

## 1. Liste des publications :

### Publications parues dans des journaux de rang A :

- [1] N. Guihéry, G. Durand, M.B. Lepetit, J. P. Malrieu, *Bistability in molecular donor acceptor complexes*, CHEM. PHYS. **183** (1994) 61
- [2] N. Guihéry, G. Durand, M.B. Lepetit, *Bistable mixed-valence molecular architectures for bit storage*, CHEM. PHYS. **183** (1994) 45
- [3] N. Guihéry, D. Maynau, et Jean-Paul Malrieu *From quinoidal to diradical structure in substituted n-para- xylylene (n=1,2,3) molecules : A Heisenberg Hamiltonian study*, CHEM. PHYS. LET. **248** (1996) 199
- [4] N. Guihéry, N. Benamor, D. Maynau, J. P. Malrieu, *Approximate Size-consistent treatments of Heisenberg Hamiltonians for large systems*, J. CHEM. PHYS. **104** (1996) 3701
- [5] S. Capponi, N. Guihéry, J. P. Malrieu, B. Miguel, D. Poilblanc, *Bond alternation of polyacetylene as a spin-Peierls distortion*, CHEM. PHYS. LET. **255** (1996) 238
- [6] N. Guihéry, J. P. Malrieu, D. Maynau, P. Wind, *A statistical multireference state-specific dressing of configuration interaction matrices : Application to Heisenberg Hamiltonian*, MOL. PHYS. **94** (1996) 209
- [7] N. Guihéry, J. P. Malrieu, D. Maynau, K. Handrick, *Unexpected CASSCF bistability phenomenon*, INT. J. OF QUANT. CHEM. **61** (1997) 45
- [8] B. Miguel, P. Wind, N. Guihéry, J.P. Malrieu, *Approaching periodic systems by a selfconsistent embedding of a finite cluster*, CHEM. PHYS. LET. **283** (1998) 77
- [9] N. Guihéry, D. Maynau, and Jean-Paul Malrieu *Search for Singlet-Triplet bistabilities in conjugated hydrocarbons*, NEW J. OF CHEM. **22** (1998) 281
- [10] B. Miguel, N. Guihéry, J. P. Malrieu, P. Wind, *Study of infinite polyacetylene from a Heisenberg Hamiltonian : Dimerization and lowest excitation energies*, CHEM. PHYS. LET. **294** (1998) 49
- [11] P. Wind, N. Guihéry, J. P. Malrieu, *Approximation of an infinite periodic system by a self-consistent embedding of a finite cluster : The Dressed Cluster method*, PHYS. REV. B **59** (1999) 2556
- [12] J.P. Malrieu, N.Guihéry, *Real Space Renormalization Group with effective interactions*, PHYS. REV. B **63** (2001) 85110-1-10
- [13] V.R. Viera, N.Guihéry, J.P. Rodriguez, P.D. Sacramento, *Decoupling of the s=1/2 antiferromagnetic zig-zag ladder with anisotropy*, PHYS. REV. B **63** (2001) 224417-1-11
- [14] N. Guihéry, J. P. Malrieu, S. Evangelisti, D. Maynau, *Correlated description of multiple bonds using localized active orbitals*, CHEM. PHYS. LET. **349** (2001) 555-561
- [15] D. Maynau, S. Evangelisti, N. Guihéry, C. Calzado, J. P. Malrieu, *Direct generation of local orbitals in multireference treatment and subsequent uses for the calculation of the correlation energy*, J. CHEM. PHYS. **116** (2002) 10060
- [16] I. de P.R. Moreira, N. Suaud, N. Guihéry, J. P. Malrieu, R. Caballol, J. M. Bofill, F. Illas, *Derivation of spin Hamiltonians from the exact Hamiltonian : Application to systems with two unpaired electrons per magnetic site*, PHYS. REV. B **66** (2002) 134430-1-14
- [17] C. Angeli, C. Calzado, R. Cimiraglia, S. Evangelisti, N. Guihéry, T. Leininger, J. P. Malrieu, D. Maynau, J.V. Pitarch Ruiz, M. Sparta, *The use of local orbitals in multireference calculations*, MOL. PHYS. **101** (2003) 1389
- [18] N. Guihéry, J. P. Malrieu, *The double exchange mechanism revisited : An ab initio study of the [Ni<sub>2</sub>(napy)<sub>4</sub>Br<sub>2</sub>]<sup>+</sup> complex*, J. CHEM. PHYS. **119** (2003) 8956
- [19] N. Guihéry, J. P. Malrieu, S. Evangelisti, *Orbital optimization : Density matrix-based procedure versus energy minimization*, J. CHEM. PHYS. **119** (2003) 11088

