, Spain, have stabilised a non-helical form of adenine by non-covalent interactions in the solid state. They hope this work will deepen understanding of the non-covalent interactions that determine the supramolecular assembly of biomimetic systems such as those that are active in the control of biorecognition processes.

Knowledge of the chemical and physical properties of both

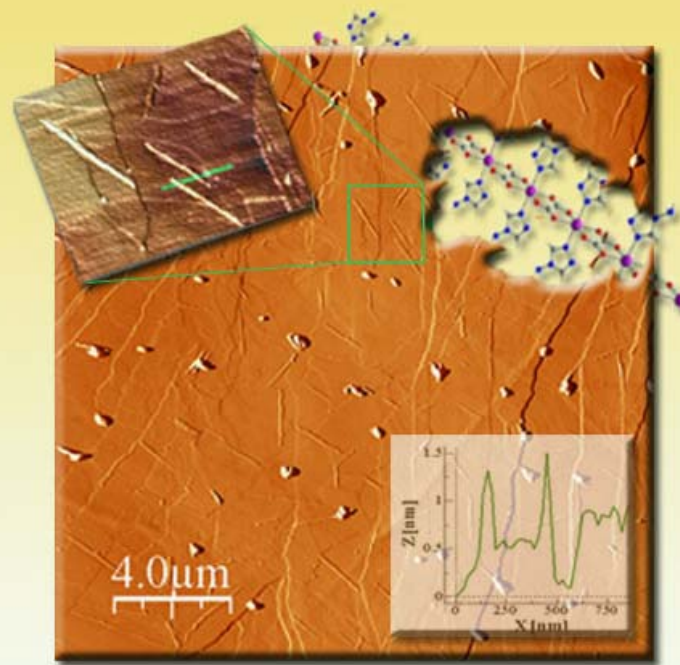


**New research stabilises nucleobases using non-covalent interactions in the solid state**

covalent and non-covalent binding of nucleobases will allow the development of advanced functional materials with potential medical and molecular science applications, say the researchers. *Helen Lunn*

