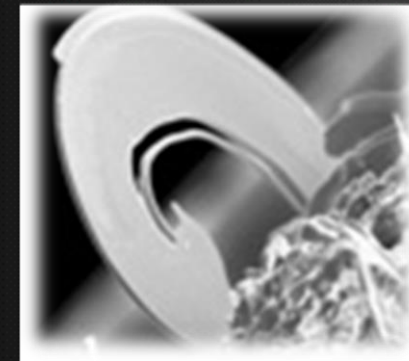
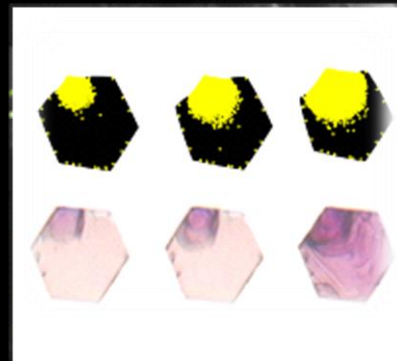
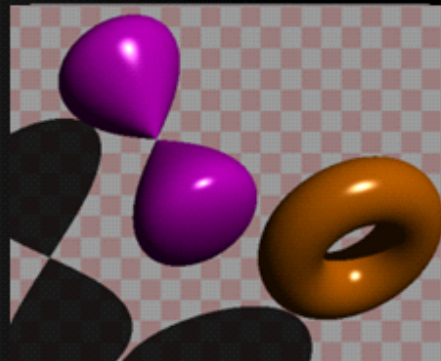
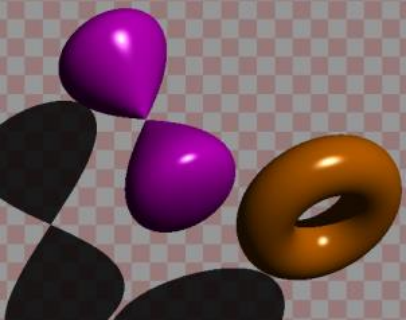


Povești despre IDEI
complexe și
oameni de succes
12 decembrie 2013



**O NOUA GENERATIE DE PARADIGME IN MAGNETISMUL MOLECULAR SI STIINTA MATERIALELOR.
ANIZOTROPIA MAGNETICA IN UNITATI COMPLEXE, SISTEME SUPRAMOLECULARE SI LA NANO-SCALA**



Rezultate obtinute in proiectul PCCE, cod CNCS 239, contract nr. 9/2010

O NOUA GENERATIE DE PARADIGME IN MAGNETISMUL MOLECULAR SI STIINTA MATERIALELOR. ANIZOTROPIA MAGNETICA IN UNITATI COMPLEXE, SISTEME SUPRAMOLECULARE SI LA NANO-SCALA

Director de proiect Conf. Dr. Marilena (Ferbinteanu) Cimpoesu

P1 –UB, Chimie, Bucuresti, coordonator, Conf. Dr. Marilena Cimpoesu

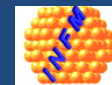
P2 –UOC, Constanta, Prof. Dr. Mihai Girtu

P3 –UAIC, Fizica, Iasi, Lect. Dr. Cristian Enachescu

P4 –ICF Bucuresti, C.S.II. Dr. Fania Cimpoesu

P5 –UAIC, Chimie, Iasi, Conf. Dr. Ionel Humelnicu

P6 –INCDFM Bucuresti, C.S.I. Dr. Petre Badica



Schema de functionare a consorțiului. Resurse umane.

Chimia sintetica coordinativa si supramoleculara, structura experimentală -generează și propune sisteme ca studii de caz în paradigma magnetismului molecular.

Corelat cu fizica teoretică și cuantica

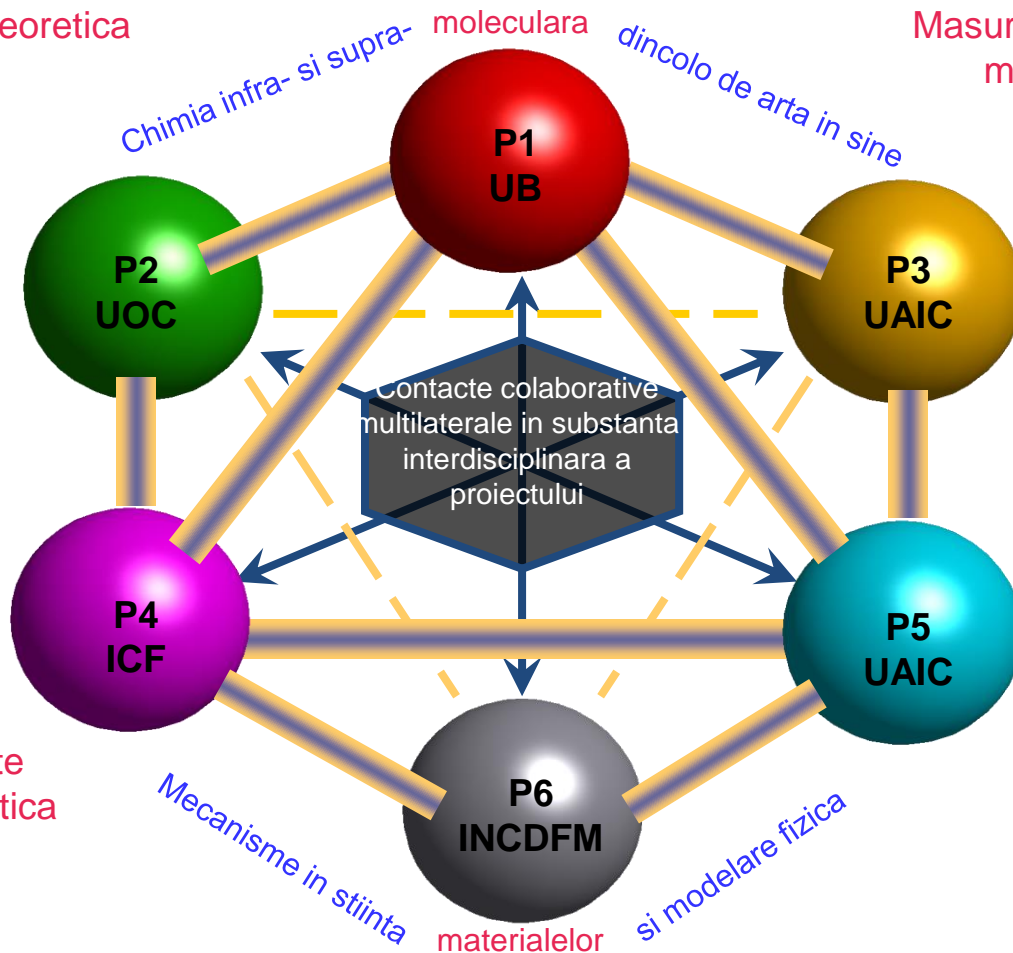
Măsurători fizice avansate și modelări numerice

Revelarea mecanismelor intra- și inter-
moleculare ale magnetismului

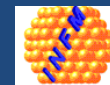
Revelarea mecanismelor intra- și inter-
moleculare ale magnetismului

Sisteme preluate de chimia teoretică

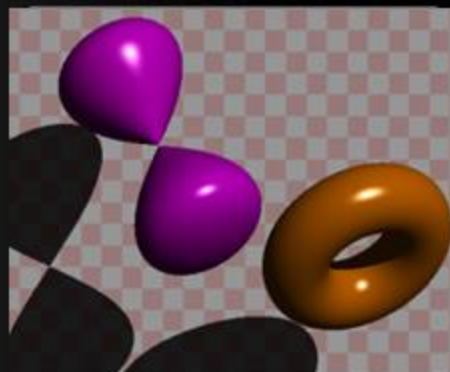
Modelarea ab initio (explicativ și predictiv)



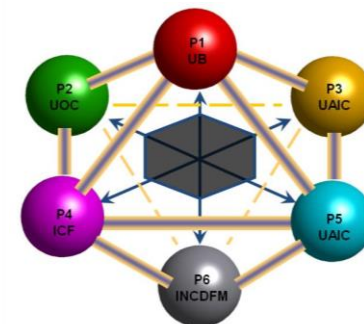
Rationalizarea la nivelul parametrilor moleculari extrapolată în complexitatea științei materialelor nano-structurate –câte ingineria fundamentală a proprietăților și aplicațiilor speciale



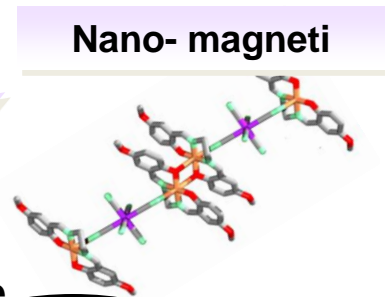
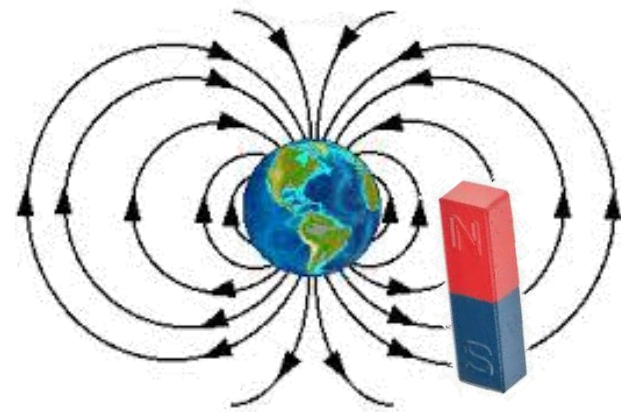
Povești despre IDEI
complexe și
oameni de succes
12 decembrie 2013



Fons et Origo.

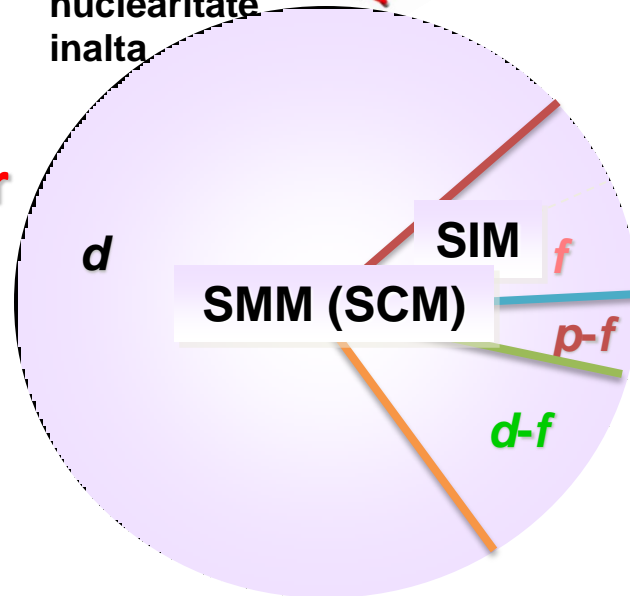


Magneti la scala nano si molecularara. Cursa pentru cel mai mic magnet.



Magnetism Molecularar

Clusteri cu
nuclearitate
inalta

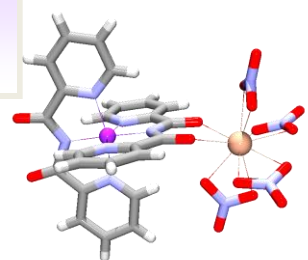


Stare fundamentala cu
spin inalt
Anizotropie magnetica

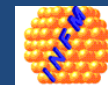
Rata redusa de relaxare
a magnetizarii

Histerezis

Rationalizarea
factorilor cauzali
Sisteme
binucleare ca
studii de caz

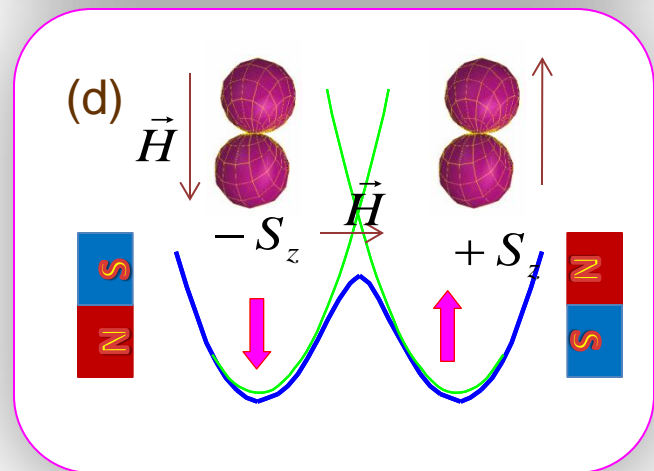
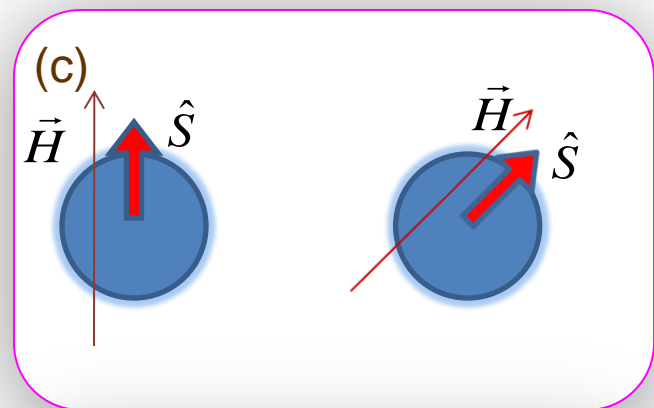
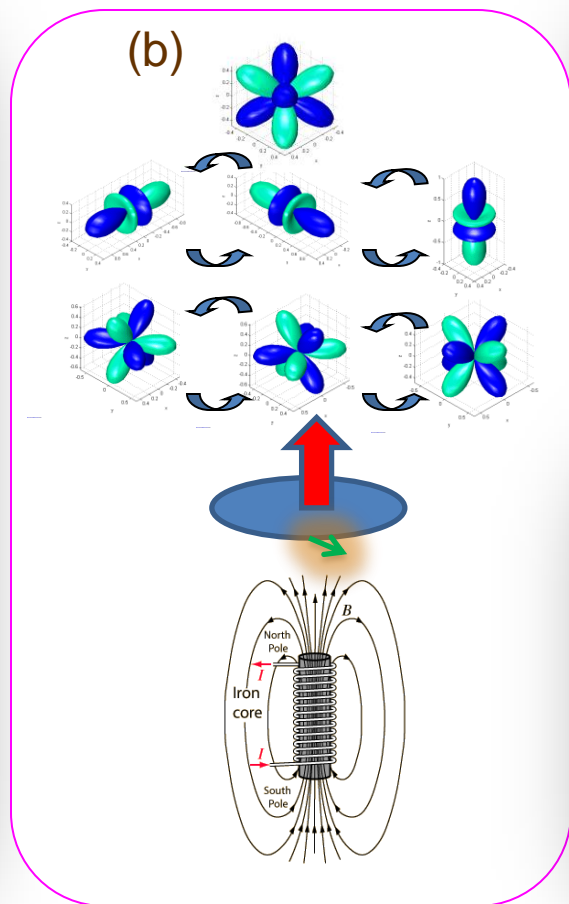
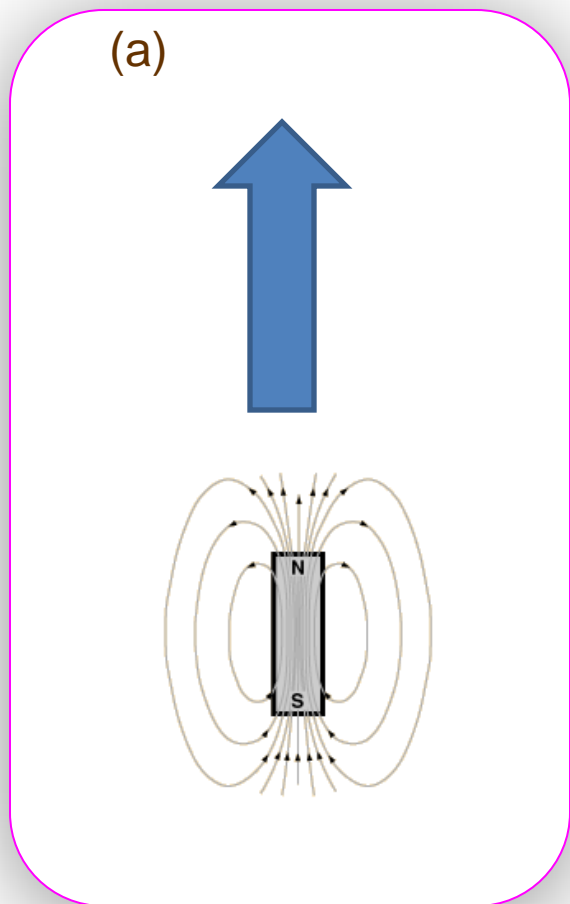


Single Chain Magnet
Single Molecule Magnet
Single Ion Magnet



Anizotropia-ingredient fundamental pentru comportamentul de magnet.

Anizotropia-subiect complex de maxim interes in magnetismul molecular din ultimii cinci ani. Multa vreme chimistii au privit subiectul ca *deus ex machina*, tratandu-l superficial sau evitandu-l. Abordarea matura presupune cooperarea intre fizica si chimie. Detinem atuuri majore in tratamentul anizotropie si prioritati ferme stabilite in literatura internationala



Sinopsis al elementelor de baza ale magnetismului atomic si molecular : (a) momentul magnetic de spin al electronului "cel mai mic magnet permanent" ; (b) magnetismul orbital, determinat de miscarea libera a electronilor intre orbitali echivalenti (degenerati) reprezinta figurativ echivalentul campului magnetic indus de o spira de curent; (c) spinul este izotrop-magnetizarea urmeaza liber campul si tensorul magnetizarii este o sfera; (d) anizotropia magnetica (ne-sferica, ex. Tensorii magnetizarii bilobali) si energia barierei dintre stari cu proiectii de spin opuse sunt premise *sine qua non* pentru constructia de sisteme care sa functioneze ca magneti moleculari.

Anizotropia magnetica

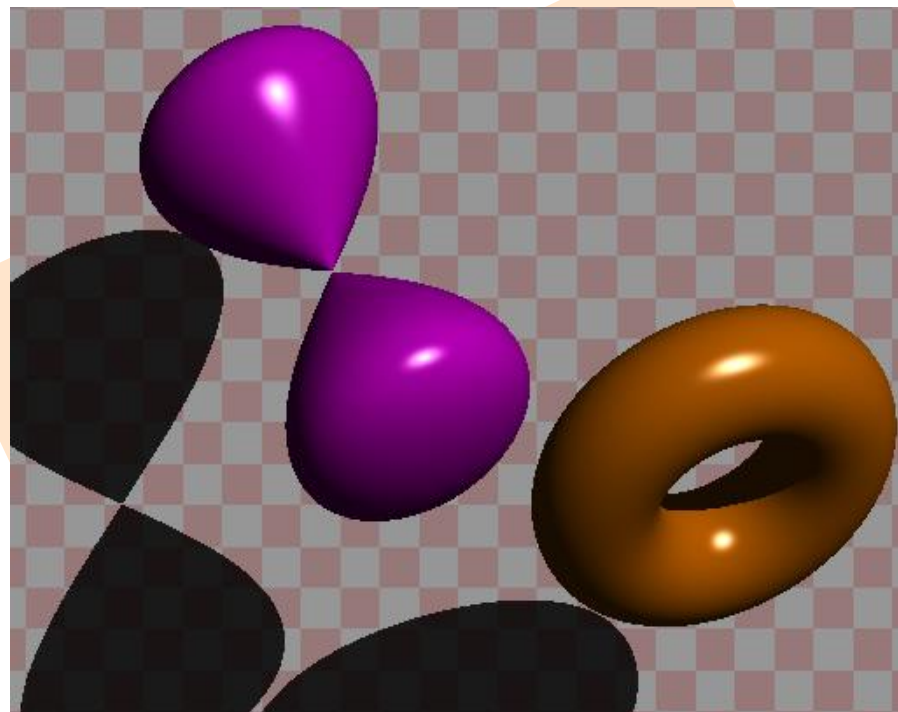
Un efect complex legat de geometria si structura electronica a unitatilor constitutive

Propus ca obiect al cercetarii interdisciplinare de catre chimisti

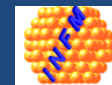
(care ofera noi edificii moleculare ca studii de caz)

si fizicieni

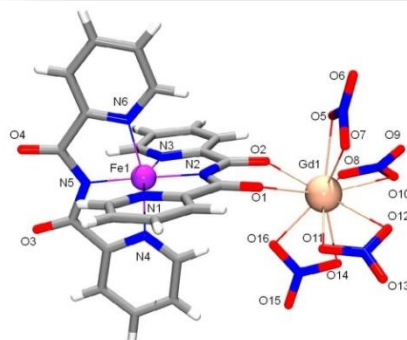
(care identifica in noile molecule parametrii sistematici)



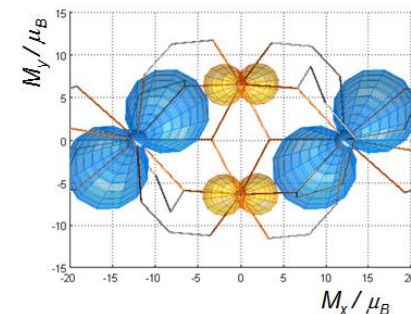
Construim puncti intre fizica si chimie plasand pe acelasi nivel experimentul si teoria.
Acesta este meritul intregii noastre echipe.