- [20] M. Al Hajj, N. Guihéry, J. P. Malrieu, P. Wind, *Theoretical study of the phase transition in the anisotropic 2D square spin lattice*, PHYS. REV. B, **70** (2004) 094415-1-6
- [21] M. Al Hajj, N. Guihéry, J. P. Malrieu, B. Bocquillon, *Real Space Renormalization Group with effective interactions : Study of phase transitions in 2D lattices*, EUR. PHYS. J. B, **41** (2004) 11
- [22] D. Taratiel, N. Guihéry, *A refined model of the double exchange phenomenon : Test on the stretched  $N+ 2$  molecule*, J. CHEM. PHYS. **121** (2004) 7127
- [23] S. Evangelisti, N. Guihéry, T. Leininger, J.-P. Malrieu, D. Maynaud, J.-V. Pitarch-Ruiz, N. Suaud, C. Angeli, R. Cimiraglia, et C. J. Calzado, *Local Orbitals for Quasi-Degenerate Systems*, J. MOL. STRUCT. (Theo. Chem.) **709** (2004) 1
- [24] Y. Carissan, J. L. Heully, N. Guihéry, F. Alary, *A study of the correlation effects upon the modelization of the double exchange phenomenon*, J. CHEM. PHYS. **121** (2004) 9453
- [25] M. Al Hajj, J. P. Malrieu, N. Guihéry, *A renormalized excitonic method*, PHYS. REV. B **72** (2005) 224412-1-8
- [26] S. Baig, B. Richard, P. Serp, C. Mijoule, K. Hussein, N. Guihéry, J.C. Barthelat and P. Kalck, *Synthesis of a series of di-palladium(I) complexes containing the  $\text{Pd}_2(\mu\text{CO})_2$  core, and DFT analysis of the Pd-CO back-donation in terminal and bridging CO*, INORG. CHEM. **45** (2006) 1935
- [27] S. Messaoudi, V. Robert, N. Guihéry, *Correlated ab initio study of the excited state of the iron-coordinated-mode noninnocent glyoxal-bis(mercaptoanil) ligand.*, INORG. CHEM. **45** (2006) 3212
- [28] R. Bastardis, N. Guihéry, C. de Graaf, *Ab initio study of the Zener polaron spectrum of half-doped manganites : Comparison of several model Hamiltonians*, PHYS. REV. B **74** (2006) 014432-1-10
- [29] B. Lévy, P. Millié, F. Spiegelman, J. S. Marin et N. Guihéry, *About the scientific contribution of Jean Paul Malrieu* article éditorial du numéro spécial de THEOR. CHEM. ACC. en l'honneur de Jean-Paul Malrieu, **116 (4-5)** (2006) 383
- [30] N. Guihéry, *The double exchange phenomenon revisited : The  $[\text{Re}_2\text{OCl}_{10}]^{3-}$  compound*, THEOR. CHEM. ACC. **116** (2006) 576
- [31] Tahra Ayed, Nathalie Guihéry, B. Tangour and Jean Claude Barthelat, *Theoretical study of the metal-metal interaction in dipalladium(I) complexes*, THEOR. CHEM. ACC. **116** (2006) 497
- [32] R. Bastardis, N. Guihéry, N. Suaud, C. de Graaf, *Competition between double exchange and purely magnetic Heisenberg models in mixed valence systems : Application to half-doped manganites*, J. CHEM. PHYS., **125** 194708-1-10 (2006)
- [33] J.P. Malrieu, N. Guihéry, C.J. Calzado, C. Angeli *Bond electron pair: Its relevance and analysis from the quantum chemistry point of view*, J. COMP. CHEM. **28** (2007) 35
- [34] R. Bastardis, N. Guihéry, N. Suaud, *Relation between double exchange and Heisenberg model spectra : Application to the half-doped manganites*, PHYS. REV. B, **75**, 132403 (2007)
- [35] R. Bastardis, N. Guihéry, C. de Graaf, *Microscopic origin of isotropic non-Heisenberg behavior in  $S=1$  magnetic systems*, PHYS. REV. B, **76** 132412 (2007)
- [36] R. Bastardis, N. Guihéry, C. de Graaf, *Ab initio study of the CE magnetic phase in half doped manganites : Purely magnetic versus double exchange description*, PHYS. REV. B, **39** **77**, 054426 (2008)
- [37] R. Bastardis, C. de Graaf, N. Guihéry, *Isotropic non-Heisenberg terms in the magnetic coupling of transition metal complexes*, J. CHEM. PHYS., **129** 154102 (2008)
- [38] P. Labèguerie, C. Boilleau, R. Bastardis, N. Suaud, J.P. Malrieu, N. Guihéry *Is it possible to determine rigorous magnetic Hamiltonians in spin  $S=1$  systems from density functional theory calculations* J. CHEM. PHYS., **129** 154110 (2008)