**Reference**  
J P Garcia-Terín et al, *Dalton Trans.*, 2006 (DOI: 10.1039/b501001d)

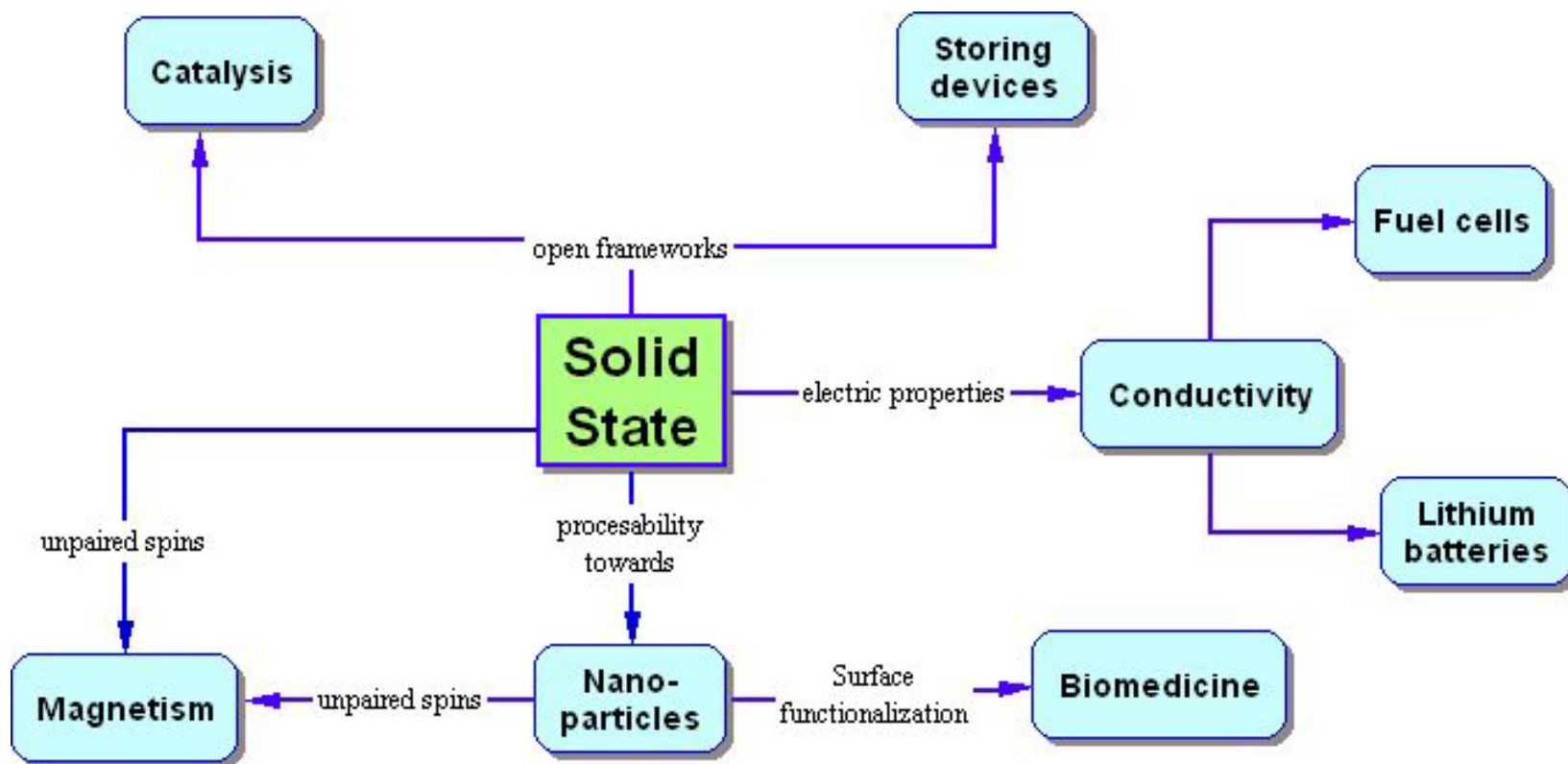
## Scanning probe microscopy characterization of single chain based on one-dimensional oxalato bridged manganese(II) complex with 4-aminotriazole



*Inorg. Chem.* 2005, 44, 8343



## Líneas de investigación



Profesor responsable:

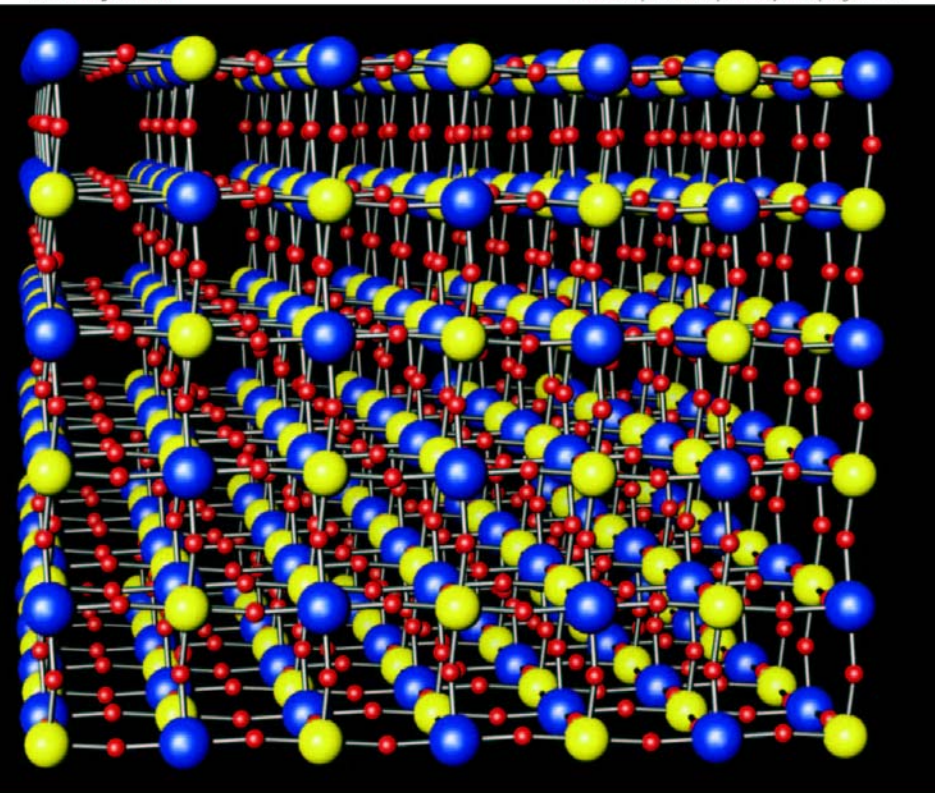
T. Rojo (Ext. 2458)