Povești despre IDEI
complexe și
oameni de succes
12 decembrie 2013

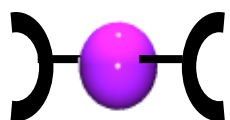


*Rerum
cognoscere
causas*



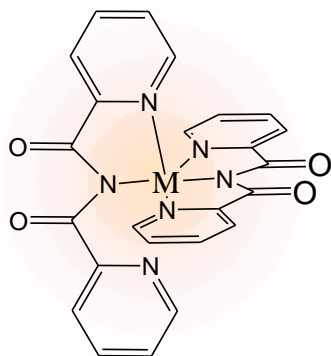
Noi dezvoltari conceptuale asupra anizotropiei magnetice

**Strategia sintetica:
asamblare coordinativa
si supramoleculara**

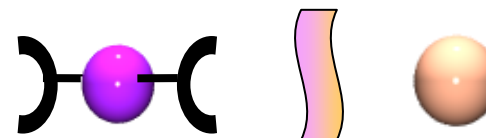


M=Fe(II, III),
Mn(III),
Ni(II)

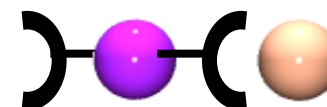
Ln=Eu, Gd, Tb,
Dy, Ho, Er, Yb



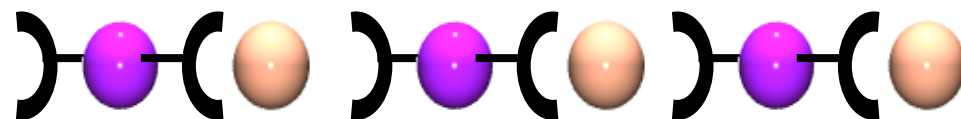
Structuri d-f disjuncte



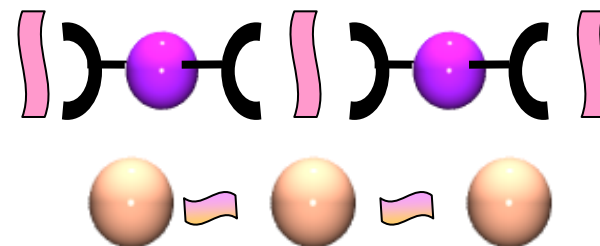
Structuri d-f dinucleare



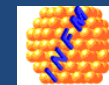
**Ansambluri
heterometalice
extinse**



**Ansambluri
homometalice extinse**

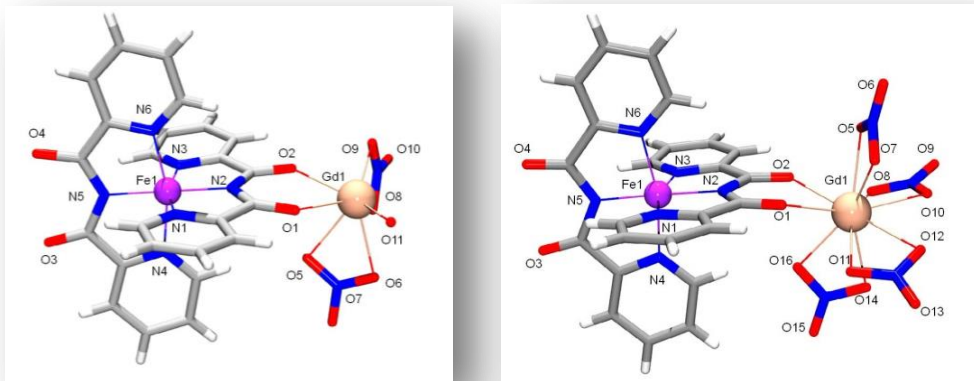


**Unitatea constitutiva este $M[bpc]_2$ cu rol de ligand complex pentru ionul de lantanid oxofil
genereaza o paleta larga de ansambluri moleculare si supramoleculare**

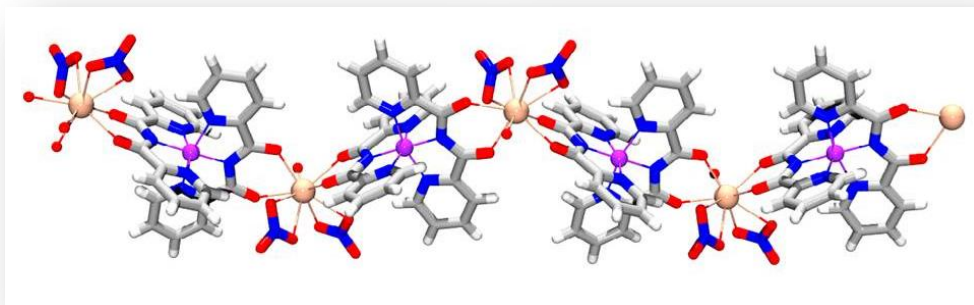


Noi dezvoltari conceptuale asupra anizotropiei magnetice

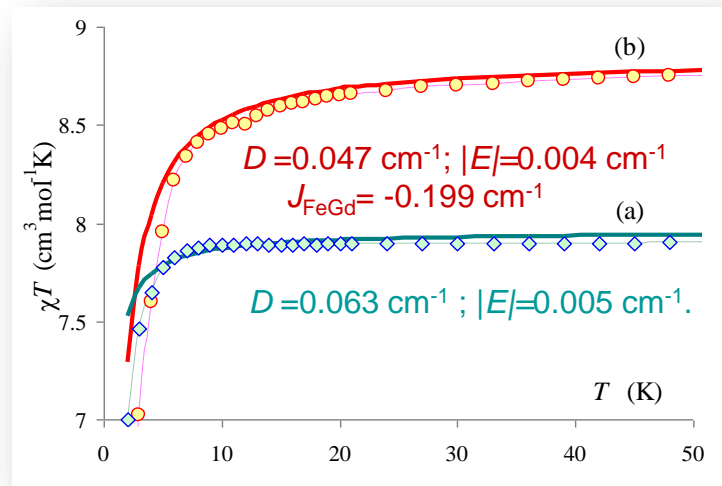
Exemple de sisteme dinucleare si monodimensionale. Imbricarea efectelor de schimb si anizotropie slaba de tip Zero Field Splitting in complexi Fe-Gd



Analiza de difractie de raze X pe monocristal



(a) Unitatea asimetrica pentru $[\text{Fe}_{\text{LS}}^{\text{II}}(\mu\text{-bpca})_2\text{Gd}(\text{NO}_3)_2(\text{H}_2\text{O})]\text{NO}_3$ (1) si pentru $[\text{Fe}_{\text{LS}}^{\text{III}}(\text{bpca})(\mu\text{-bpca})\text{Gd}(\text{NO}_3)_4]$ (2) (sus) si aranjamentul 1D al lantului $[\text{Fe}_{\text{LS}}^{\text{II}}(\mu\text{-bpca})_2\text{Gd}(\text{NO}_3)_2(\text{H}_2\text{O})]\text{NO}_3 \cdot 2\text{CH}_3\text{NO}_2$ (1)

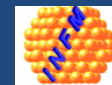


Curbele χT vs. T (simbol) si cele teoretice (linie) pentru **1** (a) si **2** (b). Curbele teoretice sunt rezultatul obtinut prin utilizarea directa a parametrilor calculului *ab initio* in modelele Hamiltonianului de spin.

$$\hat{H}_{\text{ZFS}} = D \cdot \left(S_z^2 - \frac{1}{3} S(S+1) \right) + E \cdot (S_x^2 - S_y^2)$$

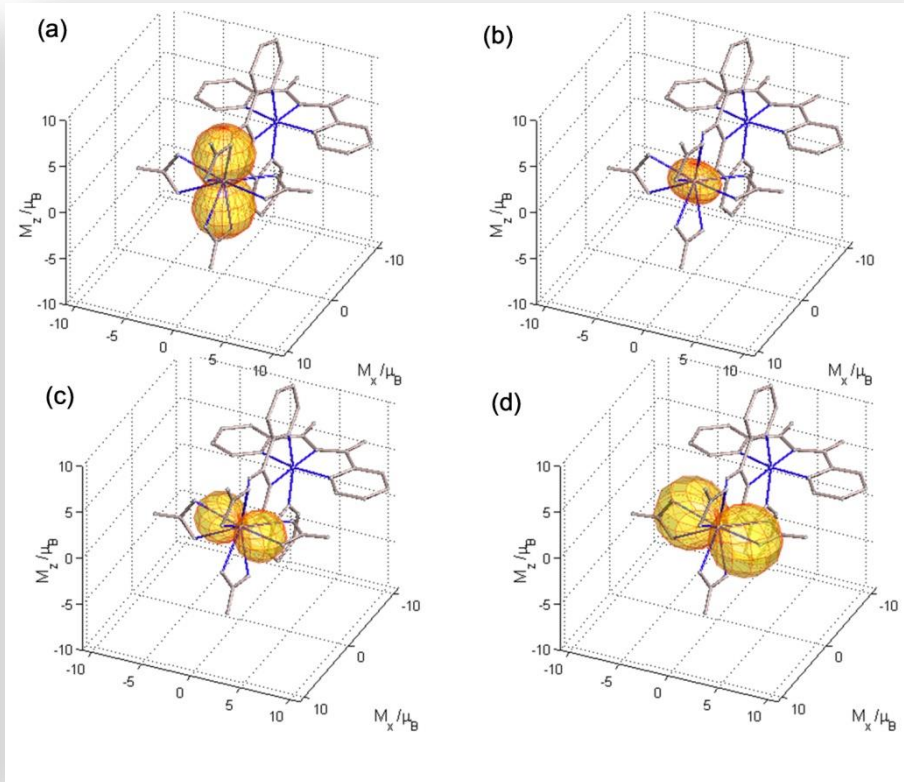
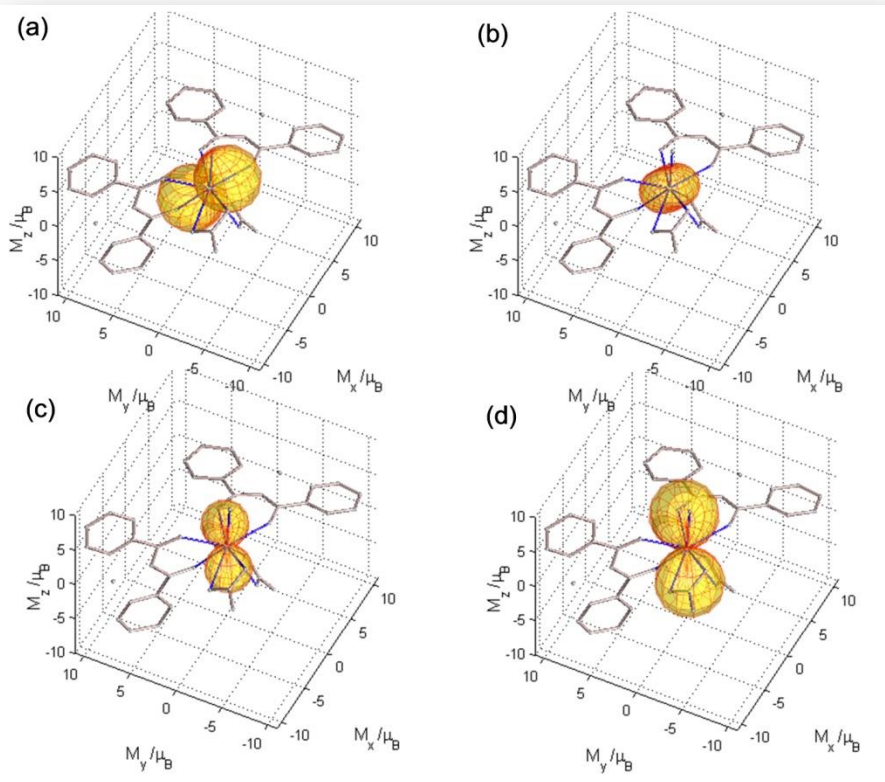
$$\hat{H}_{\text{exch}} = -2J_{\text{GdFe}} \hat{S}_{\text{Gd}} \cdot \hat{S}_{\text{Fe}}$$

$$\bar{\chi} = N_A k_B T \int_0^\pi \int_0^{2\pi} \left(\frac{d^2}{dB^2} \ln(Z(\theta, \varphi, B)) \right) \frac{1}{4\pi} \sin(\theta) d\theta d\varphi$$



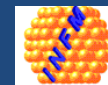
Noi dezvoltari conceptuale asupra anizotropiei magnetice

Tratamentul *ab initio* pentru anizotropia slaba de tip Zero Field Splitting si tensorii magnetizarii pentru centrii de Gd(III).



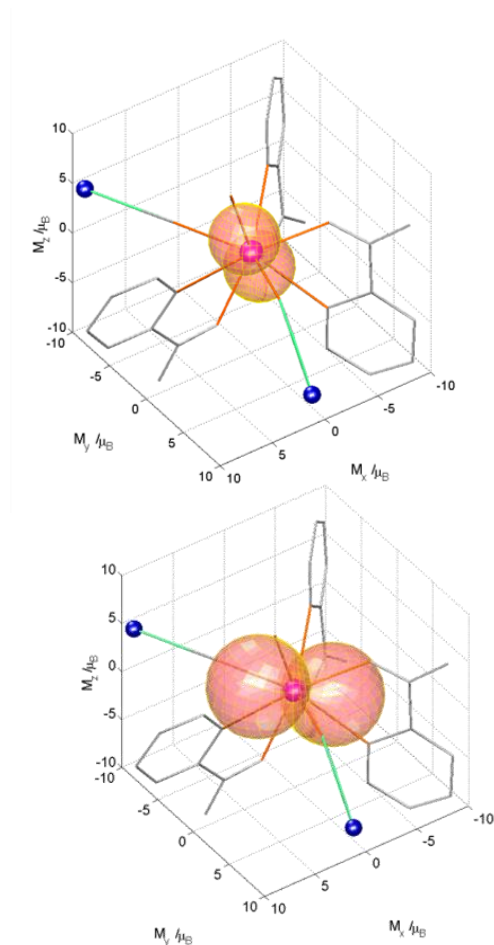
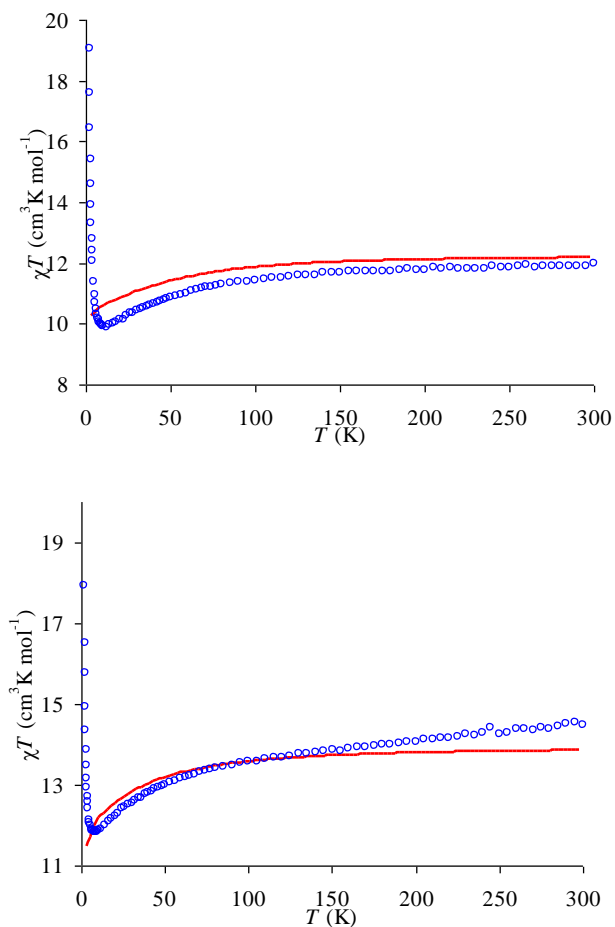
Tensorii magnetizarii au fost obtinuti printr-o procedura completa *ab initio* pentru ionii Gd(III) din **1** (stanga) si **2** (dreapta). Figurile (a)-(d) corespund perechilor de stari ZFS degenerate in ordinea energetica (a)<(b)<(c)<(d). Magnetizarile M_x , M_y , si M_z sunt reprezentate 3D in unitati (μ_B). Calcul CASSCF-SO implica stările termenii spectrali 8S , 6P , 6I , 6D , 6G , 6F , 6H ai Gd(III) (296 nivele).

$$M(\theta, \varphi) = -d\varepsilon / dB(\theta, \varphi)$$

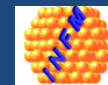


Noi dezvoltari conceptuale asupra anizotropiei magnetice

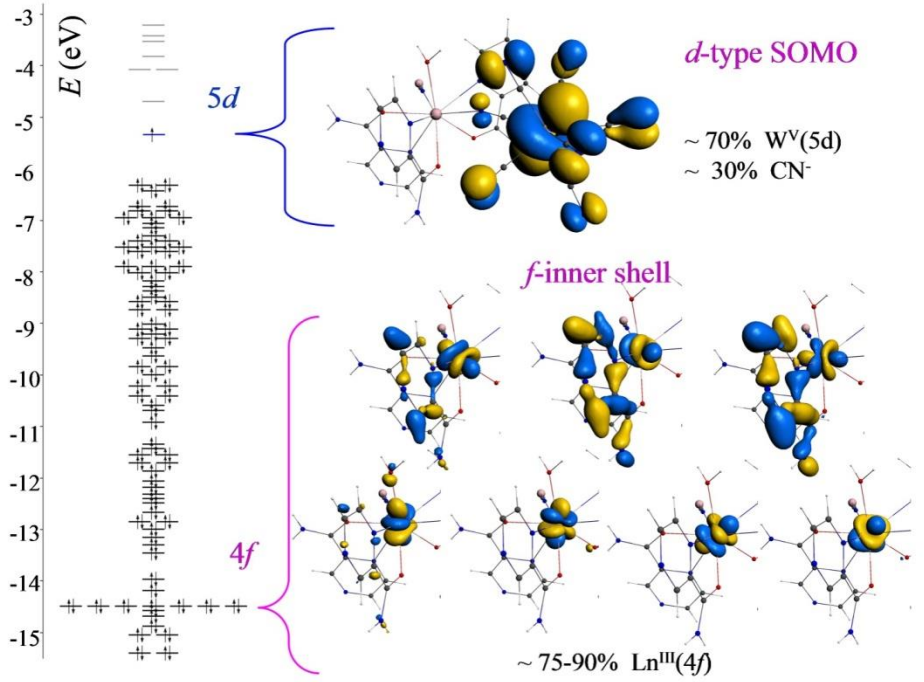
Corelatii magneto-structurale in lanturile 4f-5d cu punti ciano



Datele magnetice pentru compusii izostructurali ai Tb(III) (sus) si (b) Dy(III) (jos) , $[RE(pzam)_3(H_2O)W(CN)_8] \cdot H_2O$ (RE(III) = Gd **1**, Tb **2**, Dy **3**, pzam = pirazin-2-carboxamida) . Stanga: curbele experimentale $\chi T/T$ (simbol) si cele teoretice din date *ab initio* (lines). Dreapta: Tensorii magnetizarii calculati prin metode CASSCF-SO pentru starea fundamentala pentru centrii *f* .



