Curriculum vitae

Name: Cornelis de Graaf
Date: January 23, 2024

Personal details

Name	Cornelis
Surname:	de Graaf
DNI:	X2632706-B
Date of Birth:	30-06-1969
Place of Birth:	Alkmaar (The Netherlands)
Nationality:	Dutch
Home address:	Camí del Mig 1, 2-1
	08970 Sant Joan Despí (Barcelona)

Present professional situation

Professional category:	ICREA Research professor, started at 01-01-2006
Working place:	Universitat Rovira i Virgili
	Department of Physical and Inorganic Chemistry
Postal address:	Marcel·lí Domingo, s/n. 43007 Tarragona, Spain
Telephone	(+34) 977559568
Electronic mail:	coen.degraaf@urv.cat
Web page:	https://www.icrea.cat/Web/ScientificStaff/coen-de-graaf-367
	https://quantumchemistry.recerca.urv.cat/en
	http://orcid.org/0000-0001-8114-6658
	https://scholar.google.com/citations?user=2-6OEXUAAAAJ

Academic formation

Title:	Undergraduate degree in Chemistry
Centre:	University of Amsterdam (The Netherlands)
Date:	30-06-1993
Final thesis:	Quantum molecular dynamics simulation of an excess electron in dense He
Supervision:	prof. dr. S. W. de Leeuw
Title:	Ph. D. in Mathematics and Natural Sciences
Centre:	University of Groningen (The Netherlands)
Date:	13-03-1998
Dissertation:	Local excitations and magnetism in late transition metal oxides
Supervision:	prof. dr. W. C. Nieuwpoort and prof. dr. R. Broer

Previous scientific activities

Place:	Research assistant
Institute:	University of Groningen (The Netherlands)
Date:	01/09/1993 - 31/12/1993
Place:	Associate teacher (PhD. student)
Institute:	University of Groningen (The Netherlands)
Date:	01/01/1994 - 31/12/1997
Place:	Post-Doc (Marie Curie TMR Project)
Insititute:	University of Barcelona (Spain)
Date:	01/07/1998 - 30/09/2000
Place:	Post-Doc
Institute:	Universitat Rovira i Virgili (Tarragona, Spain)
Date:	01/10/2000 - 14/11/2001
Place:	Researcher with a full-time *Ramón y Cajal* contract
Institute:	Universitat Rovira i Virgili (Tarragona, Spain)
Date:	15/11/2001 - 31/12/2005
Place:	Honorary professor Zernike Institute of Advanced Materials
Institute:	University of Groningen (The Netherlands)
Date:	01/11/2011 - 31/10/2021

Active Research lines

Line	Development of electronic structure methods based on non-orthogonal orbitals
Centre	Universitat Rovira i Virgili, in collaboration with Oak Ridge National Laboratory (USA)
Duration	2019 -
Keywords	Orbital relaxation, Singlet fission, energy and electron transfer, massive parallelisation, GPU off-loading
Line:	Magnetism in molecular complexes
Centre:	Universitat Rovira i Virgili, in collaboration with University of Toulouse (France)
Duration:	2002 -
Keywords:	non-Heisenberg behaviour, anisotropy, heterobimetalic complexes, single-molecule magnets
Line:	Magnetism and redox properties of polyoxometalates
Centre:	Universitat Rovira i Virgili
Duration:	2002 -
Keywords:	Reduction potentials, spectroscopy, molecular conductivity, photocatalysis
Line:	Electronic properties of endohedral fullerenes
Centre:	Universitat Rovira i Virgili
Duration:	2014 -
Keywords:	Photoluminescence, actinides,