## Journal of Materials Chemistry

www.rsc.org/materials

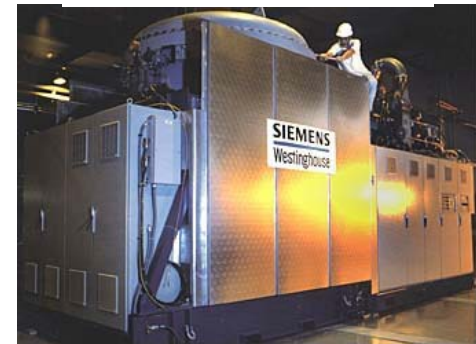
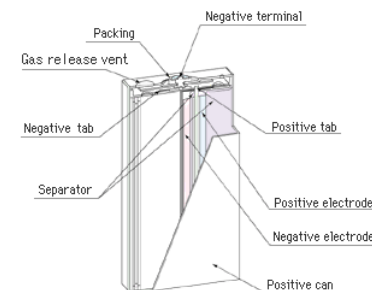
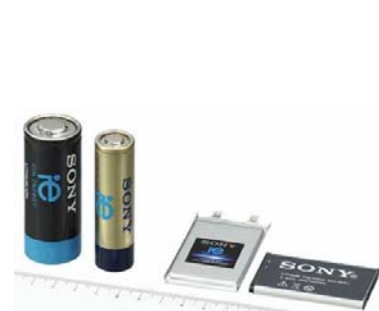
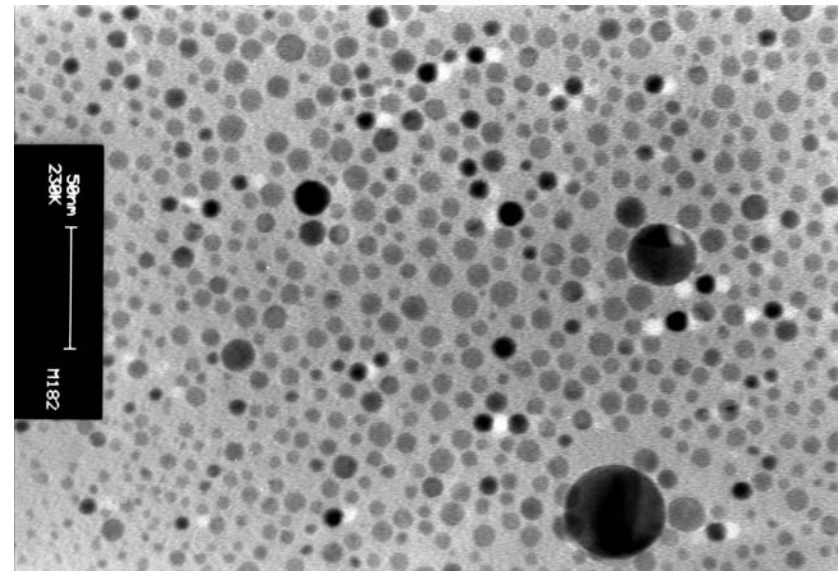
Volume 16 | Number 1 | 7 January 2006 | Pages 1-132