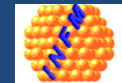
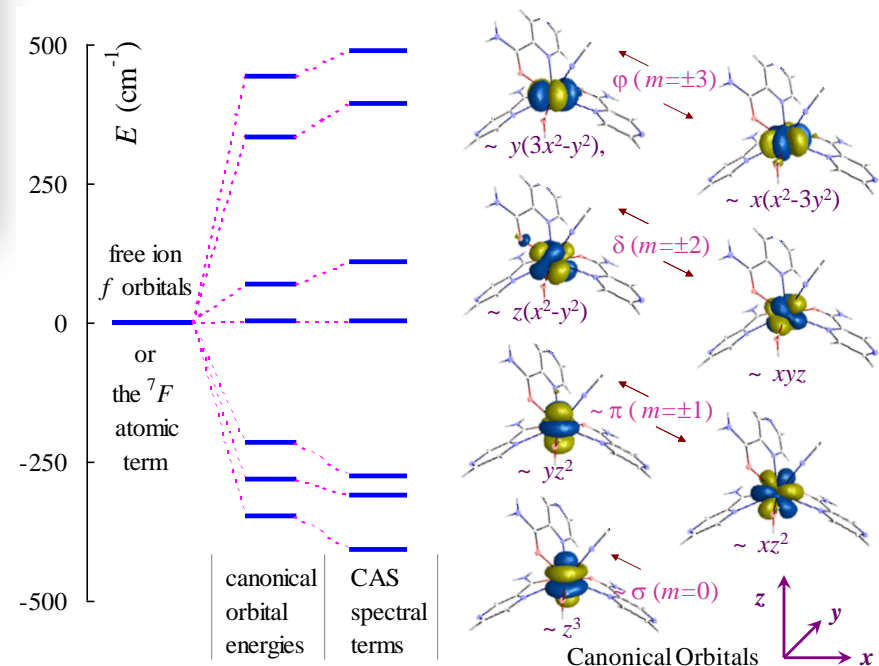
Noi dezvoltari conceptuale asupra anizotropiei magnetice



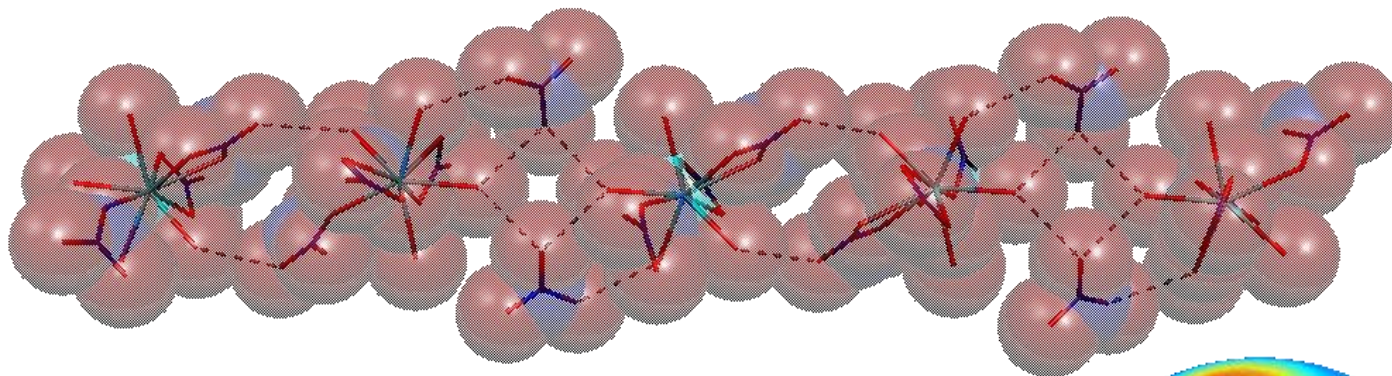
Orbitalii unitatii dinucleare $[Lu(pzam)_3(H_2O)(NClLi)][Wo(CN)_8]$
Orbitali moleculari selectati, SOMO cu caracter $5d^1$ si componente f sunt reprezentate in dreapta cu energiile corespunzatoare in stanga. Orbitalii cu contributie f sunt interiori, confirmand configuratia non-*aufbau* in cazul complexilor paramagnetici cu lantanide. Prin ionii $Lu(III)$, f^{14} , situatia non-*aufbau* este evitata.

Corelatii magneto-structurale in lanturile 4f-5d cu punti ciano

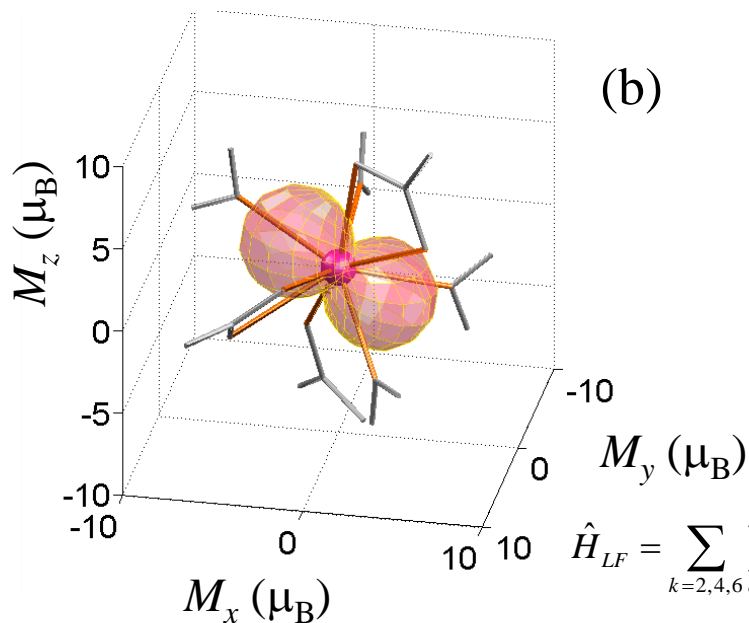
Parametrii de Camp al Liganzilor (LF) rezultate din calcule CASSCF pentru unitatea de $Tb(III)$.



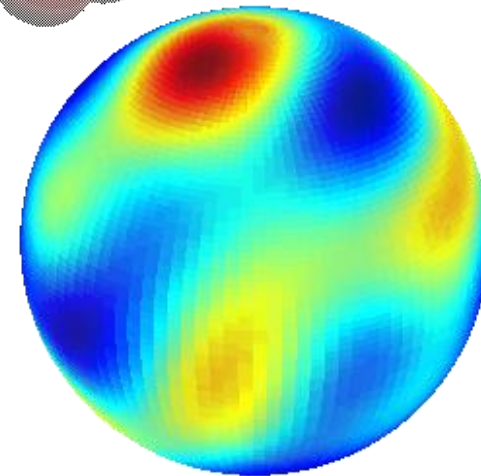
(a)



(b)



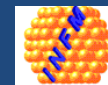
(c)



$$\hat{H}_{LF} = \sum_{k=2,4,6} \sum_{q>0} \sqrt{\frac{4\pi}{2k+1}} \left[B_q^k (Y_{k,q} + (-1)^q Y_{k,-q}) + i B_{-q}^k (Y_{k,-q} - (-1)^q Y_{k,q}) \right] + \sum_{k=2,4,6} \sqrt{\frac{4\pi}{2k+1}} B_0^k Y_{k,0}$$

Sinopsis al analizei magneto-structurale pentru unitatile $[\text{Er}(\text{NO}_3)_3(\text{H}_2\text{O})_4]$.

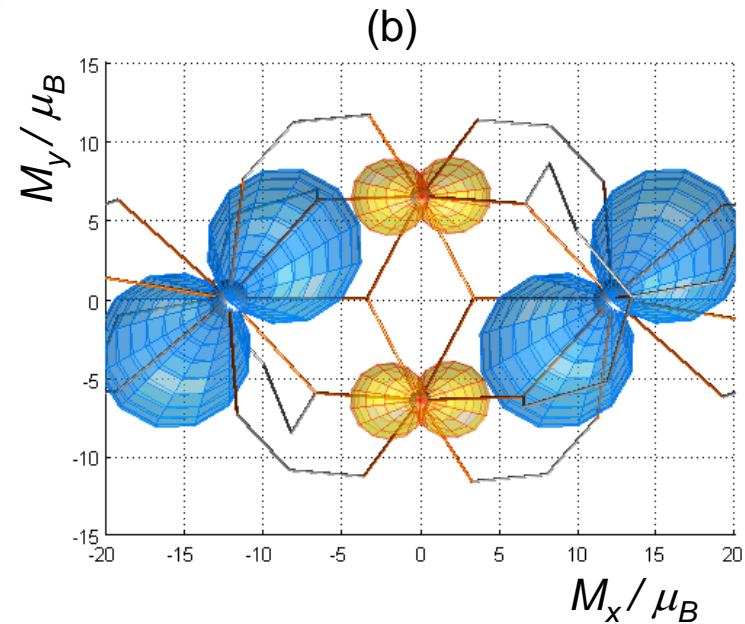
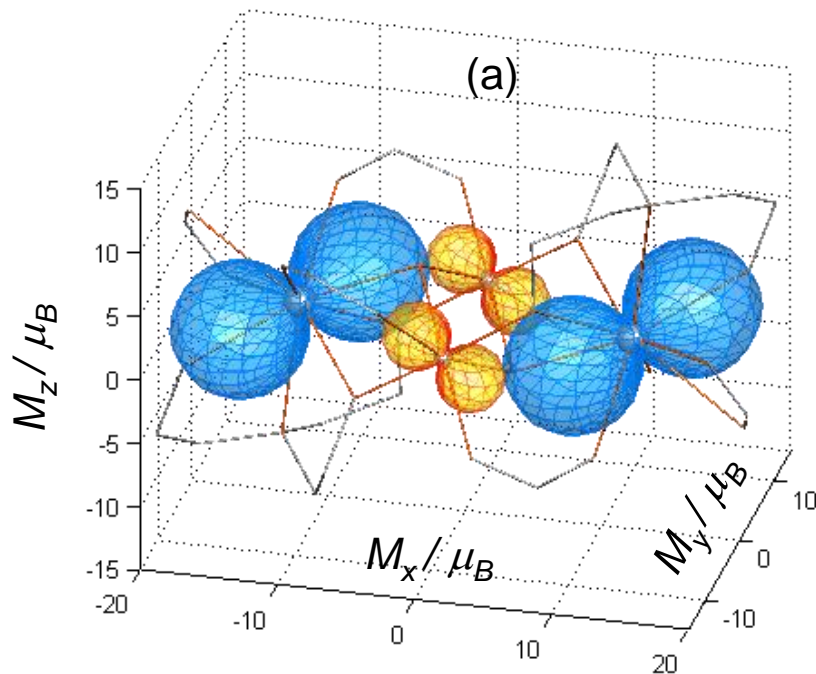
a) Structura extinsa a unitatii complexe. (b) Anizotropia magnetica in starea fundamentala. (c) Harta Campului Liganzilor. Notam coincidenta intre axa de usoara magnetizare si maximul potentialului de camp al liganzilor.



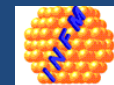
Noi dezvoltari conceptuale asupra anizotropiei magnetice

Anizotropia magnetica si cuplajul de schimb intr-o familie isostructurala de complexi $\text{Fe}^{\text{III}}_2\text{Ln}^{\text{III}}_2$

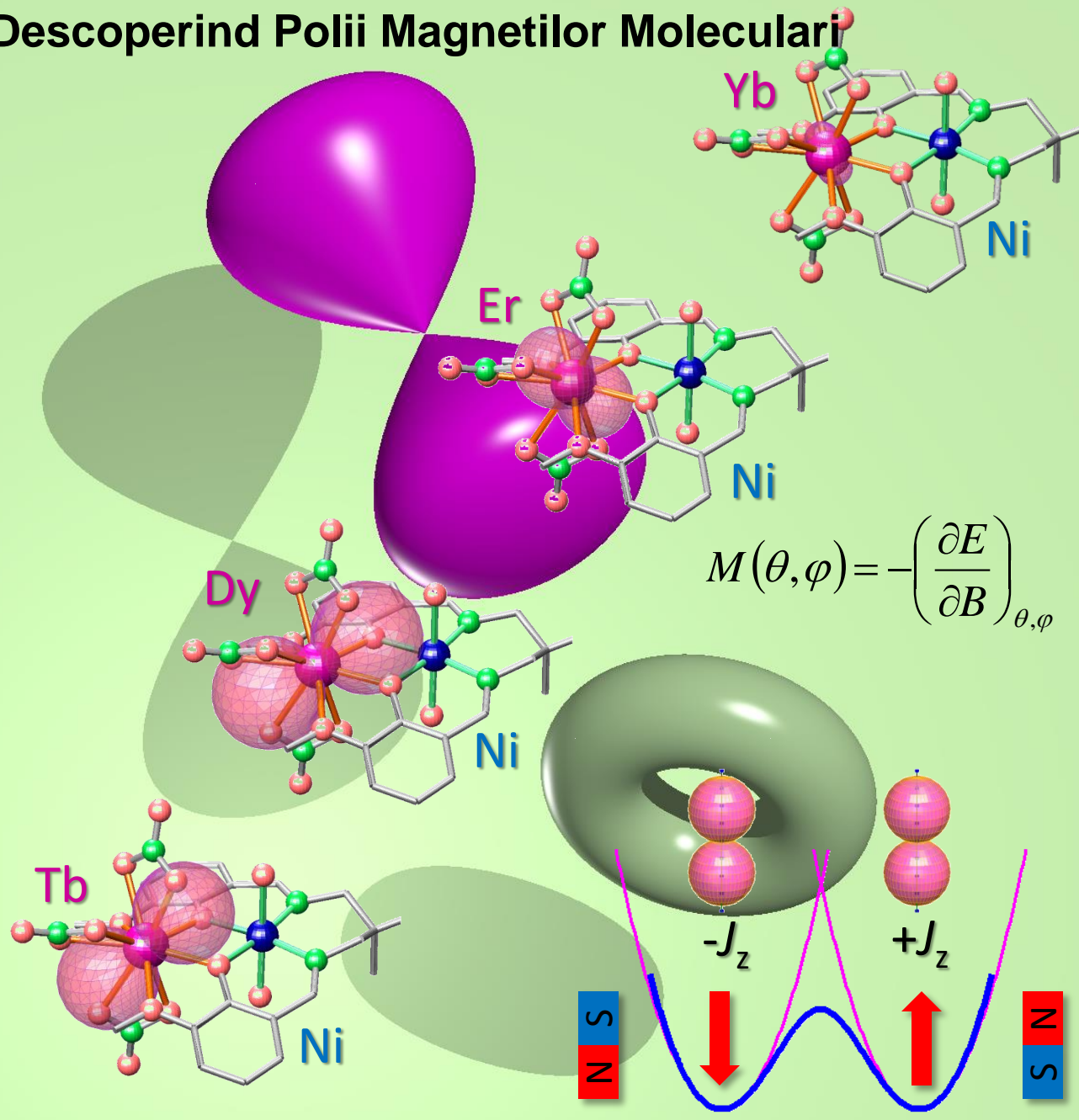
Colaborare cu Prof. A.Powell, Germania



Reprezentarea polara a functiilor $M_i(\theta, \varphi) = |dE/dB|_{(\theta, \varphi)}$ ale starilor fundamentale ale ionilor de Dy(III) -in albastru si Fe(III) in galben dintr-un sistem $\{\text{Fe}_2\text{Dy}_2\}$ compound cu puncti oxo si carboxilat. Panelurile (a) si (b) redau orientari diferite ale aceleiasi reprezentari.

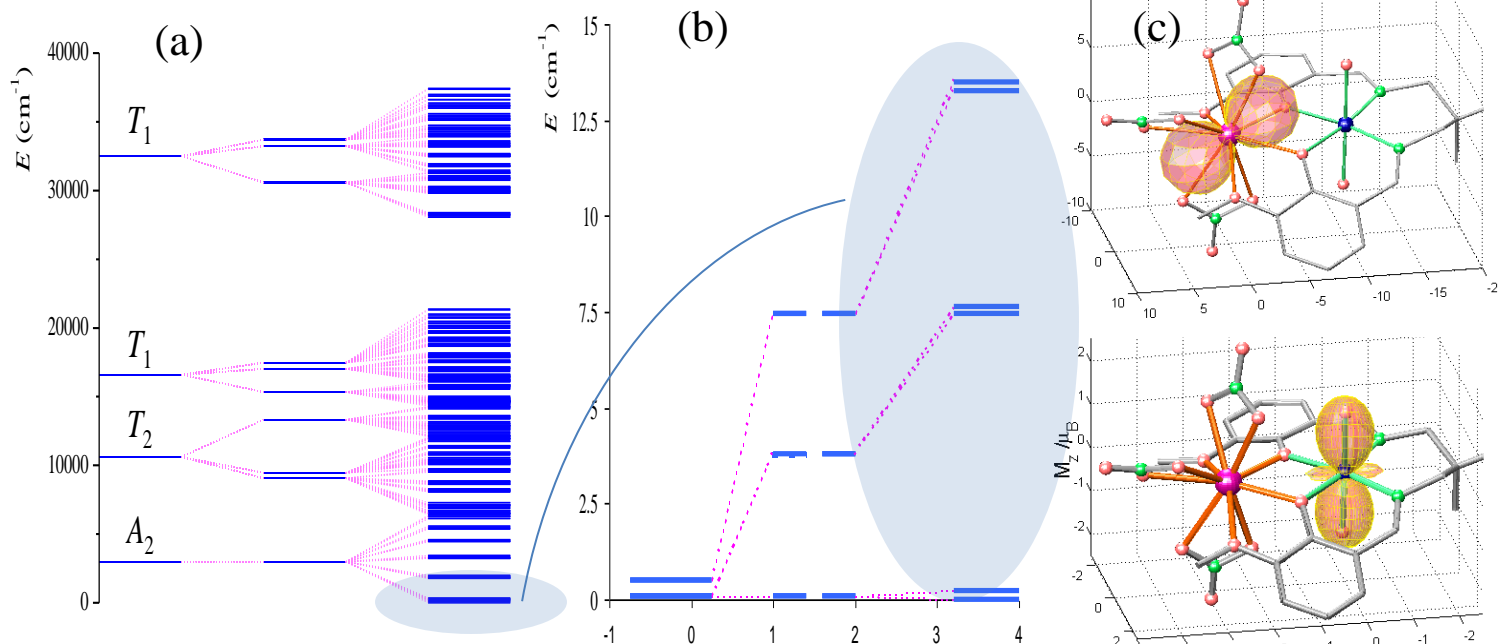


Descoperind Polii Magnetilor Moleculari

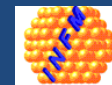


Cristalizarea chirala intr-o serie de heterobinucleari Ni-Ln: o analiza complexa a proprietatilor magnetice.

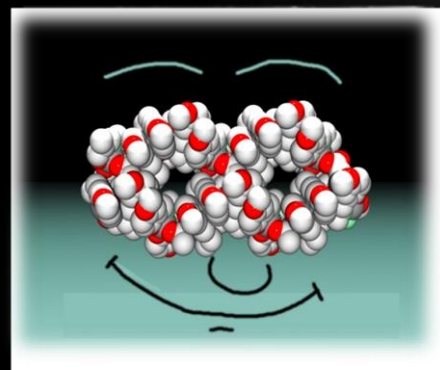
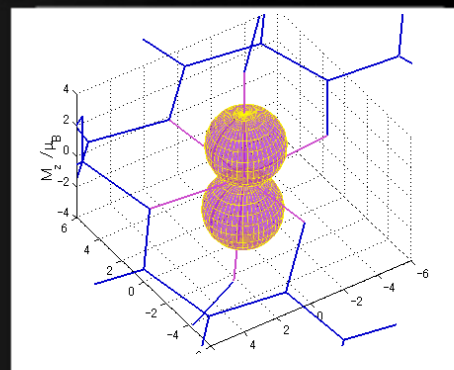
Colaborare cu Prof. J-P. Costes, Franta



Esalonarea la diverse scale a spectrului de stari determinant al efectelor optice si magnetice si anizotropiei in sistemul $[(\text{H}_2\text{O})_2\text{NiL}]\text{Tb}(\text{NO}_3)_3$ realizat cu un ligand bicameral. (a) termenii spectrali idealizati octaedric (partea stinga din graficul a) in raport de starile de cimp al liganzilor al centrului de Ni(II) (mijlocul graficului a) si intregul sistem de stari implicat de cuplajul cu ionul Tb(III) (partea dreapta din a). (b) segmentul de stari fundamentale ce justifica descrierea printr-un hamiltonian Ising a cuplajului anizotropic Ni-Tb. Aceste stari rezulta prin magnificarea partii inferioare a spectrului complex din stinga graficului din panelul (a). In (c) sint reprezentate functiile magnetizarii in starea fundamentala a ionilor Ni(II) si Tb(III) in complexul dat.