- [39] N. Guihéry, V. Robert, F. Neese *Ab initio study of intriguing coordination complexes : A metal-field theory picture*, J. PHYS. CHEM. A 112 12975 (2008)
- [40] N. Suaud, M-L Bonnet, C. Boilleau, P. LabÃ"guerie and N. Guihéry *Light-induced excited spin state trapping : ab initio study of the physics at the molecular level* , J. AM. CHEM. SOC. 132 715 (2009)
- [41] Suaud N. ; Masaro Y. ; Coronado E. ; et al. *Origin of the Paramagnetic Properties of the Mixed-Valence Polyoxometalate [GeV(14)O(40)](8-) Reduced by Two Electrons : Wave Function Theory and Model Hamiltonian Calculations* EUROPEAN JOURNAL OF INORGANIC CHEMISTRY 34, 5109-5114 (2009)
- [42] Maurice Remi ; Bastardis Roland ; de Graaf Coen ; et al. *Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians* JOURNAL OF CHEMICAL THEORY AND COMPUTATION 5 11, 2977-2984 2009
- [43] Maurice Remi ; Guihery Nathalie ; Bastardis Roland ; et al. *Rigorous Extraction of the Anisotropic Multispin Hamiltonian in Bimetallic Complexes from the Exact Electronic Hamiltonian* JOURNAL OF CHEMICAL THEORY AND COMPUTATION 6 1, 55-65 (2010)
- [44] Boilleau Corentin ; Suaud Nicolas ; Bastardis Roland ; et al. *Possible use of DFT approaches for the determination of double exchange interactions* THEORETICAL CHEMISTRY ACCOUNTS 126 3-4 231-241 (2010)
- [45] Maurice R. ; Pradipto A. M. ; Guihéry N. ; et al. *Antisymmetric Magnetic Interactions in Oxo-Bridged Copper(II) Bimetallic Systems* JOURNAL OF CHEMICAL THEORY AND COMPUTATION 6 10, 3092-3101 (2010)
- [46] Maurice Remi ; de Graaf Coen ; Guihéry Nathalie *Magnetostructural relations from a combined ab initio and ligand Field analysis for the nonintuitive zero-Field splitting in Mn(III) complexes* JOURNAL OF CHEMICAL PHYSICS 1338 Art. Num. : 084307 (2010)
- [47] Maurice Remi ; de Graaf Coen ; Guihéry Nathalie *Magnetic anisotropy in binuclear complexes in the weak-exchange limit : From the multispin to the giant-spin Hamiltonian* PHYSICAL REVIEW B 81 21 Art. Num. : 214427 (2010)
- [48] Trinquier Georges ; Suaud Nicolas ; Guihéry Nathalie ; et al. *Designing Magnetic Organic Lattices from High-Spin Polycyclic Units* CHEMPHYSICHEM 12 16, 3020-3036 (2011)
- [49] Maurice Remi ; Sivalingam Kanthen ; Ganyushin Dmitry ; et al. *Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate* INORGANIC CHEMISTRY 50 13,6229-6236 (2011)
- [50] Terencio T. ; Bastardis R. ; Suaud N. ; et al. *Physical analysis of the through-ligand long-distance magnetic coupling : spin-polarization versus Anderson mechanism* PHYSICAL CHEMISTRY CHEMICAL PHYSICS 13 26, 12314-12320 (2011)
- [51] Batchelor Luke J. et al. *Pentanuclear Cyanide-Bridged Complexes Based on Highly Anisotropic Co(II) Seven-Coordinate Building Blocks : Synthesis, Structure, and Magnetic Behavior* INORGANIC CHEMISTRY 50 23, 12045-12052 (2011)
- [52] Pradipto Abdul-Muizz ; Maurice Remi ; Guihéry Nathalie ; et al. *First-principles study of magnetic interactions in cupric oxide* PHYSICAL REVIEW B 85 art. num.: 014409 (2012)
- [53] Tabookht, Zahra; Lopez, Xavier; de Graaf, Coen; Guihery; Suaud, N; Benamor, N *Rationalization of the behavior of M2(CH3CS2)4I (M = Ni, Pt) chains at room temperature from periodic density functional theory and ab initio cluster calculations* JOURNAL OF COMPUTATIONAL CHEMISTRY 33 1748-1761 (2012)
- [54] Coulaud, Esther; Guihery, Nathalie; Malrieu, Jean-Paul; Hagebaum-Reignier, D; Siri, D; Ferre, N; *Analysis of the physical contributions to magnetic couplings in broken symmetry*