ISSN 0959-9428

**PAPER**  
Teófilo Rojo *et al.*  
Spin-glass behaviour in the double perovskite  $\text{Sr}_2\text{FeTeO}_6$  due to mis-site disorder and cation vacancy formation

**HIGHLIGHT**  
Miguel A. Correa-Duarte and Luis M. Liz-Marzán  
Carbon nanotubes as templates for one-dimensional nanoparticle assemblies





## Producción científica últimos 6 años

▲ SUMMARY

Web Of Science Results Analysis

Results Analysis

145 records. AU=(Rojo T\* OR Gutierrez-Zorrilla OR Roman P\*) AND PY=(2000-2006) AND AD=(Bilbao)

Select field to rank by:	Analyze:	Set display options:	Sort by:
Document Type ▲ Institution Name Language Publication Year ▼	<input checked="" type="radio"/> First 500 records <input type="radio"/> All (up to 2000 records)	Show the top <input type="text" value="10"/> results. Minimum record count (threshold): <input type="text" value="2"/>	<input type="radio"/> Record count <input checked="" type="radio"/> Selected field

Rank results by the selected field.

Use the checkboxes below to view the records.

**Note:** The number of records displayed may be greater than the listed Record Count if the original set contained more records than the number of records analyzed.

<input type="button" value="VIEW RECORDS"/>	Field: Publication Year	Record Count	% of 145	Bar Chart	<input type="button" value="SAVE ANALYSIS DATA TO FILE"/>
<input type="checkbox"/>	2000	19	13.1 %	<div style="width: 13.1%; height: 10px; background-color: #0056b3;"></div>	
<input type="checkbox"/>	2001	34	23.4 %	<div style="width: 23.4%; height: 10px; background-color: #0056b3;"></div>	
<input type="checkbox"/>	2002	21	14.5 %	<div style="width: 14.5%; height: 10px; background-color: #0056b3;"></div>	
<input type="checkbox"/>	2003	25	17.2 %	<div style="width: 17.2%; height: 10px; background-color: #0056b3;"></div>	
<input type="checkbox"/>	2004	18	12.4 %	<div style="width: 12.4%; height: 10px; background-color: #0056b3;"></div>	
<input type="checkbox"/>	2005	23	15.9 %	<div style="width: 15.9%; height: 10px; background-color: #0056b3;"></div>	
<input type="checkbox"/>	2006	5	3.4 %	<div style="width: 3.4%; height: 10px; background-color: #0056b3;"></div>	



## Producción científica por revistas

Field: Source Title	Record Count	% of 145	Bar Chart
INORGANIC CHEMISTRY	17	11.7 %	■
JOURNAL OF SOLID STATE CHEMISTRY	13	9.0 %	■
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE	11	7.6 %	■
EUROPEAN JOURNAL OF INORGANIC CHEMISTRY	11	7.6 %	■
JOURNAL OF MATERIALS CHEMISTRY	9	6.2 %	■
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS	8	5.5 %	■
INORGANICA CHIMICA ACTA	7	4.8 %	■
JOURNAL OF THE CHEMICAL SOCIETY-DALTON TRANSACTIONS	7	4.8 %	■
CHEMISTRY OF MATERIALS	6	4.1 %	■
INORGANIC CHEMISTRY COMMUNICATIONS	6	4.1 %	■
JOURNAL OF PHYSICS-CONDENSED MATTER	5	3.4 %	■
POLYHEDRON	4	2.8 %	■
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	3	2.1 %	■
DALTON TRANSACTIONS	3	2.1 %	■
INTERNATIONAL JOURNAL OF INORGANIC MATERIALS	3	2.1 %	■
MATERIALS RESEARCH BULLETIN	3	2.1 %	■
NEW JOURNAL OF CHEMISTRY	3	2.1 %	■
ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE	3	2.1 %	■
CHEMICAL COMMUNICATIONS	2	1.4 %	■
CHEMISTRY-A EUROPEAN JOURNAL	2	1.4 %	■
JOURNAL DE PHYSIQUE IV	2	1.4 %	■
JOURNAL OF ALLOYS AND COMPOUNDS	2	1.4 %	■
JOURNAL OF INORGANIC BIOCHEMISTRY	2	1.4 %	■
PHYSICA B-CONDENSED MATTER	2	1.4 %	■
PHYSICAL REVIEW B	2	1.4 %	■