Closed Research lines

Line:	Quantum Molecular Dynamics
Centre:	University of Amsterdam
Duration:	1992 - 1993
Keywords:	Quantum Molecular Dynamics, excess electrons in dense He
Line:	Study of the electronic structure of ionic solids
Centre:	University of Groningen
Duration:	1993 - 1997
Keywords:	Optical and X-ray spectroscopy, magnetism, transition metal compounds
Line:	Magnetism in low-dimensional Heisenberg systems
Centre:	University of Barcelona
Duration:	1998 - 2000
Keywords:	Magnetism, spin ladders, spin chains, Heisenberg Hamiltonian
Line:	Impurities and defects in ionic and covalent materials
Centre:	University of Barcelona, Universitat Rovira i Virgili (Tarragona, Spain)
Duration:	1998 - 2006
Keywords:	Defects, spectroscopy, local geometry

Line:	Electronic structure parameters in transition metal oxides
Centre:	Universitat Rovira i Virgili
Duration:	2000 - 2015
Keywords:	Magnetism, effective Hamiltonians, electronic structure parameters, embedded cluster approach
Line:	Extended metal atom chains
Centre:	Universitat Rovira i Virgili
Duration:	2012 - 2018
Keywords:	Molecular conductivity, electronic structure, metal-metal bonding
Line:	Light-induced magnetism in transition metal complexes
Centre:	Universitat Rovira i Virgili
Duration:	2006 - 2022
Keywords:	Spin-crossover, photomagnetism, LIESST

Publications

1. Authors: B. Boltjes, C. de Graaf, R. P. H. Rettschnick, S. W. de Leeuw
   Title: QMD simulation of an excess electron in dense helium
   Ref.: Journal of Chemical Physics 97, 408-416 (1992)

2. Authors: B. Boltjes, C. de Graaf, S. W. de Leeuw
   Title: Computation of the energy V_o of an excess electron in dense helium and argon
   Ref.: Journal of Chemical Physics 98, 592-601 (1993)

3. Authors: C. de Graaf, R. Broer, W. C. Nieuwpoort
   Title: Electron correlation effects on the d-d excitations in NiO
   Ref.: Chemical Physics 208, 35-42 (1996)

4. Authors: C. de Graaf, F. Illas, R. Broer, W. C. Nieuwpoort
   Title: On the magnetic coupling of NiO
   Ref.: Journal of Chemical Physics 106, 3287-3291 (1997)

5. Authors: C. de Graaf, R. Broer, W. C. Nieuwpoort
   Title: Comparison of the superexchange interaction in NiO and in a NiO[100] surface
   Ref.: Chemical Physics Letters 271, 372-376 (1997)

6. Authors: C. de Graaf, R. Broer, W. C. Nieuwpoort, P. S. Bagus
   Title: On the role of relaxed charge-transfer excitations: Ni 3s hole states in NiO
   Ref.: Chemical Physics Letters 272, 341-346 (1997)

7. Authors: F. Illas, I. de P. R. Moreira, C. de Graaf, O. Castell, J. Casanovas
   Title: Absence of collective effects in Heisenberg systems with localized magnetic moments
   Ref.: Physical Review B 56, 5069-5072 (1997)

8. Authors: C. de Graaf, W. A. de Jong, R. Broer, W. C. Nieuwpoort
   Title: Theoretical study of the crystal field excitations in CoO
   Ref.: Chemical Physics 237, 59-66 (1998)

9. Authors: P. S. Bagus, R. Broer, C. de Graaf, W. C. Nieuwpoort
   Title: The electronic structure of NiO for Ni-3s hole states including full orbital relaxation and localization
   Ref.: Journal of Electron Spectroscopy and Related Phenomena 98-99, 303-319 (1999)

10. Authors: C. de Graaf, C. Sousa, R. Broer
    Title: Ionization and excitation energies in CuCl and NiO within different embedding schemes
    Ref.: Journal of Molecular Structure (TheoChem) 458, 53-60 (1999)

11. Authors: M. Geleijns, C. de Graaf, R. Broer, W. C. Nieuwpoort
    Title: Theoretical study of local electronic transitions in the NiO (100) surface
    Ref.: Surface Science 421, 106-115 (1999)