*density functional theory approach* JOURNAL OF CHEMICAL PHYSICS 137 art. num. 114106 (2012)

[55] Suaud, Nicolas; Ruamps, Renaud; Guihery, Nathalie; Malrieu, Jean Paul; *A Strategy to Determine Appropriate Active Orbitals and Accurate Magnetic Couplings in Organic Magnetic Systems*; JOURNAL OF CHEMICAL THEORY AND COMPUTATION 8 4127-4137 (2012)

[56] Boilleau, Corentin; Suaud, Nicolas; Guihery, Nathalie; *Ab initio study of the influence of structural parameters on the potential energy surfaces of spin-crossover Fe(II) model compounds*; JOURNAL OF CHEMICAL PHYSICS 137 art. num. 224304 (2012)

[57] Ruamps, Renaud; Batchelor, Luke J.; Maurice, Remi; Gogoi, N ; Jimenez-Lozano, P; Guihery, N; de Graaf, C; Barra, AL; Sutter, JP; Mallah, T; *Origin of the Magnetic Anisotropy in Heptacoordinate Ni-II and Co-II Complexes* CHEMISTRY-A EUROPEAN JOURNAL 19 950-956 (2013)

[58] Ruamps, Renaud; Maurice, Remi; Batchelor, Luke; ; Boggio-Pasqua, M; Guillot, R; Barra, AL ; Liu, JJ; Bendeif, E; Pillet, S; Hill, S; Mallah, T; Guihery, N; *Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory*; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY; 135 3017-3026 (2013)