## Producción científica por autores

<input type="checkbox"/>	Field: Author	Record Count	% of 145	Bar Chart	<input type="checkbox"/>
<input checked="" type="checkbox"/>	Rojo, T	101	69.7 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Lezama, L	67	46.2 %		<input type="checkbox"/>
<input type="checkbox"/>	Arriortua, MI	56	38.6 %		<input type="checkbox"/>
<input type="checkbox"/>	Pizarro, JL	44	30.3 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Mesa, JL	39	26.9 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Roman, P	34	23.4 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Luque, A	32	22.1 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Castillo, O	25	17.2 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Insausti, M	21	14.5 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Vitoria, P	19	13.1 %		<input type="checkbox"/>
<input checked="" type="checkbox"/>	Gutierrez-Zorrilla, JM	18	12.4 %		<input type="checkbox"/>
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<input type="checkbox"/>	Reinoso, S	10	6.9 %		<input type="checkbox"/>
<input type="checkbox"/>	Bazan, B	9	6.2 %		<input type="checkbox"/>
<input type="checkbox"/>	Fernandez, S	9	6.2 %		<input type="checkbox"/>



## Tesis Doctorales en los últimos 6 años

1. Jose M<sup>a</sup> Rojo, 2000 (INSHT)
2. Tomás Hernández, 2001 (Univ. Auton. Puebla, México)
3. Izaskun Gil, 2001 (UPV/EHU)
4. Zuriñe Serna, 2001 (Prof. Ikastola)
5. Oscar Castillo, 2001 (UPV/EHU)
6. Ricardo López, 2002 (UPV/EHU)
7. Susana Martín, 2002 (Universidad Francisco de Vitoria)
8. Jaione Escobal, 2002 (Fraternidad Muprespa)
9. Jose Julio Blanco, 2002 (Fundición Palacios)
10. Sergio Fernández, 2003 (UPV/EHU)
11. Begoña Bazán, 2003 (UPV/EHU)
12. Alazne Peña, 2003 (UPV/EHU)
13. Noelia de la Pinta, 2004 (Empresa Privada)
14. Iñaki Muga, 2004 (Prof. Instituto)
15. Santiago Reinoso, 2005 (Post. Doc., Univ. Int. Bremen)
16. Luis Ortega, 2005 (Post. Doc., Univ. Edimburgo)
17. Iratxe de Meatza (CIDETEC)
18. Imanol de Pedro (SIBELCO Minerales, S.A.)



## Colaboración con centros públicos

**Results Analysis**

145 records. AU=(Rojo T\* OR Gutierrez-Zorrilla OR Roman P) AND PY=(2000-2006) AND AD=(Bilbao)

Select field to rank by:	Analyze:	Set display options:	Sort by:
Author Country/Territory Document Type Institution Name	<input checked="" type="radio"/> First 500 records <input type="radio"/> All (up to 2000 records)	Show the top 25 results. Minimum record count (threshold): 2	<input checked="" type="radio"/> Record count <input type="radio"/> Selected field

Rank results by the selected field.