**Povești despre IDEI
complexe și
oameni de succes**
12 decembrie 2013

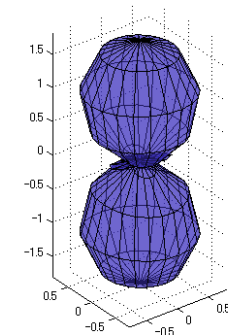
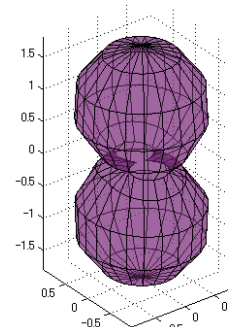
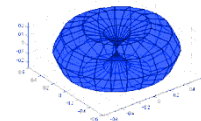
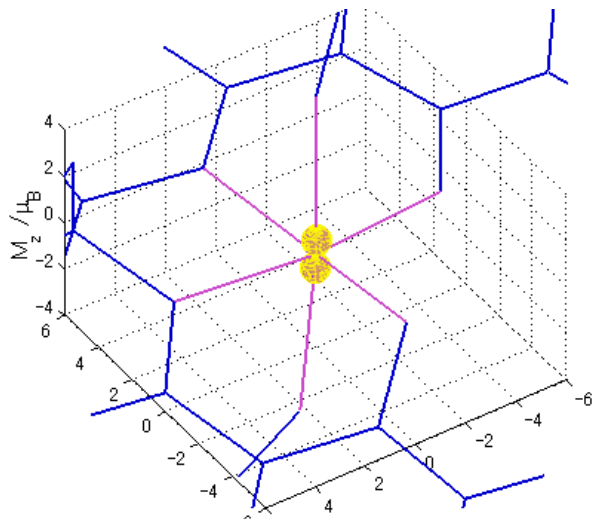


Inter caetera

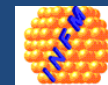
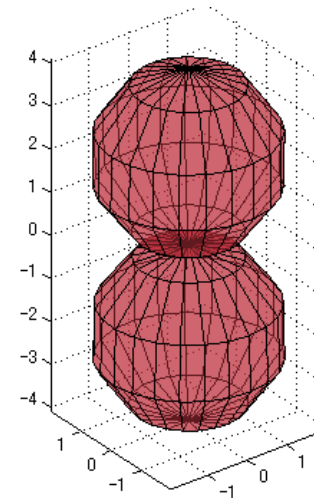
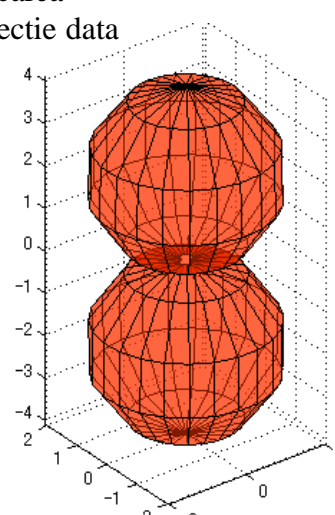
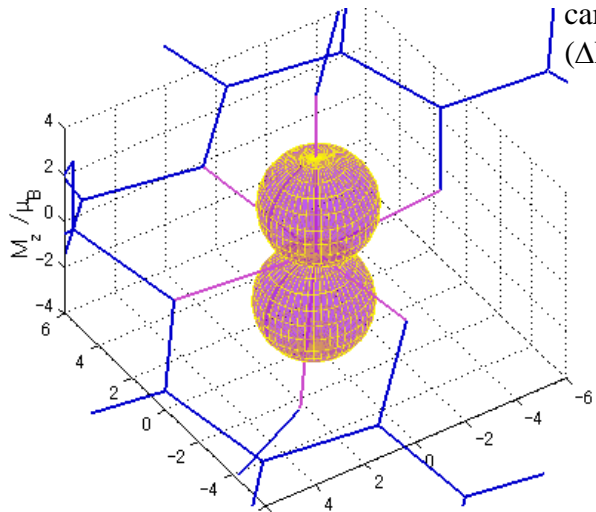


Anizotropia magnetica a starilor ZFS ale unitatilor cu $D < 0$

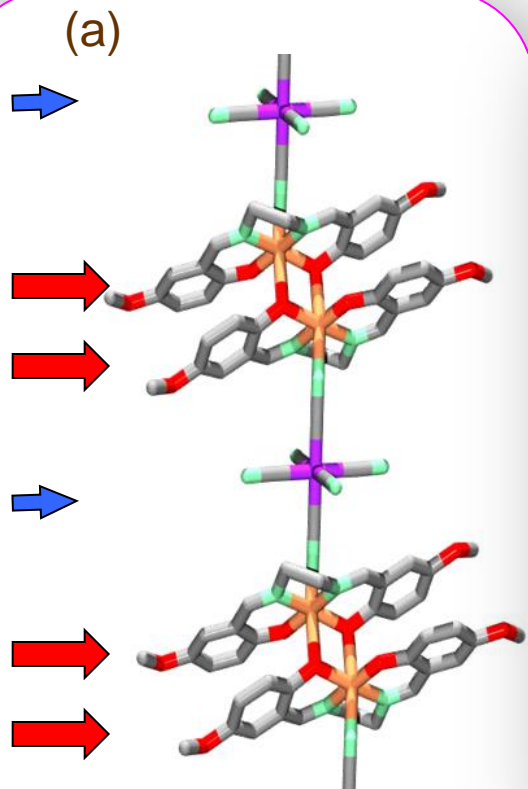
[Mn^{III}(5MeoSalen)]⁺



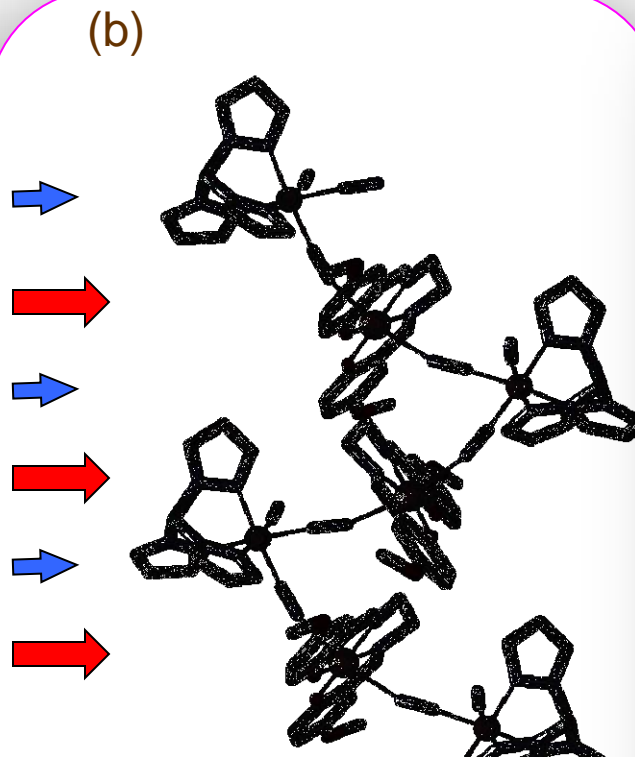
Calculate ca raspuns la aplicarea
 campului magnetic pe o directie data
 ($\Delta E_i / \beta H$)



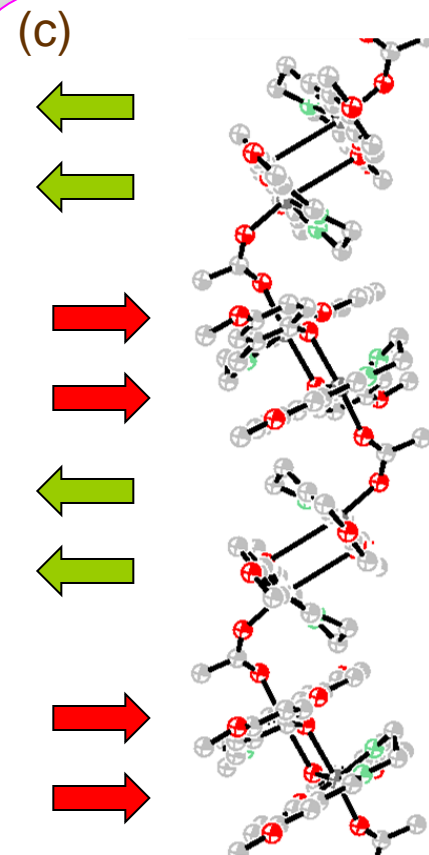
Anizotropia magnetica a starilor ZFS ale unitatilor cu $D < 0$



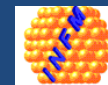
SCM



METAMAGNET



SMM-uri cuplate antifero

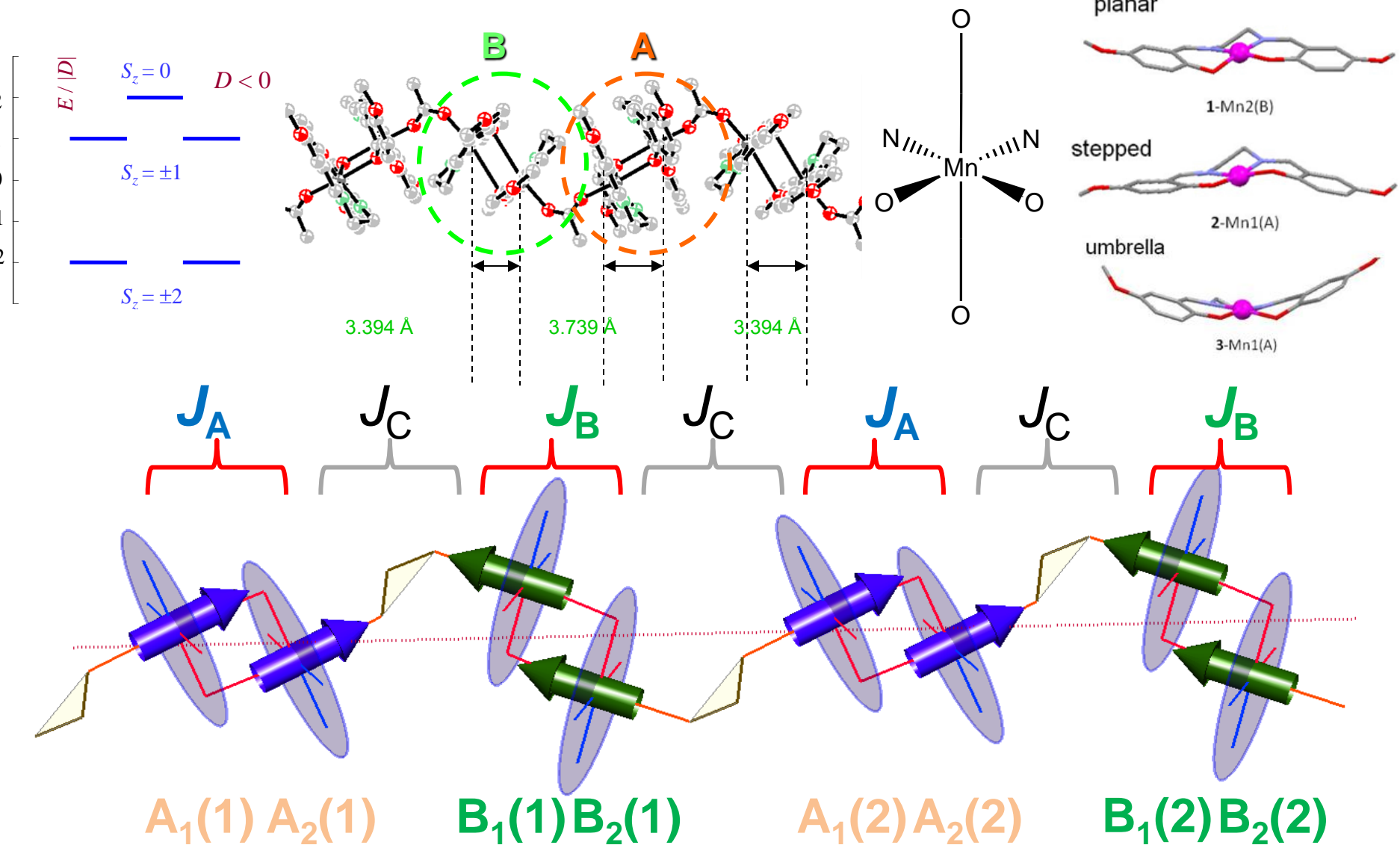


Sisteme cu un magnetism complex $[\text{Mn}_2(5\text{MeOsalen})_2(\text{CH}_3\text{COO})\text{X}]$, $\text{X} = \text{ClO}_4, \text{PF}_6, \text{CF}_3\text{SO}_3$

Cuplaj feromagnetic in unitatile $\{\text{Mn}_2\}$ si cuplaj antiferomagnetic intre ele.

Anizotropia magnetica pentru toate unitatile Mn este $D < 0$

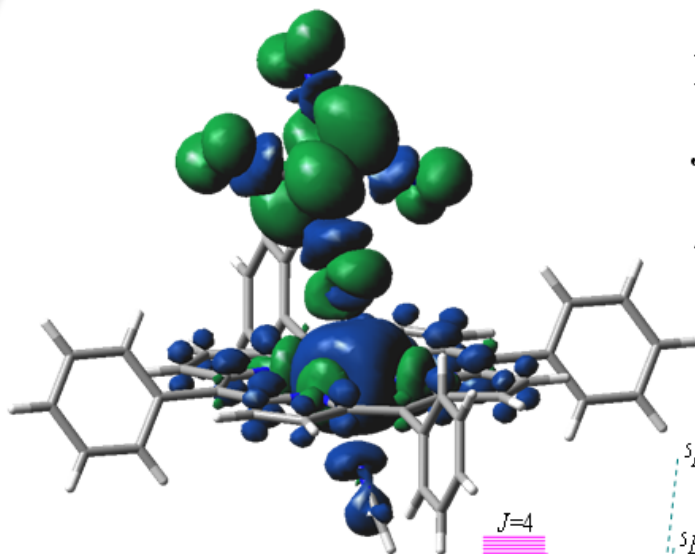
Geometria fiecarui ion Mn (III) este Oh alungit planar



Sisteme prototipice pentru anizotropia ionilor tranzitionali d

Studiul complexelor de Mn(III) și derivati de porfirina, cu topologie de octaedru alungit, care, asamblati cu liganzi purtatori de spin (e.g. tetraciano-etilena) conduc la compusi de tip magnet unidimensional.

S-a realizat tratamentul DFT al proprietatilor de schimb (parametri J) și anizotropie (parametri $D < 0$ in Hamiltonianul ZFS), cu explicitarea rolului campului liganzilor.



and



$J=4$
 $J=3$
 $J=2$
 $J=1$
 $J=0$

SO

${}^5B_{2g}$
 5E_g
 5D
 ${}^5A_{1g}$
 ${}^5B_{1g}$

LF (D_{4h})

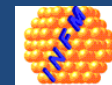
${}^5A_{1g}$
 ${}^5B_{1g}$
 $D > 0$
 $D < 0$
LF (D_{4h})+SO \equiv ZFS

$s_z = \pm 2$
 $s_z = \pm 1$
 $s_z = 0$
 $s_z = 0$
 $s_z = \pm 1$
 $s_z = \pm 2$

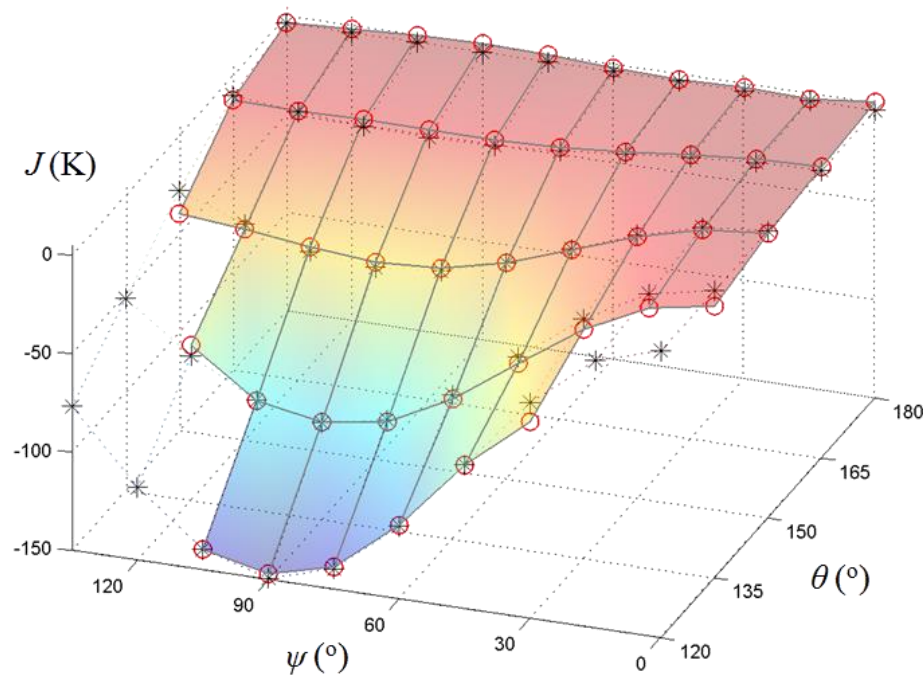
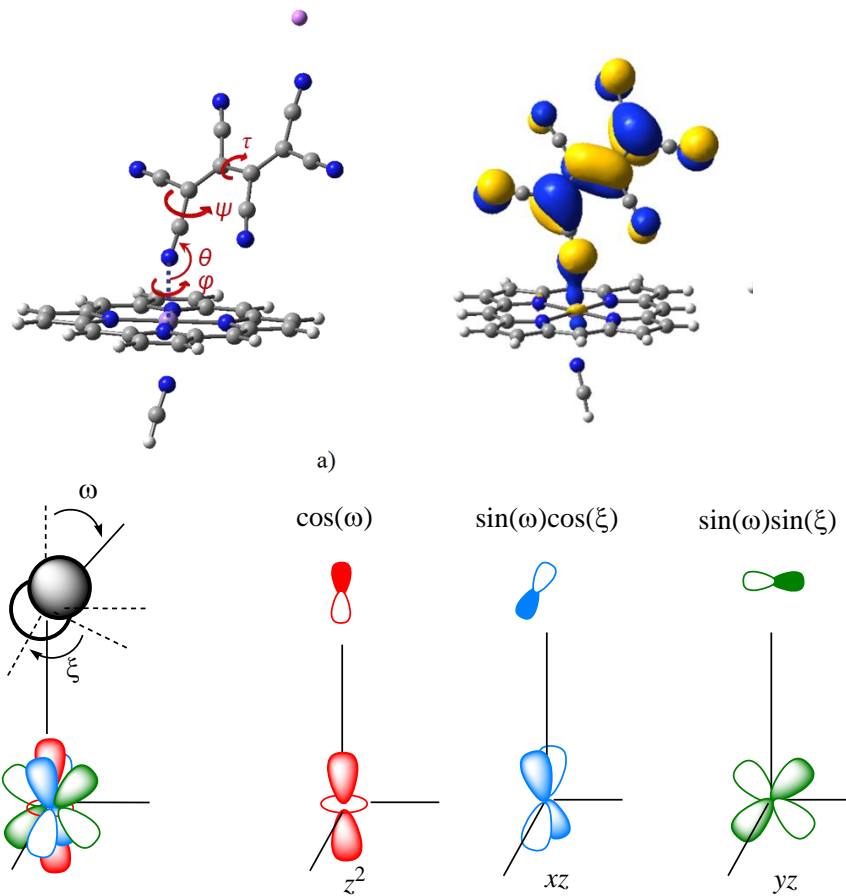
DFT Broken Symmetry

J vs. geometry

ZFS vs. Ligand Field



[MnOEP][HCBD] & [MnTtBuPP][HCBD] vs. [MnTPP][TCNE]

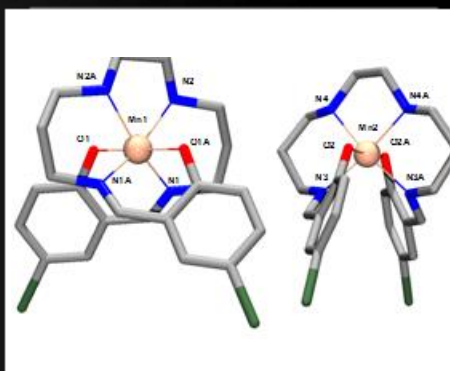


$$2J = \frac{1}{4} (2K - U_{\sigma} S_{\sigma}^2 \cos^2(\omega) - U_{\pi} S_{\pi}^2 \sin^2(\omega))$$

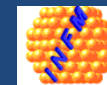
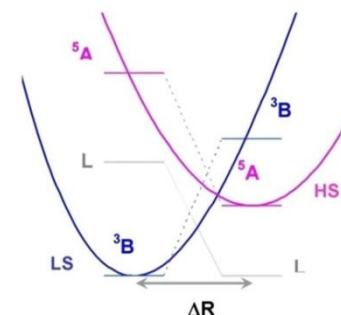
$$\cos(\omega) = \sin(\theta) \sin(\varphi)$$

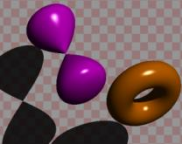
Fitarea rezultatelor calculelor a reliefat rolul determinat al suprapunerii $d_{z^2}-\pi^*$, prin unghiul θ , si al torsiunii scheletului butadienic prin unghiul τ .