[59] Coulaud, Esther; Malrieu, Jean-Paul; Guihery, Nathalie; et al., *Additive Decomposition of the Physical Components of the Magnetic Coupling from Broken Symmetry Density Functional Theory Calculations* JOURNAL OF CHEMICAL THEORY AND COMPUTATION; 9 3429-3436 (2013)

[60] Maurice, Remi; de Graaf, Coen; Guihery, Nathalie, *Theoretical determination of spin Hamiltonians with isotropic and anisotropic magnetic interactions in transition metal and lanthanide complexes*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 15 18784-18804 (2013)

[61] Jean-Paul Malrieu, Rosa Caballol, Carmen J. Calzado, Coen de Graaf, Nathalie Guihéry, *Magnetic interactions in molecules and highly correlated materials: Physical content, analytical derivation and rigorous extraction of magnetic Hamiltonians from wave-function theory and density functional theory*". CHEMICAL REVIEW DOI 10.1021/cr300500z

[62] *Singly occupied MOs in Mono- and diradical conjugated hydrocarbons: comparison between variational single-reference, fully correlated and Huckel descriptions*, N. Suaud, R. Ruamps, J. P. Malrieu and N. Guihéry, in press JOURNAL OF CHEMICAL PHYSICS, DOI 10.1021/jp4120892

[63] *Interplay between local anisotropies in bi-nuclear complexes*, R. Ruamps, R. Maurice, C. de Graaf and N. Guihéry, accepted INORGANIC CHEMISTRY

## 2. Chapitres de livres :

[1] M. Al Hajj, N. Guihéry, J.P. Malrieu, *Introduction of effective interactions in Real Space Renormalization Techniques* World Scientific, Review Book, *Strongly correlated systems, coherence and entanglement* (2007)

[2] Roland Bastardis, Nathalie Guihéry *Competition between several model Hamiltonians in half-doped manganites* World Scientific, Review Book, *Strongly correlated systems, coherence and entanglement* (2007)

### 3. Conférences invitées, Conférences obtenues sur propositions, Cours dans des écoles thématiques ou masters internationaux et Séminaires invités