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**Note:** The number of records displayed may be greater than the listed Record Count if the original set contained more records than the number of records analyzed.

<input type="button" value="VIEW RECORDS"/>	Field: Institution Name	Record Count	% of 145	Bar Chart	<input type="button" value="SAVE ANALYSIS DATA TO FILE"/>
<input type="checkbox"/>	Univ Pais Vasco	136	93.8 %	<div style="width: 93.8%;"></div>	
<input type="checkbox"/>	Univ Burgos	13	9.0 %	<div style="width: 9.0%;"></div>	
<input type="checkbox"/>	Inst Chim Mat Condensee Bordeaux	8	5.5 %	<div style="width: 5.5%;"></div>	
<input type="checkbox"/>	Univ Cantabria	8	5.5 %	<div style="width: 5.5%;"></div>	
<input type="checkbox"/>	Univ Valencia	8	5.5 %	<div style="width: 5.5%;"></div>	
<input type="checkbox"/>	UNICAMP	6	4.1 %	<div style="width: 4.1%;"></div>	
<input type="checkbox"/>	CNRS	5	3.4 %	<div style="width: 3.4%;"></div>	
<input type="checkbox"/>	Univ Coruna	5	3.4 %	<div style="width: 3.4%;"></div>	
<input type="checkbox"/>	Univ Estadual Campinas	5	3.4 %	<div style="width: 3.4%;"></div>	
<input type="checkbox"/>	UPV	4	2.8 %	<div style="width: 2.8%;"></div>	
<input type="checkbox"/>	CSIC	3	2.1 %	<div style="width: 2.1%;"></div>	
<input type="checkbox"/>	Inst Max Von Laue Paul Langevin	3	2.1 %	<div style="width: 2.1%;"></div>	
<input type="checkbox"/>	Univ Maine	3	2.1 %	<div style="width: 2.1%;"></div>	
<input type="checkbox"/>	UPV EHU	3	2.1 %	<div style="width: 2.1%;"></div>	
<input type="checkbox"/>	Fac Ciencias	2	1.4 %	<div style="width: 1.4%;"></div>	

(22 Institution Name value(s) outside display options.)

1. Universidad de Burgos
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3. Universidad de Cantabria
4. Universidad de Valencia
5. UNICAMP. Sao Paulo, Brasil
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9. Inst Max Von Laue Paul Langevin
10. Univ. Maine
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## Colaboración con empresas

1. AZTERLAN
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3. IKERLAN
4. CIDETEC
5. FAGOR
6. LABEIN
7. RHODIA
8. DERIVADOS DEL FLUOR S.A.
9. TS Fundiciones

## Proyectos de investigación en los 6 últimos años

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1. Europeas: 1
2. Nacionales: 7
3. Gobierno Vasco: 2
4. UPV/EHU: 2

Importe Total de la Financiación: **1.186.030,48 €**



## Equipamiento científico

Laboratorios



Línea de vacío



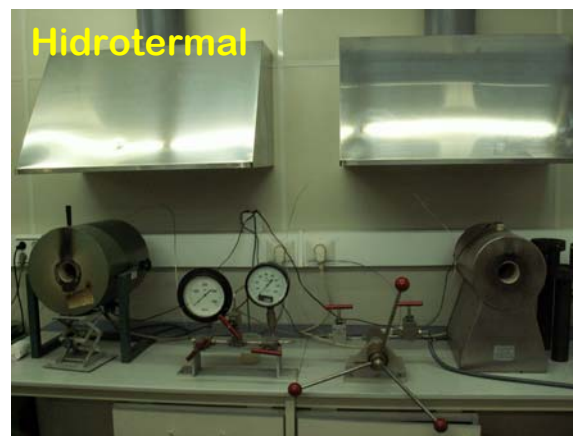
Caja de guantes



Hornos



Hidrotermal



Ablación por láser





## Equipamiento científico