Povești despre IDEI
complexe și
oameni de succes
12 decembrie 2013



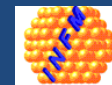
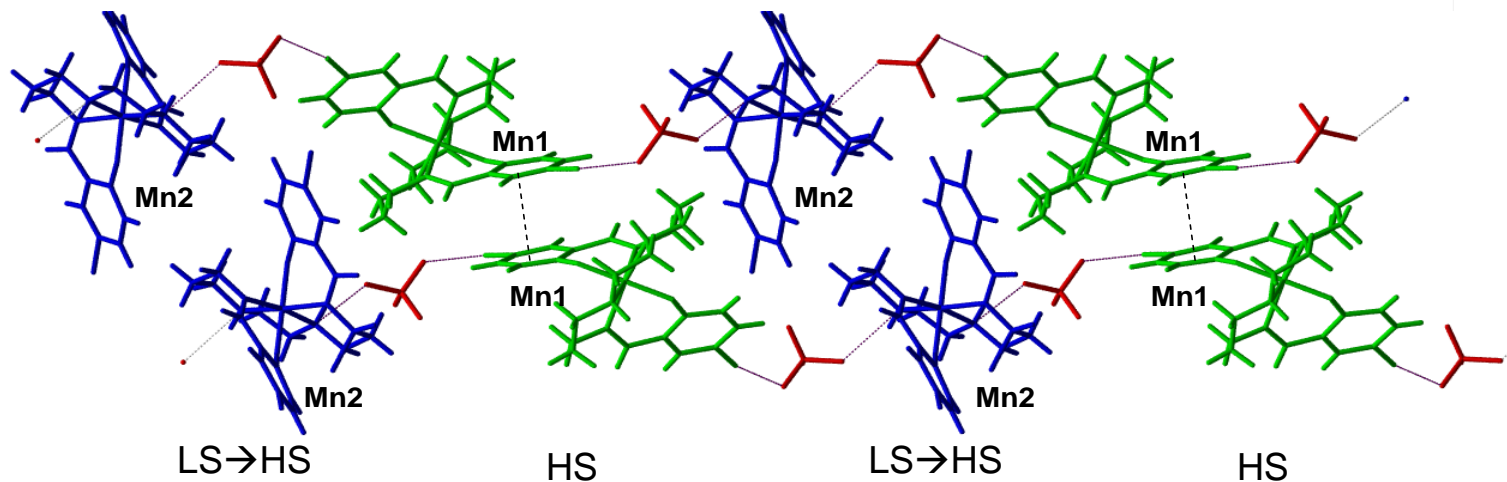
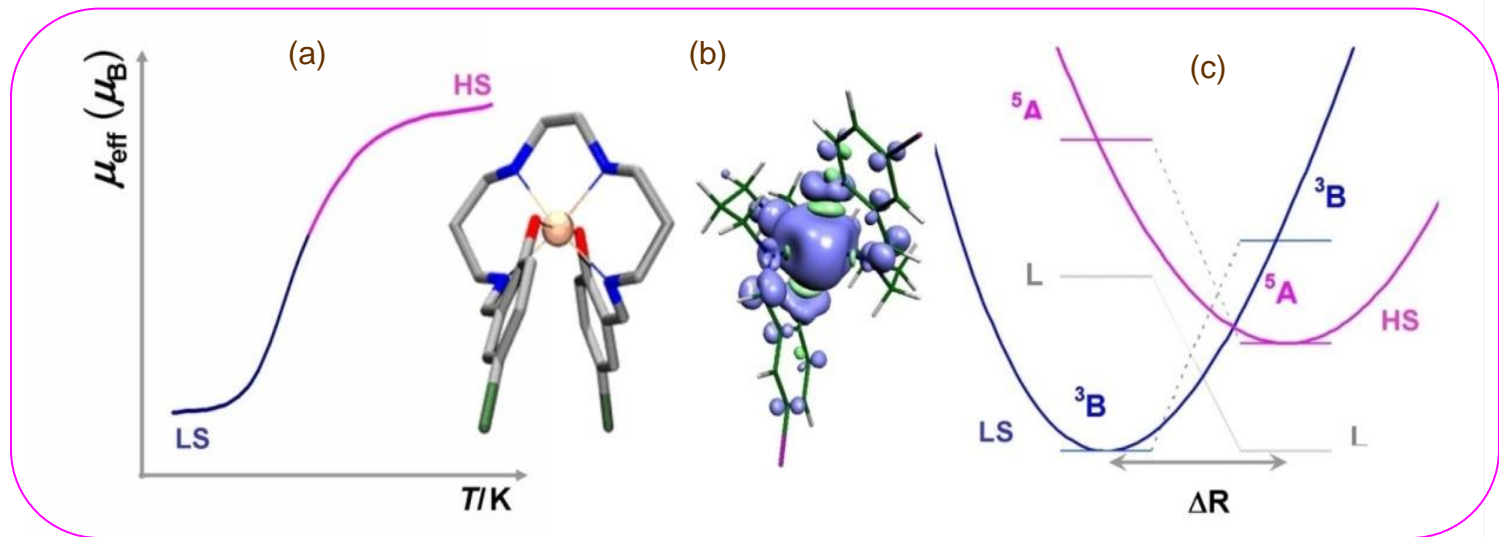
*Ita res
accendent
lumina rebus*

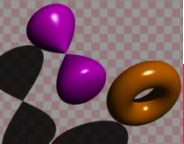




Tranzitie de spin in complexi de Mn(III). Anizotropie de tip D>0

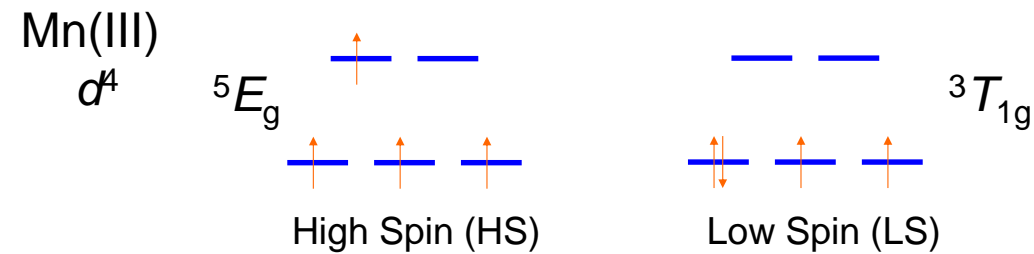
Studiul de caz al unui efect rar: analiza experimentală și teoretică a unui sistem de Mn(III) cu tranziție de spin



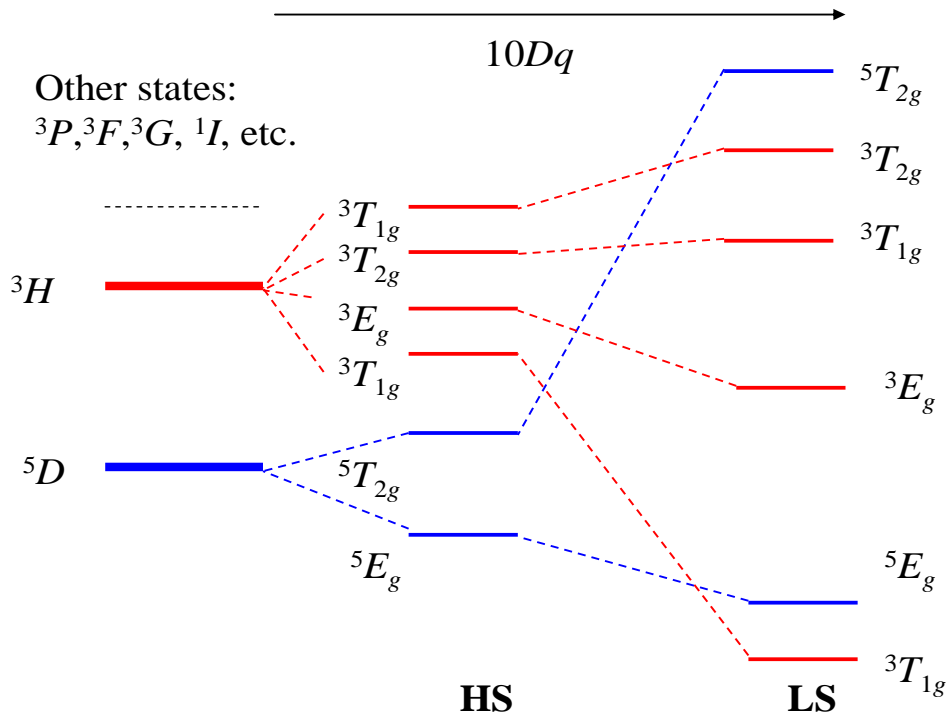


Tranzitie de spin in complexi de Mn(III). Anizotropie de tip D>0

Dependenta de taria campului liganzilor a tranzitiei de spin in complexii octaedrici ai Mn(III)



Energia de stabilizare in camp cristalin (LFSE) vs. energia de imperechere a spinilor.

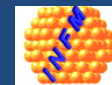


$$d^4 \left\{ \begin{array}{l} 10Dq \sim 6B + 5C \\ C \sim 4B \\ 10Dq \sim 26B \end{array} \right.$$

$$d^6 \left\{ \begin{array}{l} 10Dq \sim 2.5B + 4C \\ C \sim 4B \\ 10Dq \sim 18.5B \end{array} \right.$$

Termenii spectrali ai d^4 implicati in tranzitia de spin.

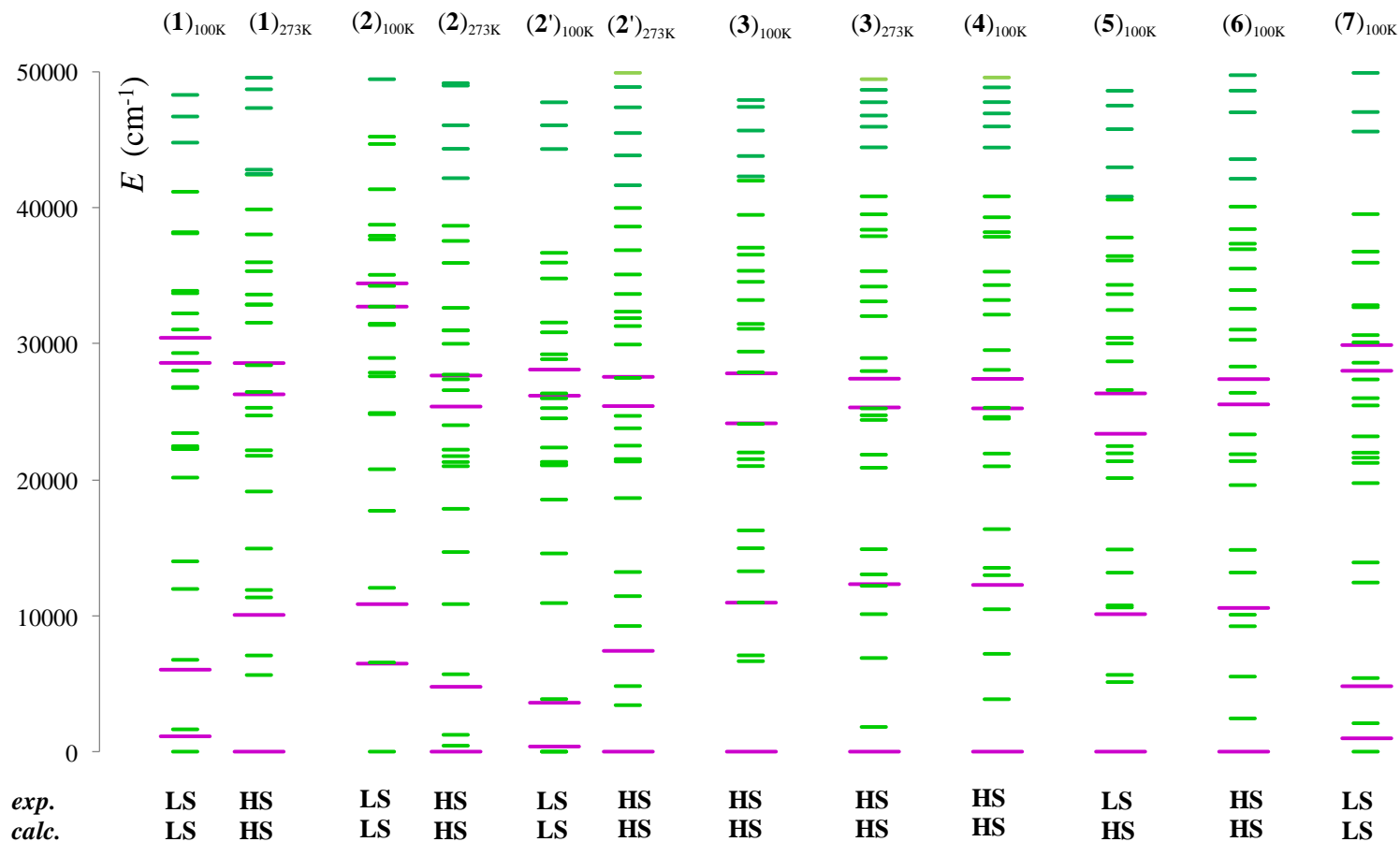
Comparand cu tranzitia d^6 ($^1A \rightarrow ^5T$), tranzitia d^4 ($^3T \rightarrow ^5E$) cere campuri mai inalte pentru a egala energia de imperechere a spinilor.



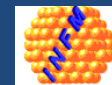


Tranzitie de spin in complecsi de Mn(III). Anizotropie de tip D>0

Termenii spectrali HS (violet) si LS (verde). Calcul vs. experiment

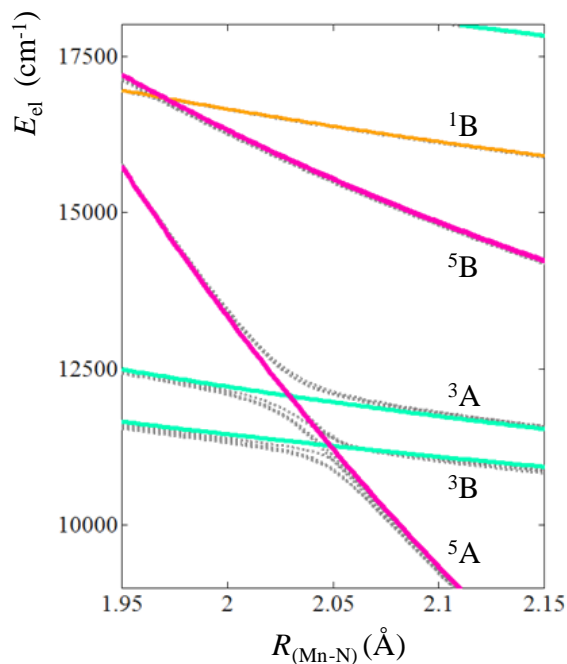


(1) Formele LS si HS ale speciilor active ale sistemului [Mn(5-Br-sal-N-1,5,8,12)]⁺; (2) si (2') doua specii cristalografice [Mn(3,5-Cl-sal-N-1,5,8,12)]⁺, fiecare in formele LS si HS la 100K vs. 273K, respectiv, (3) [Mn(3MeO-sal-N-1,5,9,13)]⁺ ; (4) [Mn(5-tert-butyl-sal-N-1, 5, 8, 12)]⁺; (5) [Mn(5-NO₂-sal-N-1, 5, 8, 12)]⁺; (6) [Mn(2-aceton-sal-N-1,5,8,12)]⁺; (7) [Mn(5-Cl-sal-N-1,5,8,12)]⁺.

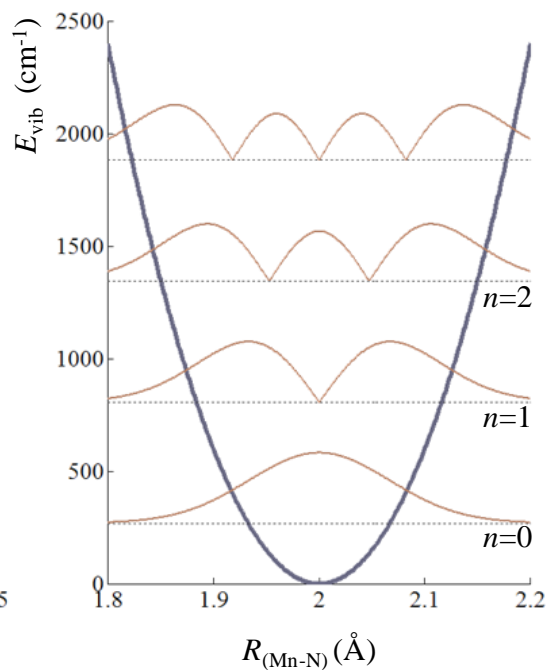




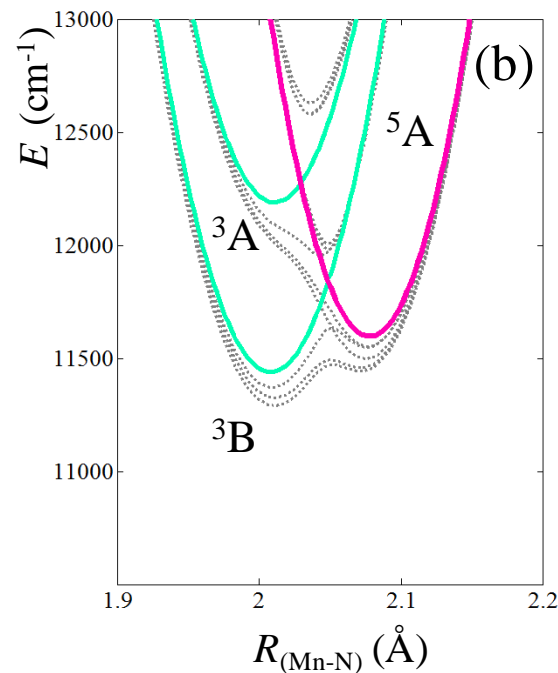
Factori concurenti: structura electronica, cuplaj spin-orbita si vibratie moleculara



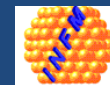
Incrucisarea termenilor HS-LS



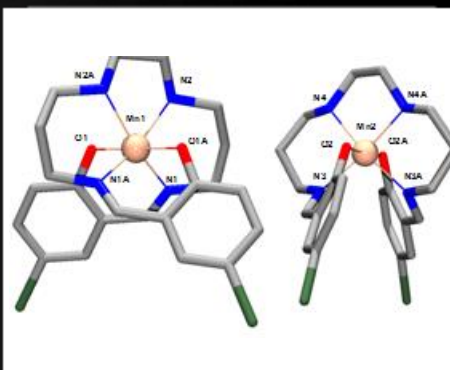
Vibratii armonice moleculare



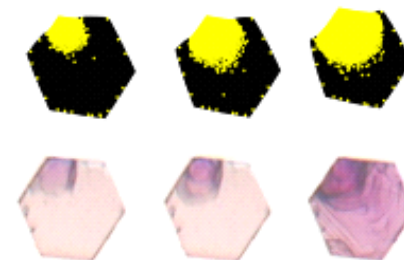
Suma componentelor electronice si vibrationale



Povești despre IDEI
complexe și
oameni de succes
12 decembrie 2013



*Ita res
accendent
lumina rebus*

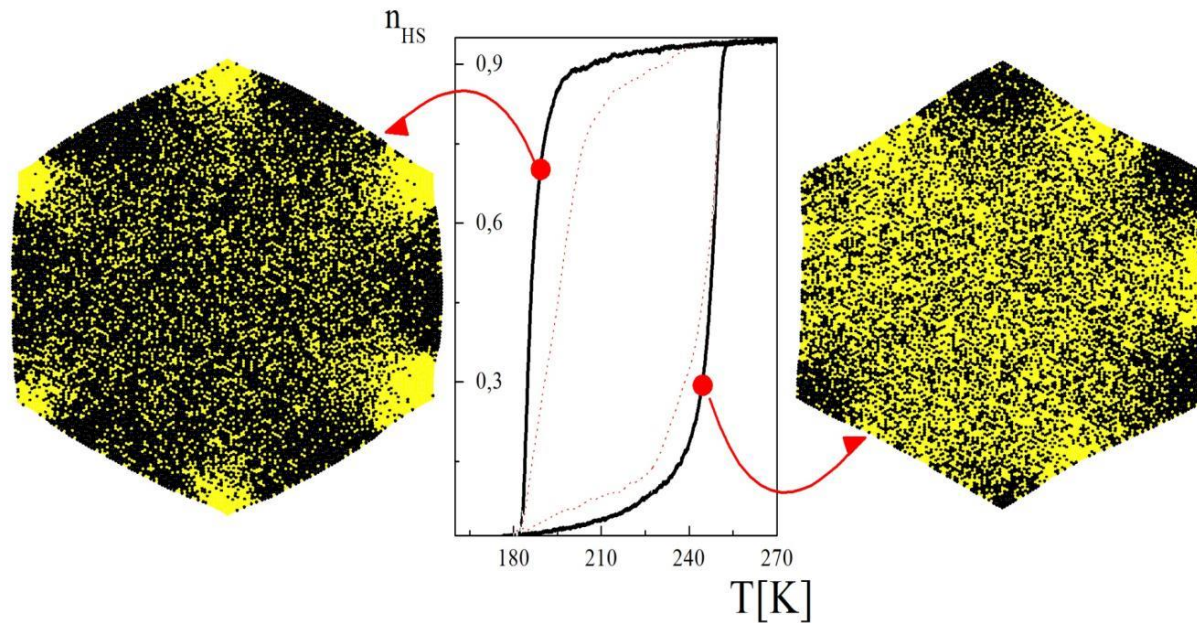


Model de interactiuni elastice pentru magnetii molecularari cu tranzitie de spin

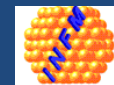
C. Enachescu, M. Nishino, S. Miyashita, A. Hauser, A. Stancu, L. Stoleriu, EPL, 2010