#### 3.1 Liste des conférences invitées : les plénières (CP) apparaissent en premier

- [1] CP1 : *Some missions of quantum theoreticians in the domain of magnetism* MOLECULAR MATERIALS (MOLMAT 2006), Lyon, June 7th-10th 2006.
- [2] CP2: *Determination of magnetic interactions in extended magnetic systems*, THETIS, Pisa, Italy 18th-20th February 2009
- [3] CP3: *Accurate calculation of the Zero Field Splitting parameters in transition metal complexes* Congrès de Chimie Théorique d'expression latine CHITEL 2010 Anglet, France, Septembre 2010
- [4] CP4 : *Magnetic anisotropy in mono and bi-nuclear transition metal compounds: Combining wave function based calculations and the effective Hamiltonian theory*, 48th Symposium on Theoretical Chemistry STC, September 23th-27th 2012 Karlsruhe (Germany)
- [5] *From quinoidal to diradical structure in (para - xylylenen) (n=1,2,3) : bistability or progressive mixing?* Quantum Theory Conference, September 17th-20th 1994, University of Sheffield, Angleterre
- [6] *Localized description in multireference contexts*, 6th World Congress of Theoretically Oriented Chemists WATOC, 4-9 Aout 2002 Lugano, Suisse
- [7] *Possible use of quantum chemistry for the study of physical and chemical properties of magnetic systems*, The 1st French-Syrian conference on Chemistry, Novembre 2003, Homs, Syrie
- [8] *Etude et détermination d'interactions électroniques fondamentales dans les composés magnétiques à partir de calculs ab initio*, Les journées "Magnétisme" de l'UMR de chimie, Novembre 2004, Ecole normale Supérieure de Lyon.
- [9] *Ab initio study of the physics of Zener polarons in half-doped manganites* CECAM Workshop, Lyon, Juillet 18-21, 2006.
- [10] *Magnetic interactions in conjugated diradicals* International Symposium on Novel Aromatic Compound (ISNA-13) Satellite meeting Diradicals and Multiradicals: Theory and Experiment, Namur, Belgique, Juillet 2009
- [11] *Extraction of anisotropic spin Hamiltonian from the effective Hamiltonian theory and correlated ab initio calculations* Satellite de l'ECMM (European Congress of Molecular Magnetism), Wroclaw, Pologne, Octobre 2009
- [12] *Extraction of model Hamiltonians from the effective Hamiltonian theory: applications to molecular magnetism* atelier "Magnétisme" du GDR DFT, ENS Lyon, Novembre 2010.
- [13] *Combining high spin organic units to generate ferromagnetic, antiferromagnetic and ferrimagnetic systems* (WATOC) satellite meeting: Theoretical modeling of materials, Barcelone, Espagne, Juillet 2011.
- [14] *Theoretical description of anisotropy in mono- and bi-nuclear transition metal complexes* World Association of Theoretical and computational chemists (WATOC), Santiago de Compostela, Espagne, Juillet 2011.
- [15] *How to build appropriate magnetic orbitals for accurate evaluation of magnetic couplings?* Conference in honor of Ria Broer, Gröningen (The Netherlands) Auguts 30th - September 1rst 2012.
- [16] *How many spins can be aligned by a single hole ?* Theoretical Chemistry in Spain told by women, January 30th-31st 2013 Tarragona, Spain
- [17] *Synergy and Destructive Interferences Between Local Anisotropies in Binuclear Complexes: New Insights from Theory* 2nd International Conference in Bimetallic Complexes 2013, 23th-25th September 2013, Karlsruhe, Germany

### 3.2 Liste des contributions orales :

- [18] *A statistical multireference state-specific dressing of configuration interaction matrices : application to Heisenberg Hamiltonian*, Mars 1998, Réunion du réseau TMR QUCEX, Knokke de Zoute, Belgique
- [19] *Possible use of localized orbitals in the calculations of magnetic couplings*, Franco-Spanish PICS meeting, Juin 2002, Tarragona, Espagne
- [20] *The use of local orbitals in multireference calculations* COST D26 meeting, November 2002, Toulouse
- [21] *Revised double exchange model : application to the  $[Ni_2(napy)_4Br_2]^+$  compound*, Franco Spanish PICS meeting, Mars 2003, Toulouse
- [22] *Magnétisme dans les complexes à double échange*, Congrès des Chimistes théoriciens d'Expression Latine (CHITEL), Septembre 2004, Porto, Portugal
- [23] *Zener polaron localization in half-doped manganites*, European Workshop on Molecular Magnetism, JIJOLS II, Jujols, Juin 23-26, 2006
- [24] *Competition between double exchange and purely magnetic Heisenberg models in half-doped manganites*, European Conference on Molecular Magnetism (ECMM), Octobre 10-15, 2006, Tomar, Portugal
- [25] *Role of the non-Hund states in magnetic systems having two open shells per centre*, Rencontre du PICS Franco-Espagnol, Novembre, 2007, Tarragona, Spain
- [26] *Rôles possible du chimiste quanticien dans les domaines du magnétisme et de la commutation moléculaire*, Rencontre du GDR Magnétisme moléculaire et commutation, Décembre, 2007, Dourdan
- [27] *Rigorous extraction of the Heisenberg Hamiltonian for spin  $S=1$  systems: the role of the three-body operator*; European Workshop on Molecular Magnetism, JIJOLS III Perpignan, septembre 2008.
- [28] *Possible rationalization of the anisotropic parameters in mononuclear and binuclear transition metal complexes*, European Workshop on Molecular Magnetism, JIJOLS IV, Groningen, Pays Bas, mai 2009.
- [29] *Theoretical study of magnetic organic system*, Rencontre du PICS franco-Italien, Toulouse, Février 2010.
- [30] *Magnétisme moléculaire dans les composés organiques* Rencontre du GDR MCM, Montpellier, Juillet 2010
- [31] *Design of high spin organic magnetic units from simple rules*, European Workshop on Molecular Magnetism, JIJOLS V, Horta de Sant Joan, Espagne, Novembre 2010.
- [32] *On the possible use of the multi-spin and giant spin Hamiltonians for the description of the anisotropy in binuclear complexes* COST CODECS (CONvergent Distributed Environment for Computational Spectroscopy) Meeting, Avril 2011, Pise, Italie
- [33] *Zero-Field Splitting in Copper-acetate : on the importance of the correlation effects*. Rencontre du PICS Franco-italien, Ferrare, Italie Juin 2011
- [34] *Correlation between  $T(LIESST)$  and structural features in spin crossover complexes*, European Workshop on Molecular Magnetism, JIJOLS VI, Seville, Espagne, Février 2012
- [35] *Giant Ising-type magnetic anisotropy in trigonal Ni(II) complexes : competition between first order spin orbit coupling and Jahn Teller effect*. Conference TACC : Theory and Applications in Computational Chemistry: 2-6th september 2012 Pavie (Italie)
- [36] *Interplay between local magnetic anisotropies in polynuclear transition metal complexes*, European Workshop on Molecular Magnetism , JIJOLS VII, 13th -17th January 2014, Mulheim, Allemagne