L. Stoleriu, P. Chakraborty, A. Hauser, A. Stancu, C. Enachescu Phys Rev B, 2011

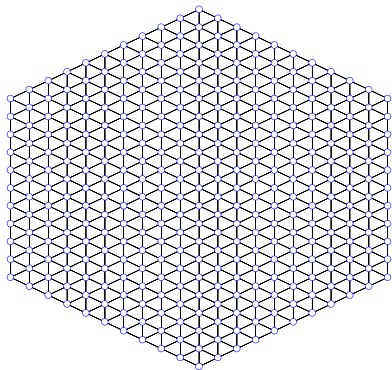
C. Enachescu, M. Nishino, S. Miyashita, A. Stancu, L. Stoleriu, Phys Rev B, submitted



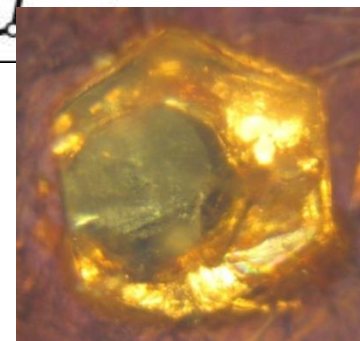
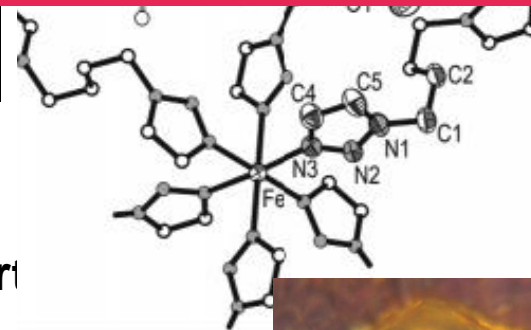
Folosind o singura constanta elastica, pentru ambele tipuri de interactiuni (scurte si lungi) din modelele precedente, am reprodus corect, pentru prima data, nu numai curbele macroscopice ci si evolutia clusterilor in sistem de la colturi.



Caracteristici



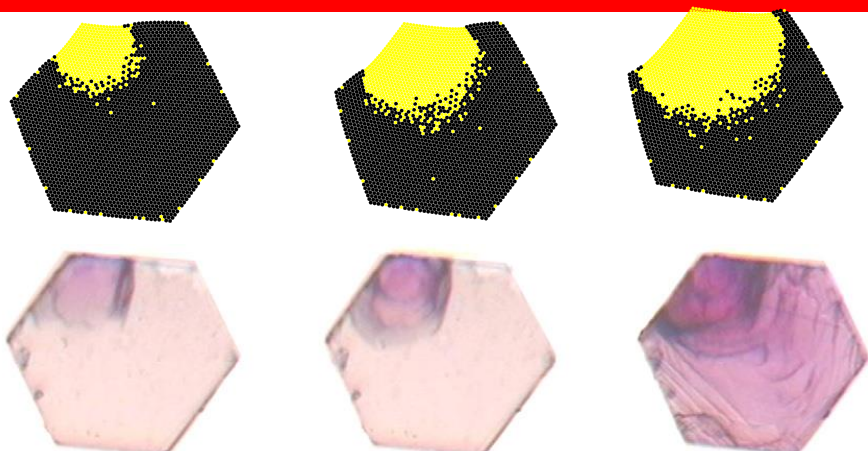
Sistem hexagonal
Margini libere
Molecule conectate prin resorti



Similar sistemului $[\text{Fe}(\text{bbtr})_3](\text{ClO}_4)_2$ studiat experimental in

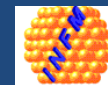
I. Krivokapic, C. Enachescu, A. Hauser et al, Inorg. Chem 2011

**Unul din putinele cazuri in care simularea a precedat si incurajat experimental:
Datele obtinute din model au fost confirmate experimental dupa un an.**



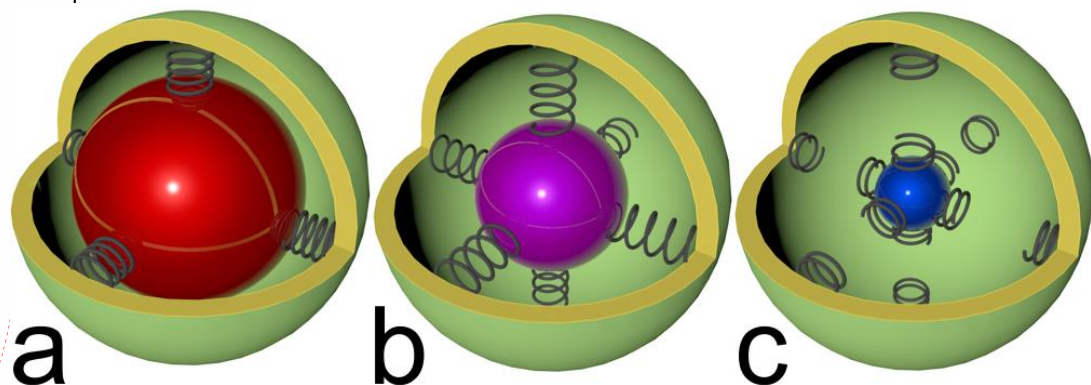
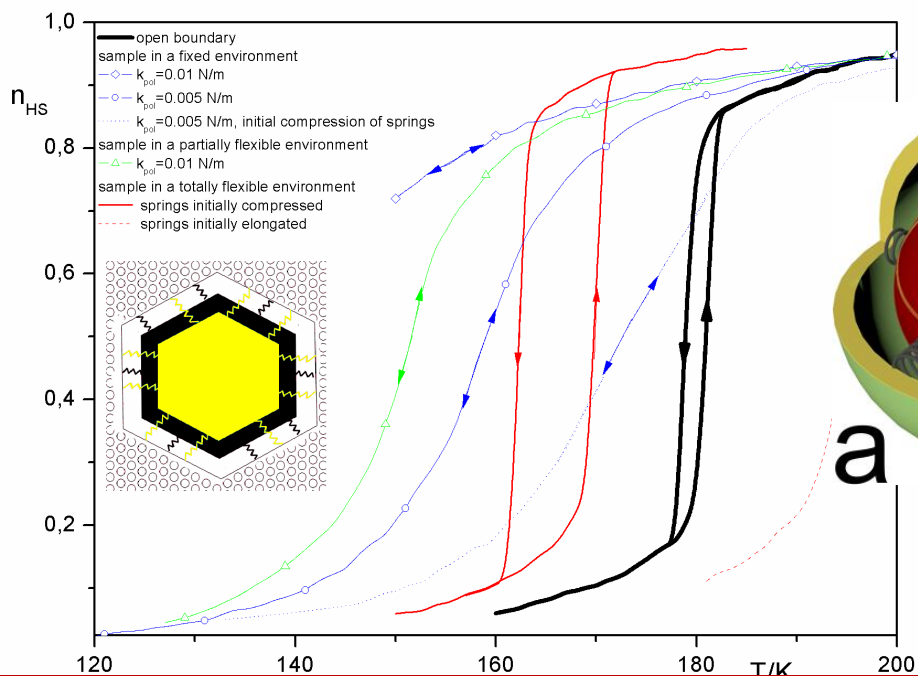
Model:
C. Enachescu, et al, Phys Rev Lett. 2009,
EPL 2010

Experiment:
F. Varret, et al, Phys Rev B. 504, 29,
2011(optical microscopy)



Pentru prima data s-a reusit explicarea histerezisului in nanoparticulele cu tranzitie de spin (masurat din 2008!!!), folosind modelul mecanoelastic ingloband sistemele in matrici:

- Ingustarea histerezisului;
- tranzitie incompleta si graduala
- deplasarea catre temperaturi mai mici

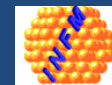


Interacțiunile dintre particulele cu tranziție de spin și polimer prezente inițial (a), se amplifică (b) și apoi dispar (c)

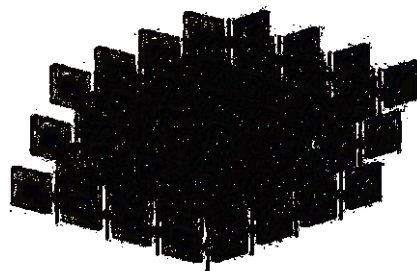
L. Stoleriu, A. Hauser, A. Stancu, C.Enachescu Phys Rev B, 2011

A. Tissot, M.L.Boillot, C.Enachescu J. Mater. Chem., 2012

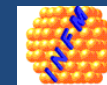
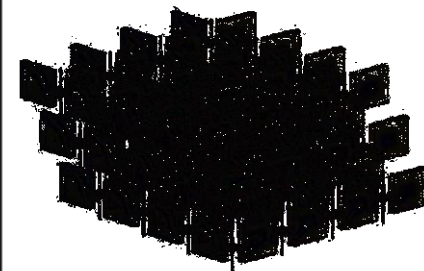
R. Tanasa, M.L.Boillot, C.Enachescu Appl. Phys. Lett., 2014



**Povești despre IDEI
complexe și
oameni de succes**
12 decembrie 2013



***Ubi Materia,
Ibi Geometria***

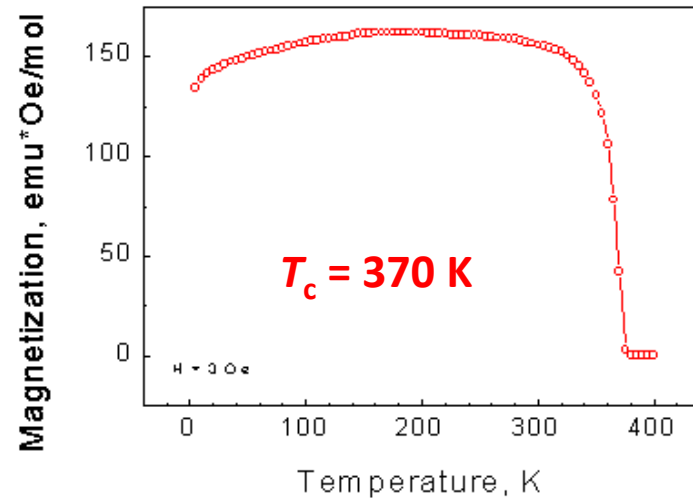
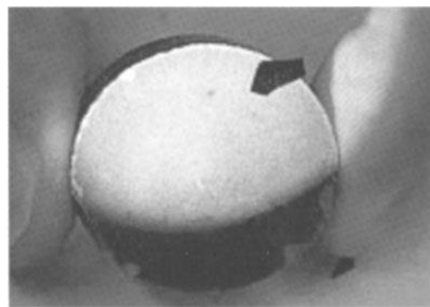
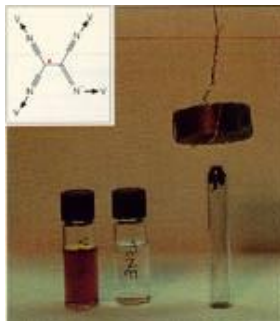




V[TCNE]_x - Primul magnet molecular la temperatura camerei

Aplicatii in spintronica – Valve de spin organice

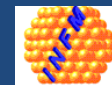
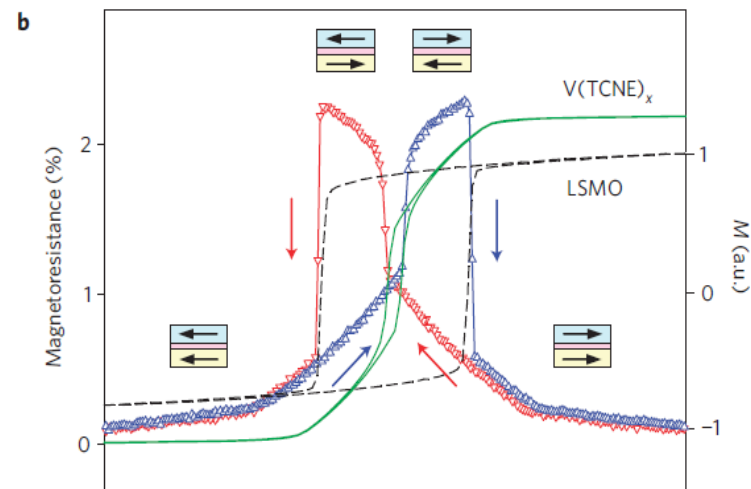
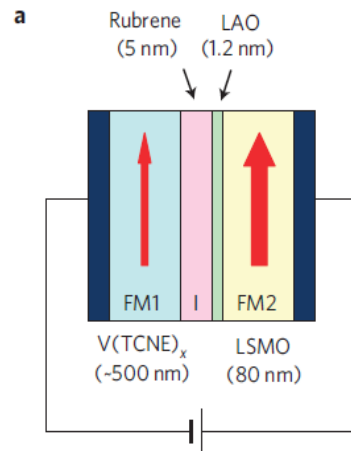
Miller & coworkers, Science **1991**, 252, 1415



Epstein & coworkers, Nature materials **2010**, 9, 638

Valve de spin:

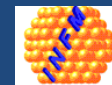
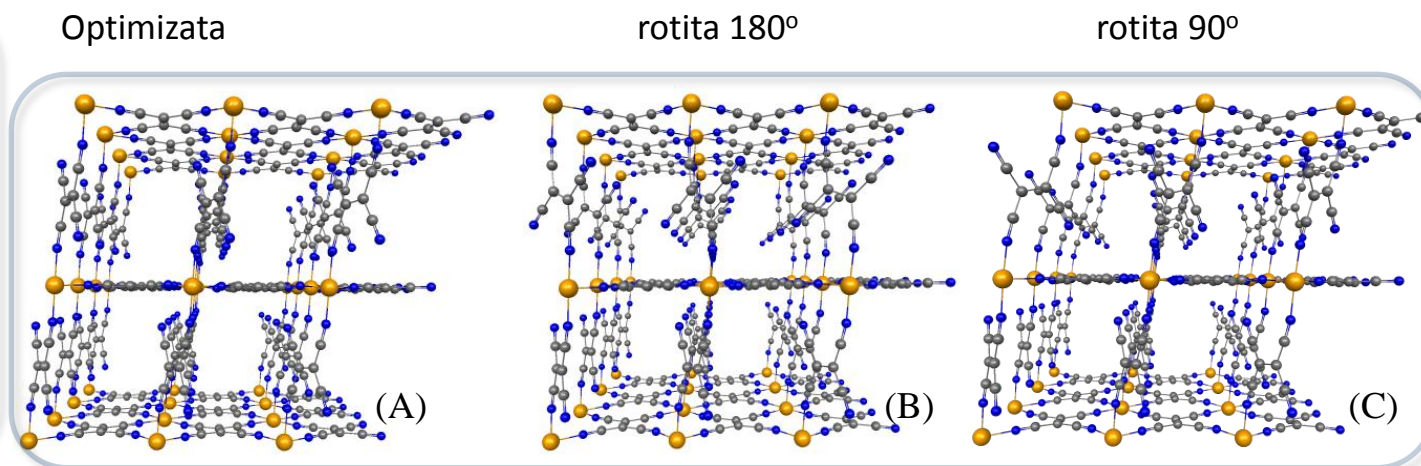
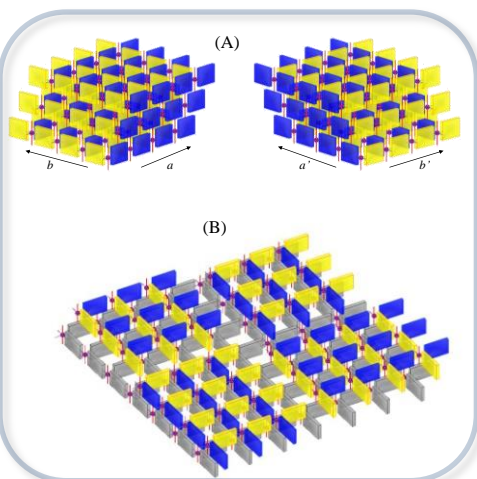
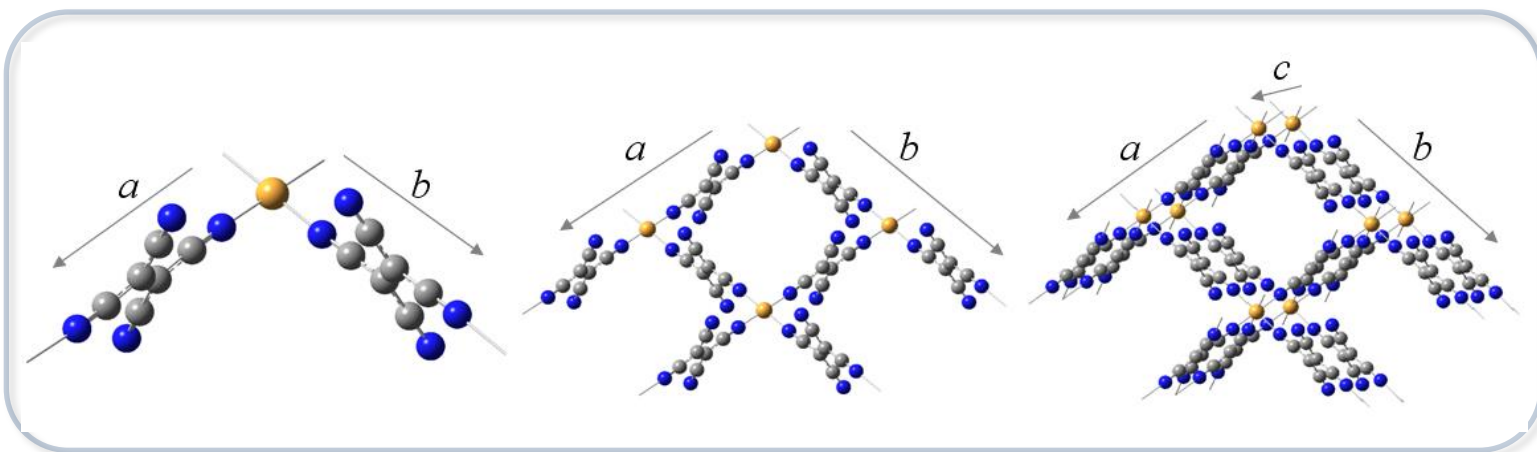
- Doua straturi magnetice conductoare separate de unul izolator.
- Rezistenta dispozitivului se modifica in functie de orientarea relativa a spinilor din cele doua straturi.



V[TCNE]_x – Structura. Originea dezordinii structurale

- *trans* TCNE-V-TCNE
- *ac* - TCNE coord-2
- *bc* - TCNE coord-4

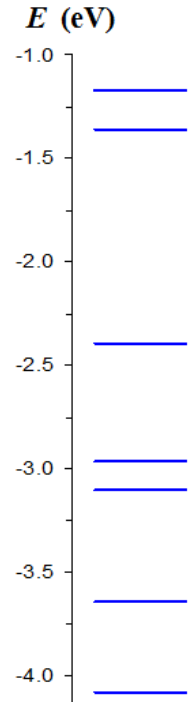
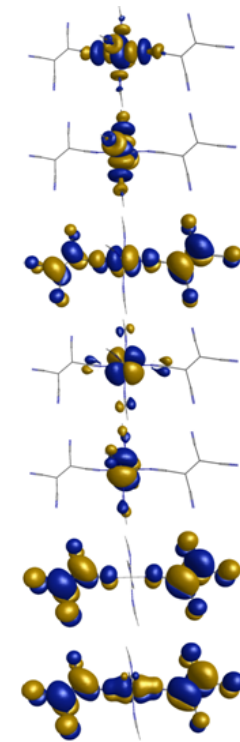
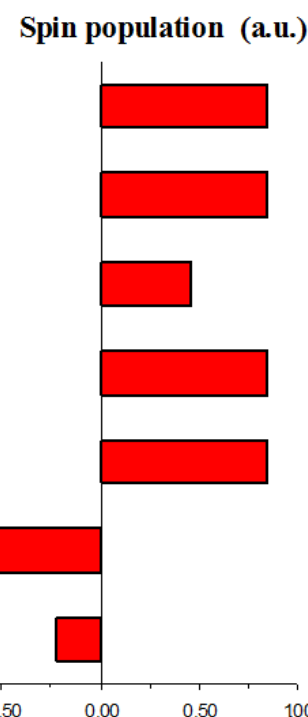
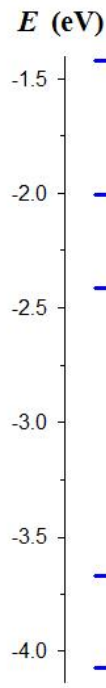
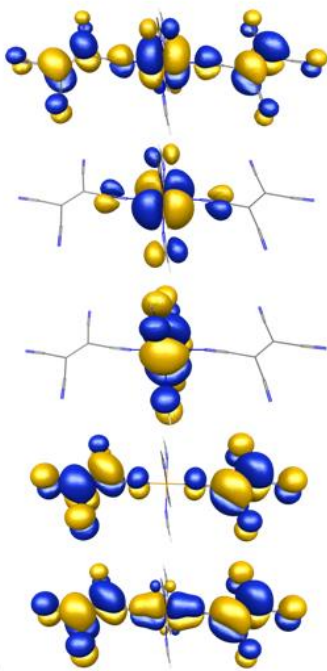
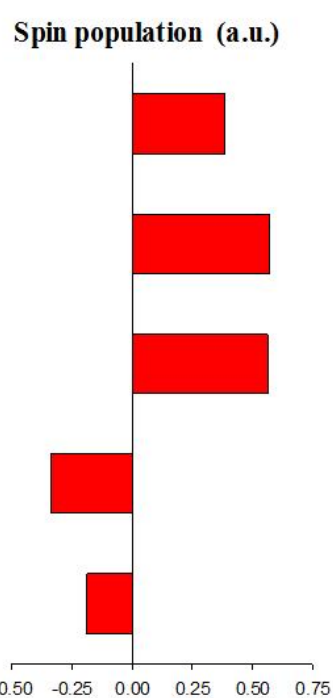
- amestec racemic a doi enantiomeri



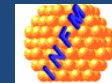
Taria interactiunii magnetice:

TCNE-V-TCNE vs. TCNE-Mn-TCNE

Traseele de superschimb pentru V mai numeroase si mai puternice decat pentru Mn.



Spini α pe V sau Mn, β pe TCNE.



V[TCNE]_x – Magnet molecular cu anizotropie aleatoare

$$\mathcal{H} = 2J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j - D_c \sum_i (\mathbf{n} \cdot \mathbf{S}_i)^2 - D_r \sum_i (\mathbf{n}_i \cdot \mathbf{S}_i)^2 - g\mu_B \sum_i \mathbf{H} \cdot \mathbf{S}_i$$

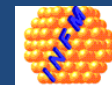
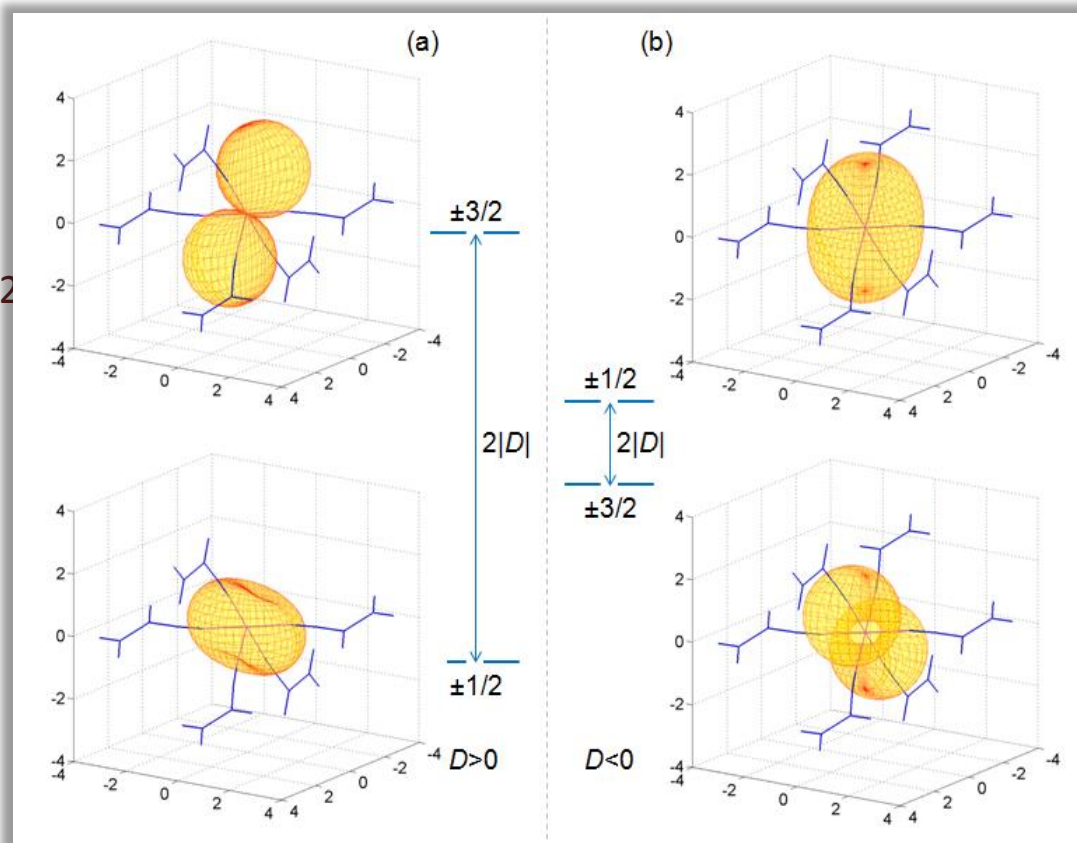
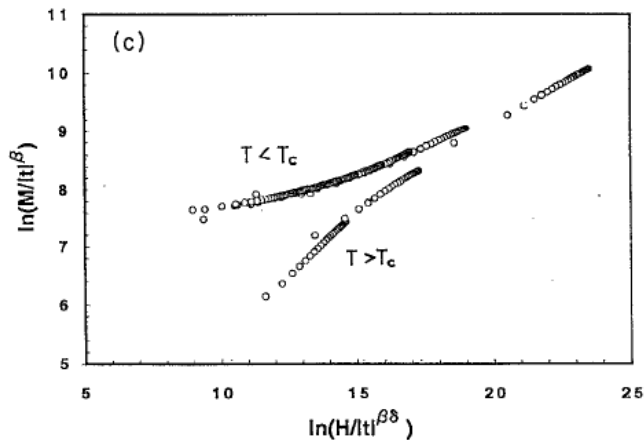
Calculul CASSCF:

$$10Dq \sim 18400 \text{ cm}^{-1}$$

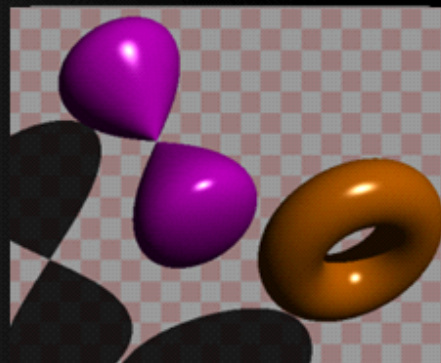
$$D_c \sim -0.03 \text{ K}$$

$$D_r \sim 0.45 \text{ K}$$

Epstein & coworkers, Phys. Rev. B **1993**, *48*, 132
 V[TCNE]_x – magnet cu anizotropie aleatoare



**Povești despre IDEI
complexe și
oameni de succes**
12 decembrie 2013

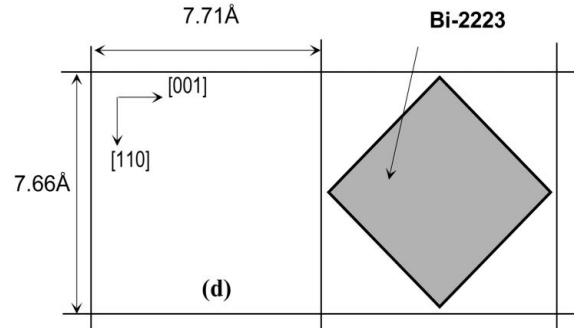
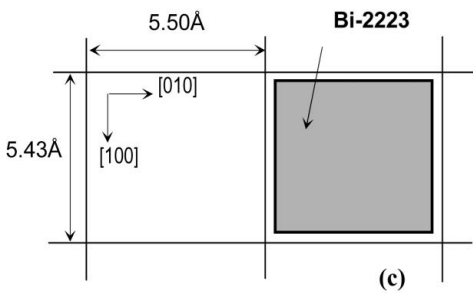
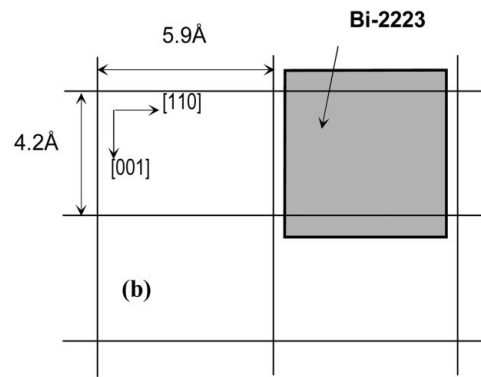
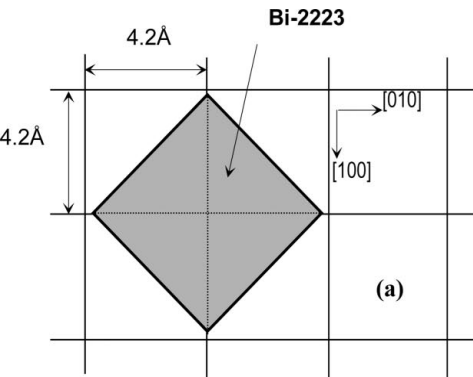


***Ubi Materia,
Ibi Geometria***

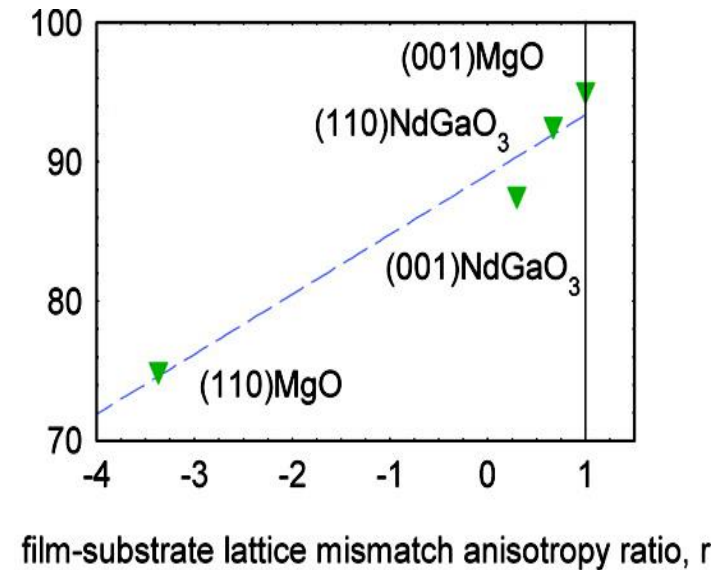


(001) $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ Superconducting Thin Films on Substrates with Large Film-Substrate Lattice Mismatch and Different Film-Substrate Lattice Mismatch Anisotropy

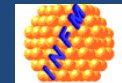
(001) Bi2223 straturi subtiri epitaxiale crescute pe diferite substraturi:
(a)- (001)MgO, b)- (110)MgO, c)- (001) NdGaO₃ si d)- (110) NdGaO₃.



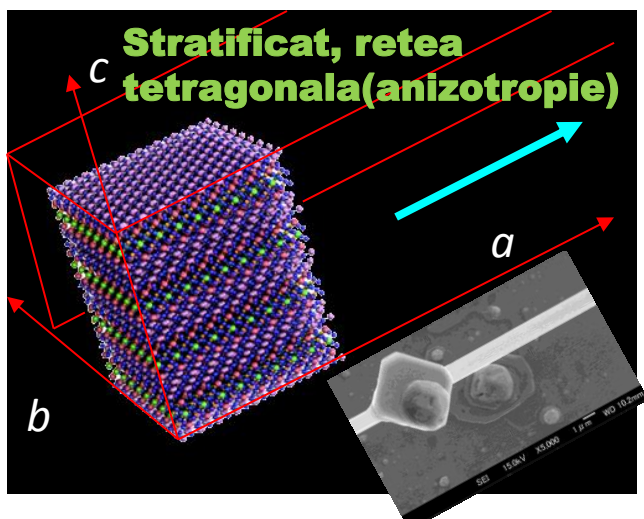
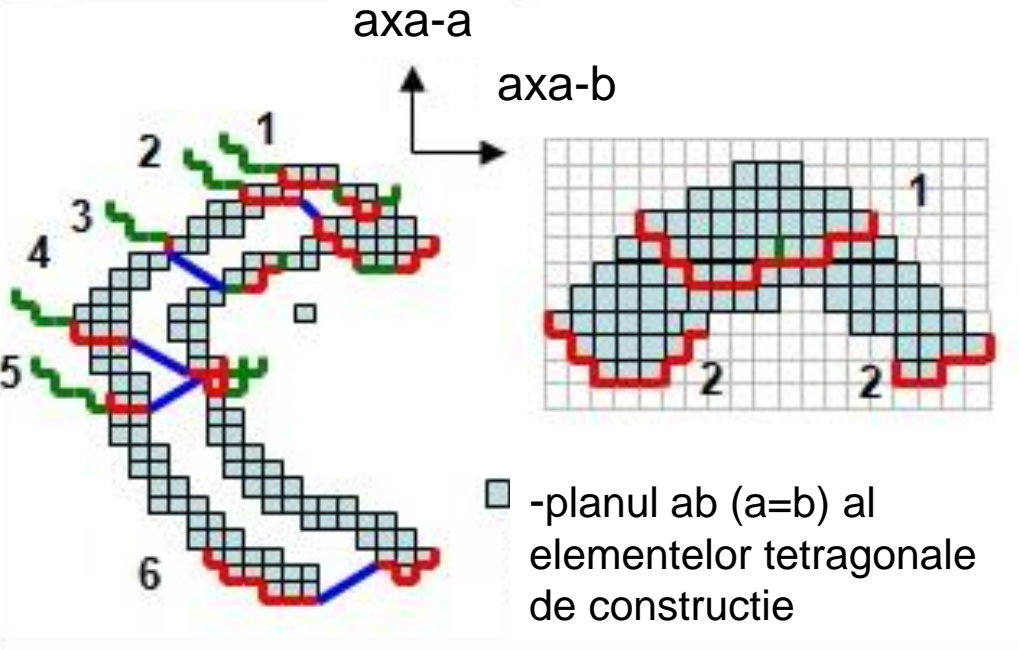
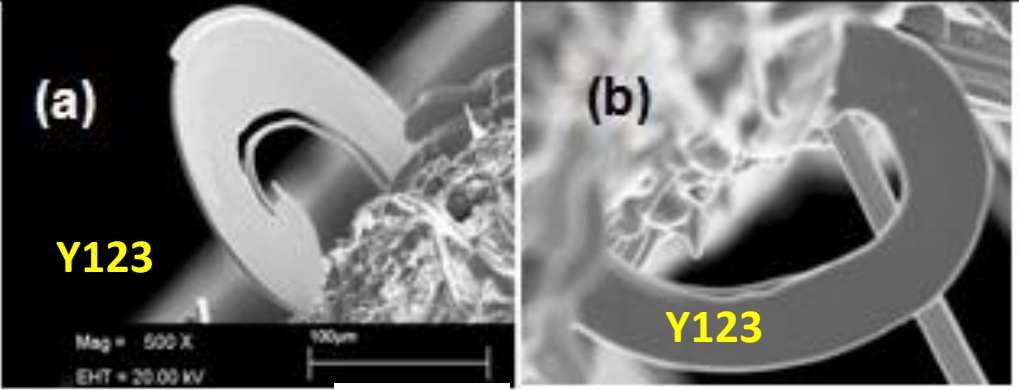
zero resistance critical temperature T_{c0} (K)



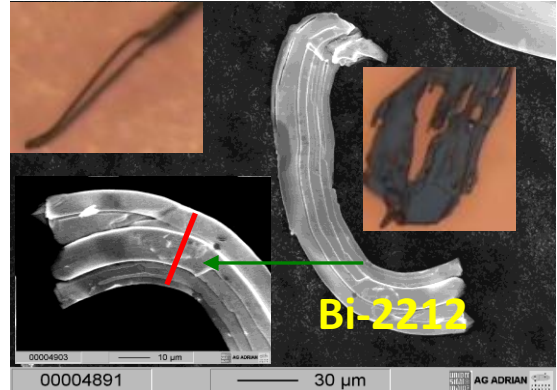
Prin aceasta abordare se pot controla propr. supraconductoare a straturilor subtiri practice: de ex. Bi2223 pe substrat de MgO poate fi un potential candidat pentru aplicatii de microunde (filtre de banda, rezonatoare, altele).



**Obiecte cristaline (epitaxie 3D ca pentru cristalele clasice)
oxidice supraconductoare anisotrope neliniare: curcubeu
sau inel**



De obicei se obtin cristale aciculare drepte!

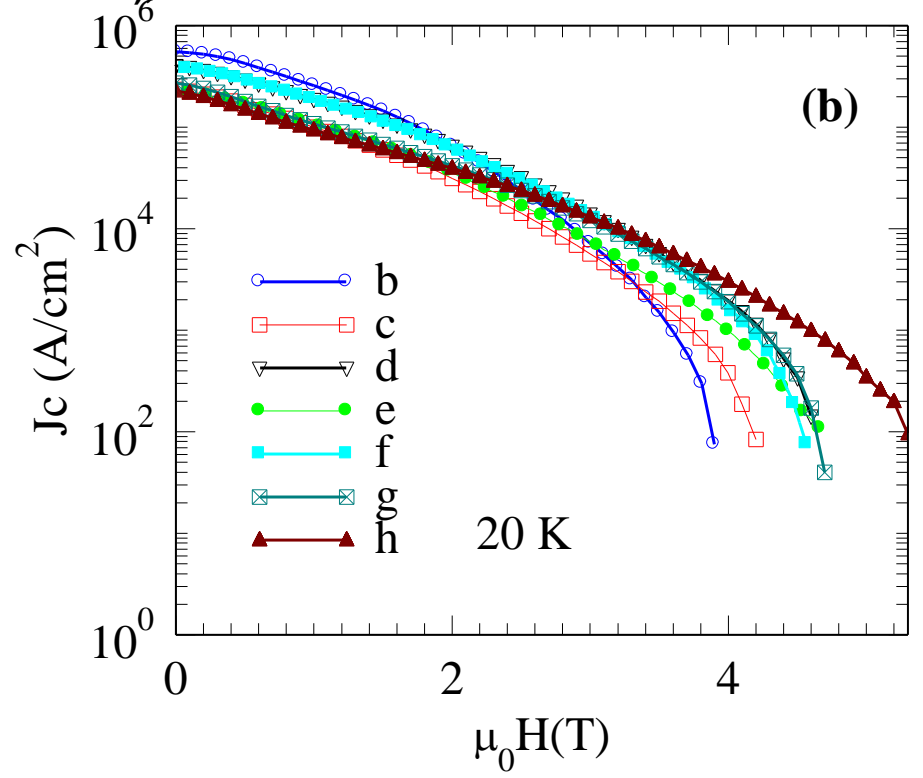
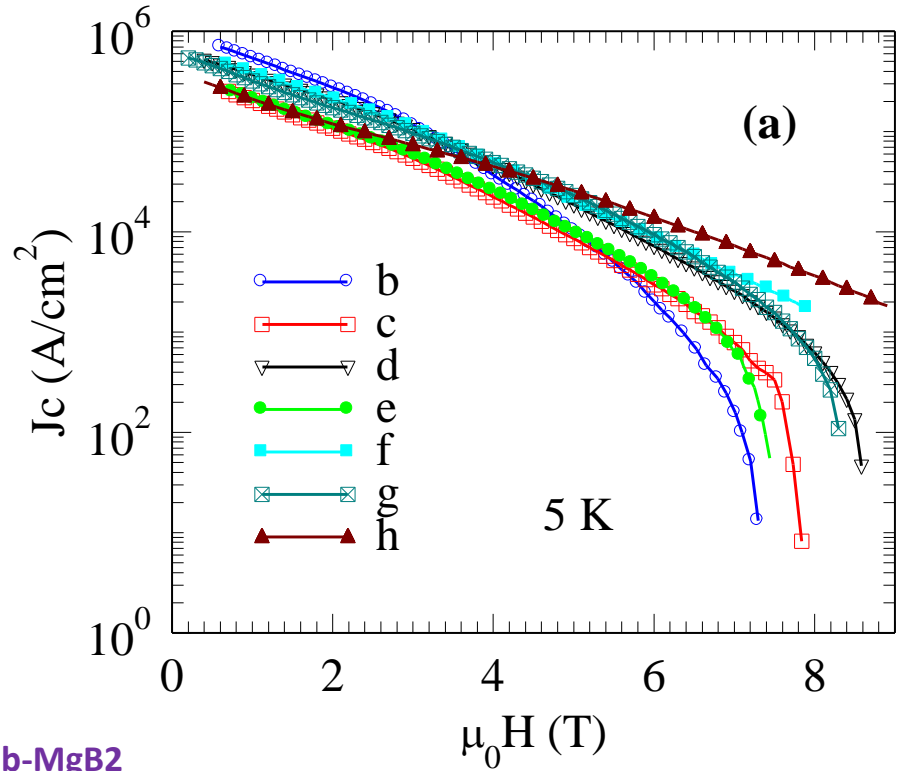


Formarea liniei curbate este in planul ab.
**Aceste obiecte pot fi utile ca interconexiuni
sau electromagneti in electronica
supraconductoare.**

Interfata de crestere la anumite momente de timp in timpul cresterii: forma si pozitia acesteia se modifica; obiectele curbate sunt 'bucati taiate' dintr-un cristal perfect de tip clasic!