### **3.3 Liste des séminaires invités (11)**

- [1] *Bistabilité dans les composés donneur-accepteur : utilisation possible pour le stockage d'information*, Mars 1996, Laboratoire du CEA, Paris, France
- [2] *Self-Consistent Size-Consistent dressing of Multireference Truncated Configuration Interactions*, Novembre 1998, Torun, Pologne
- [3] *Phase transition of the anisotropic Heisenberg Hamiltonian in spin lattices*, Avril 1999, centro de Fisica das Interaccoes Fundamentais, Instituto Superior Tecnico, Lisbonne, Portugal
- [4] *Real Space Renormalization Group with effective interactions : applications to 1D and 2D spin lattices*, Mai 2000, Dipartimento di Chimica, Universita degli Studi di Ferrara, Ferrare, Italie

### **3.4 Liste des cours invités:**

- [1] *La corrélation électronique*, 1iere Ecole de Carthage de Chimie et Physique théoriques, 22-28 mars 2006
- [2] *Magnetism from a quantum chemist point of view*, Cours : Institute of Theoretical and Computational Chemistry, Nanjing University, 3-6 Juillet 2007
- [3] *Real Space Renormalization Group theory and effective interactions*, Cours: Institute of Theoretical and Computational Chemistry, Nanjing University, 3-6 Juillet 2007
- [4] "Magnétisme" Cours à l'école du Réseau Français des chimistes théoricien, Dourdan, France Novembre 2011.
- [5] Multireference Configuration Interaction method I : the treatment of non-dynamic correlation, Intensive course of the Erasmus Mundus Mater II on Chemistry and Computational Modelling September 2012, Perugia (Italy)
- [6] Multireference Configuration Interaction method II : the treatment of dynamic correlation, Intensive course of the Erasmus Mundus Mater II on Chemistry and Computational Modelling September 2012, Perugia (Italy)
- [7] Multireference Configuration Interaction method I : treatment of non-dynamic correlation, Intensive course of the Erasmus Mundus Mater II on Chemistry and Computational Modelling September 2013, Madrid (Spain)
- [8] Multireference Configuration Interaction method II : treatment of dynamic correlation, Intensive course of the Erasmus Mundus Mater II on Chemistry and Computational Modelling September 2013, Madrid (Spain)