MgB₂ cu diferite adaosuri: C substituie B (modificand anisotropia), iar celelalte nu produc efecte de substitutie dar introduc centrii de fixare: ambele efecte pot duce la marirea Jc la campuri mari !

MgB₂ are potential in aplicatiile: de putere (transformatoare, motoare fara zgomot pentru vapoare, submarine, etc) energie (stocatoare de energie 'fly wheel', lagare fara frecare pentru generatoarele eoliene, etc), transport (trenuri cu levitatie magnetica, scuturi passive electromagnetice pentru statiile orbitale, etc), medicina (tomografele cu rezonanata magnetica nucleara), etc



- b- MgB₂
- c- MgB₂ + Sb₂O₃
- d- MgB₂ + Bi₂O₃
- e- MgB₂ + TeO₂
- f- MgB₂ + Te
- g- MgB₂ + SiC
- h- MgB₂ + Te + SiC

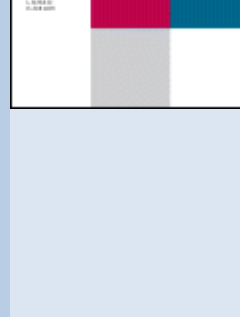
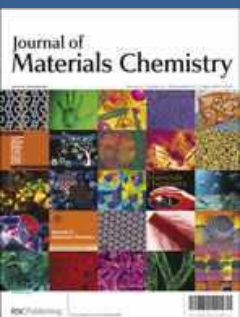
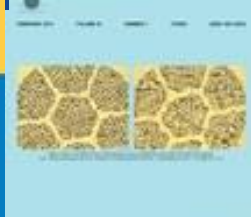
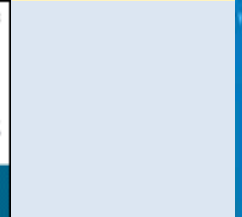
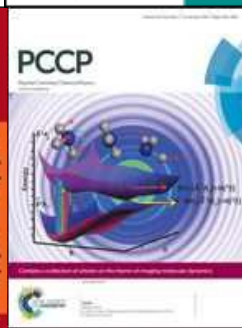
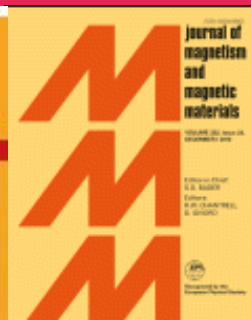
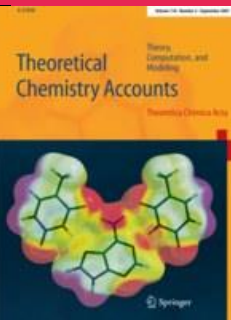
Metoda de procesare: Ex-situ Spark Plasma Sintering

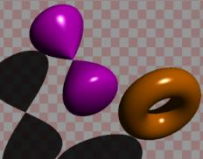
20K: Jc(MgB₂) < Jc(MgB₂+Sb₂O₃) < Jc(MgB₂+Bi₂O₃) < Jc(Te,TeO₂) ~ Jc(SiC) < Jc(Te+SiC)

Cel mai eficient este Te+SiC si nivelul atins de Jc la campuri mari si la 20K este comparabil cu probele record din literatura obtinute pentru materii prime speciale. In ac. caz am folosit materii prime comerciale.

Criteria minime de performanta contractate (2010-2013): 21 articole ISI, 50 factor de impact cumulat.

Publicatii •44(41 ISI), FI: ~104, 2 capitole de carte





Workshop International ADVANCES IN STRUCTURE-PROPERTY CORRELATIONS, THE GATE FOR SPECIAL PROPERTIES AT MOLECULAR AND NANO-SCALE LEVELS, ADSPECPRO 2012, Bucuresti, 20-21.09.2012

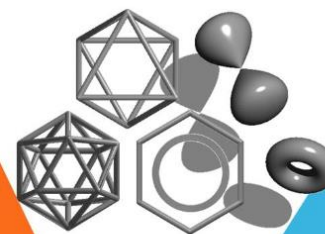
In cadrul proiectului s-a organizat workshop-ul international **ADSPECPRO 2012**, cu participanti din Romania, China, Italia, Serbia si Germania (10% participanti straini)

ADSPECPRO 2012



Va invitam sa participati la lucrarile workshop-ului international

ADVANCES IN STRUCTURE-PROPERTY CORRELATIONS, THE GATE FOR SPECIAL PROPERTIES AT MOLECULAR AND NANO-SCALE LEVELS



**ADSPECPRO 2012,
September 20-21st
Bucharest, Romania**

Lucrarile se vor desfasura in sala Roma a hotelului Siqua, Calea Plevnei 59 A, Sector 1, Bucuresti.

Informatii suplimentare si contact:
http://stoner.phys.uaic.ro/projects/PCCE_239_2010/Events_IC.html
E-mail:
marilena.cimpoesu@g.unibuc.ro

Workshop-ul este organizat in cadrul proiectului de cercetare PNII-PCCE-9/2010, *A new generation of paradigms in the molecular magnetism and material sciences. The magnetic anisotropy in complex units, supramolecular systems and at nano-scale*, cu sprijinul CNCS-UEFISCDI.

Parteneri



Workshop International
ADVANCES IN STRUCTURE-PROPERTY CORRELATIONS, THE GATE FOR SPECIAL PROPERTIES AT
MOLECULAR AND NANO-SCALE LEVELS, ADSPECPRO 2012,
Bucuresti, 20-21.09.2012



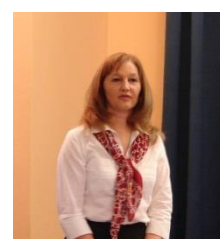
Horst Bormann
*Max Planck Institute Chemical
 Physics of Solids, Dresden,
 Germany*



Mircea Diudea
*Faculty of Chemistry
 and Chemical
 Engineering, Babes-
 Bolyai University, Cluj*



Alessandro Stroppa
University of L'Aquila, Italy



Snezana Zaric
*University of Belgrade,
 Department of Chemistry, Serbia*

Invitati



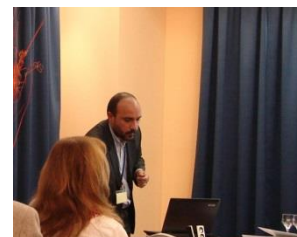
Shi Wang
*Institute of Advanced Materials
 (IAM), Nanjing University of Posts
 & Telecommunications, Nanjing,
 China*



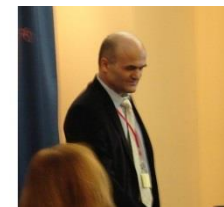
Mihai Viorel Putz
*Universitatea de Vest,
 Timisoara, Bucharest,
 Romania*



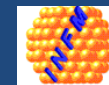
Stefania Tanase Grecea
*Van't Hoff Institute for Molecular
 Sciences, University of Amsterdam,
 Holland*

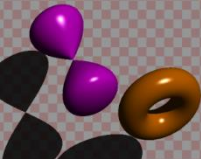


Radu Silaghi-Dumitrescu
*Institute of Technology Babes-Bolyai,
 Faculty of Chemistry and Chemical
 Engineering, Center for Computational
 Quantum Chemistry and Molecular
 Modelling, Cluj, Romania*



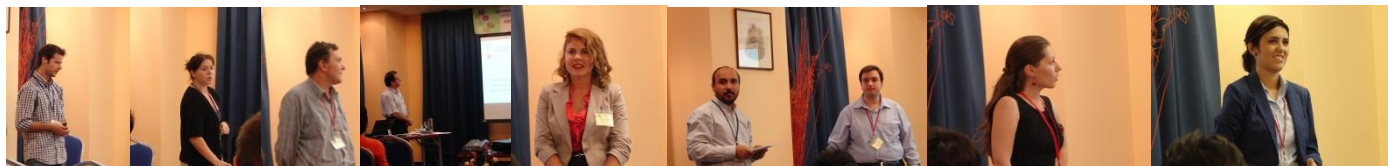
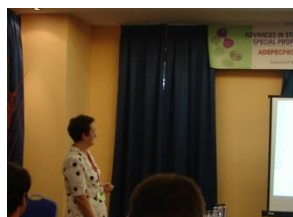
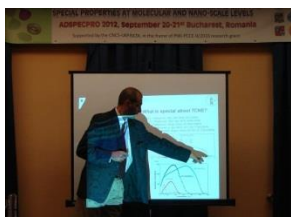
**Mangalagiu
 Ionel**
*The Alexandru Ioan Cuza
 University of Iasi, Organic
 Chemistry Dep., Romania
 Referent proiect*



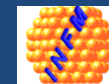


Workshop International ADVANCES IN STRUCTURE-PROPERTY CORRELATIONS, THE GATE FOR SPECIAL PROPERTIES AT MOLECULAR AND NANO-SCALE LEVELS, ADSPECPRO 2012, Bucuresti, 20-21.09.2013

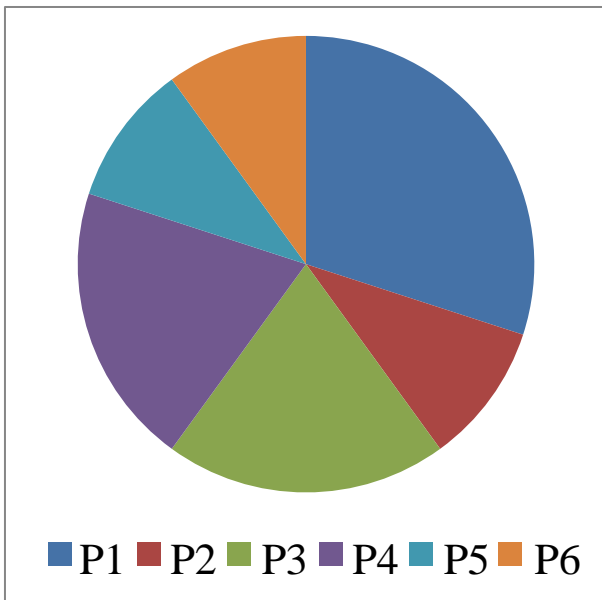
Keynote presentations



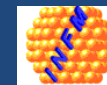
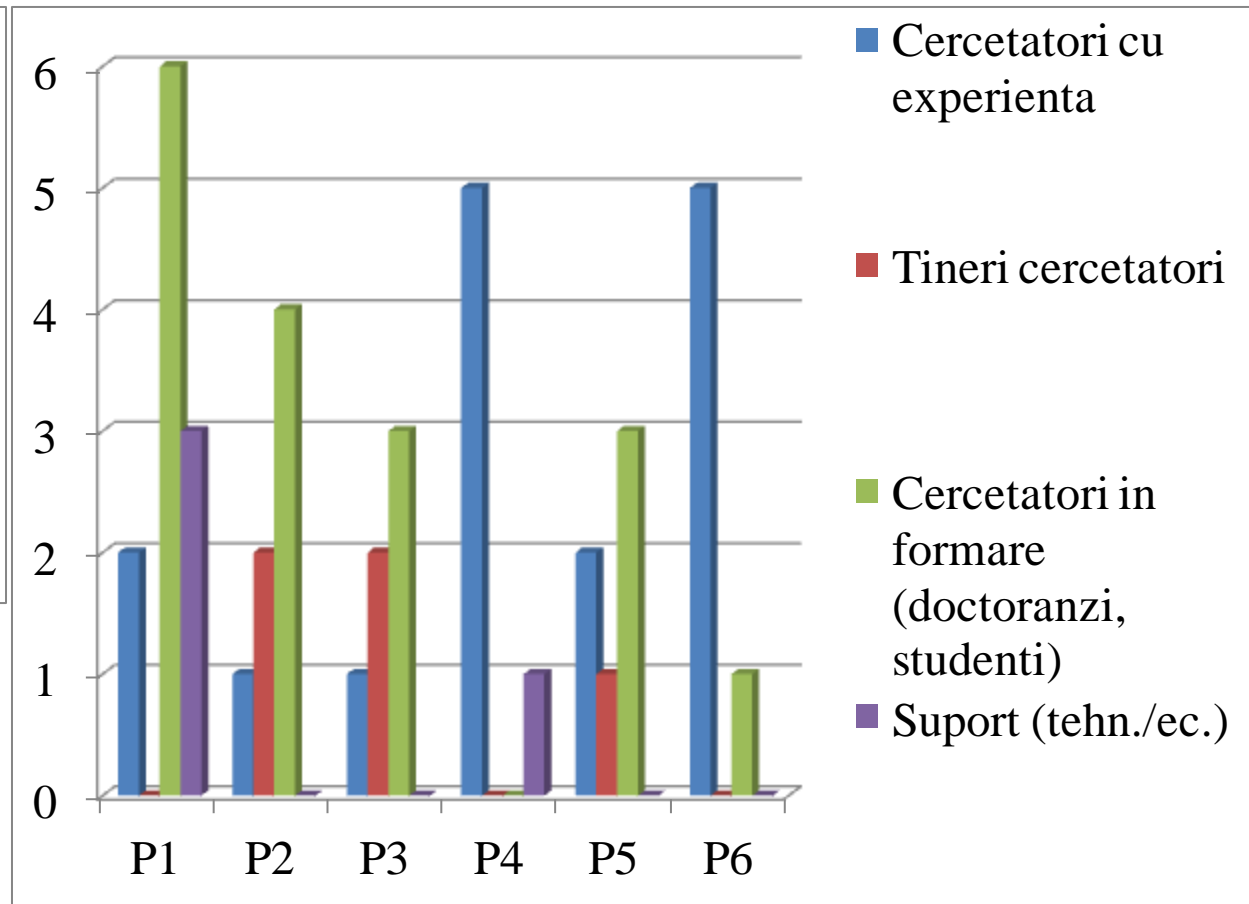
Short oral presentations



Gradul de implicare al coordonatorilor

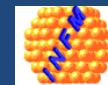
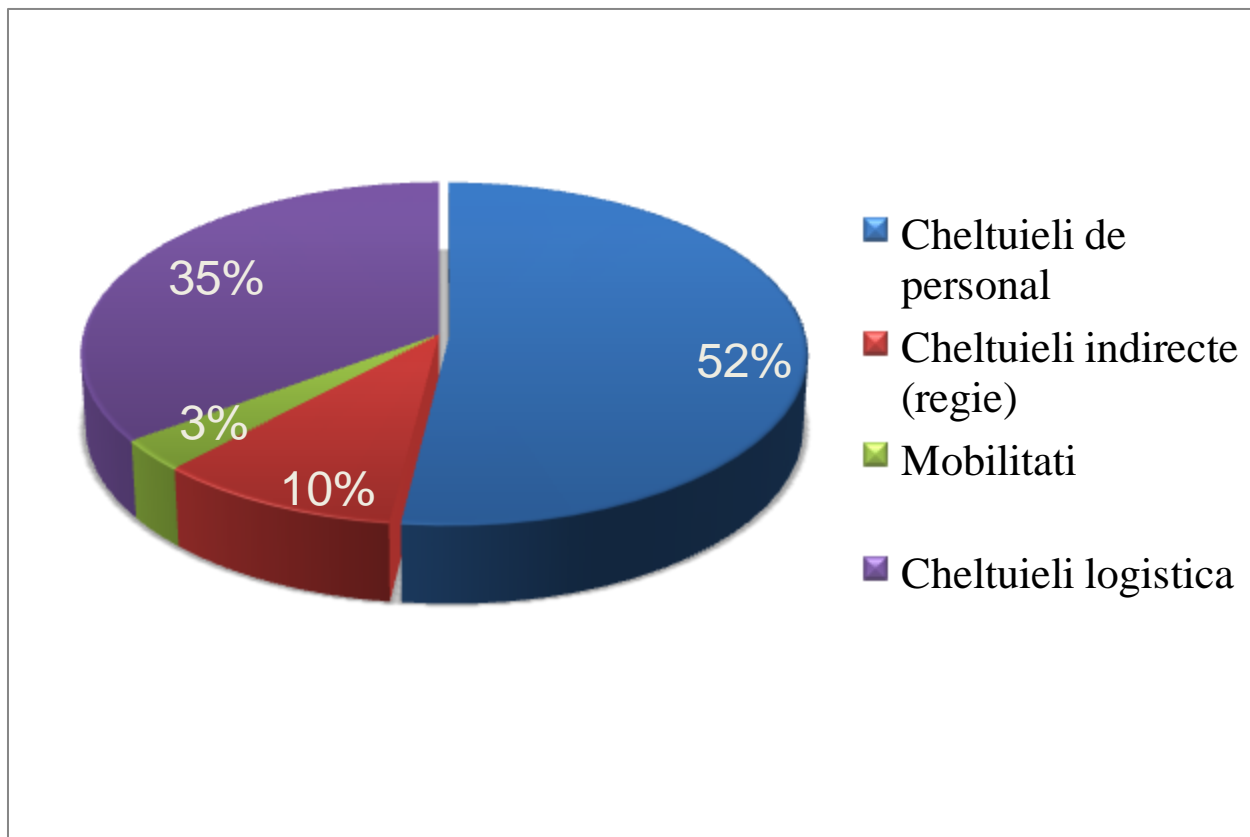


Structura echipelor de cercetare



Structura bugetului (pe capitole de buget).

Total **7000000** RON , repartizati pe ani **1000000** RON (2010), **3000000** RON (2011), **2000000** RON (2012), **1000000** RON (2013)



Laborator infiintat in intregime cu suportul financiar acordat de
CNCS-UEFISCDI acordat proiectului PNII-PCCE-9/2010

Echipamente

Difractometru de raze X pe monocristal (Rigaku R-AXIS RAPID II)



Caracteristici

Curved imaging plate chemical crystallography system

Imaging plate (IP) and scanner: Detector: Cylindrical IP with vertical translation axis;

Radius: 127.4 mm; 2θ range: Tangential direction -60° to 144° ; Active area: 460 mm x 256 mm

Goniometer (Partial- χ , 3-axis goniometer): ω axis: -85° to 265° 0.002° /step, χ axis: -15° to 55° 0.0002° /step; φ axis: 360° 0.002° /step' Sphere of confusion: $\leq 20 \mu\text{m}$;

Camera: 1/3" camera for sample alignment and observation; 70X magnification color image displayed on host computer

X-ray generator: 5 kW rotating anode: Mo

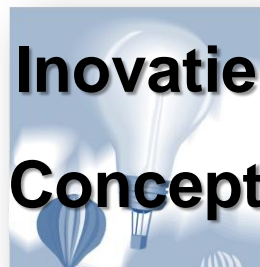
Computer: PC with Windows®

Software: CrystalClear™ automated measurement/processing software; Software for face indexing using CCD video camera; TwinSolve twinned crystal integration software; CrystalStructure™ single-crystal structure solution refinement and reporting suite .





Idei
Complexitate
Creatie



Inovatie
Concept
Originalitate



Pionierat
Prioritate
Brand

Citius
Altius
Fortius