12. Authors: C. de Graaf, I. de P. R. Moreira, F. Illas, R. L. Martin
    Title: Ab initio study of the magnetic interactions in the spin-ladder compound $SrCu_2O_3$
    Ref.: Physical Review B 60, 3457-3464 (1999)

13. Authors: P. Reinhardt, I. de P. R. Moreira, C. de Graaf, R. Dovesi, F. Illas
    Title: Detailed ab-initio analysis of the magnetic coupling in CuF_2
    Ref.: Chemical Physics Letters 319, 625-630 (2000)

14. Authors: F. Illas, I. de P. R. Moreira, C. de Graaf, V. Barone
Title: Magnetic coupling in biradicals, binuclear complexes and wide-gap insulators: a survey of ab initio wave function and density functional theory approaches
Ref.: Theoretical Chemistry Accounts 104, 265-272 (2000)

15. Authors: C. de Graaf, R. Broer
Title: Midinfrared spectrum of undoped cuprates: d-d transitions studied by ab initio methods
Ref.: Physical Review B 62, 702-709 (2000)

16. Authors: C. de Graaf, I. de P. R. Moreira, F. Illas
Title: Magnitude of the first and second neighbour magnetic interactions in the spin chain compound Li_2CuO_2
Ref.: International Journal of Molecular Sciences 1, 28-38 (2000)

17. Authors: C. Sousa, C. de Graaf, F. Illas
Title: Core exciton energies of MgO, Al_2O_3 and SiO_2
Ref.: Physical Review B 62, 10013-10021 (2000)

18. Authors: J. Cabrero, N. Ben Amor, C. de Graaf, F. Illas, R. Caballol
Title: Ab Initio Study of the Exchange Coupling in Oxalato-Bridged Cu(II) Dinuclear Complexes
Ref.: Journal of Physical Chemistry A 104, 9983-9989 (2000)

19. Authors: J. A. Aramburu, M. Moreno, I. Cabria, M. T. Barriuso, C. Sousa, C. de Graaf, F. Illas
Title: Neutral atoms in ionic lattices: Stability and ground-state properties of KCl:Ag^0
Ref.: Physical Review B 62, 13356-13365 (2000)

20. Authors: C. Sousa, C. de Graaf, F. Illas, M. T. Barriuso, J. A. Aramburu, M. Moreno
Title: Neutral atoms in ionic lattices: Excited states of KCl:Ag^0
Ref.: Physical Review B 62, 13366-13375 (2000)

21. Authors: C. Sousa, D. Domínguez-Ariza, C. de Graaf, F. Illas
Title: Electric field effects on the ionic-neutral curve crossing of alkali halide molecules
Ref.: Journal of Chemical Physics 113, 9940-9947 (2000)

22. Authors: C. Sousa, C. de Graaf, F. Illas, G. Pacchioni
Title: Excited states in metal oxides by configuration interaction and multireference perturbation theory
Ref.: in: Progress in Theoretical Chemistry and Physics Vol. 7, 227-245 (2000) – *book chapter*

23. Authors: C. de Graaf, F. Illas
Title: Electronic structure and magnetic interactions of the spin-chain compounds Ca_2CuO_3 and Sr_2CuO_3
Ref.: Physical Review B 63, 014404 (2001)

24. Authors: C. Sousa, C. de Graaf, G. Pacchioni
Title: Optical properties of peroxy radicals in silica: Multiconfigurational perturbation theory calculations
Ref.: Journal of Chemical Physics 114, 6259-6264 (2001)

25. Authors: I. de P. R. Moreira, F. Illas, D. Muñoz, C. de Graaf, M. A. Garcia-Bach
Title: A relationship between electronic structure and T_c in monolayered cuprate superconductors
Ref.: Chemical Physics Letters 345, 183-188 (2001)

26. Authors: C. de Graaf, C. Sousa, I. de P. R. Moreira, F. Illas
Title: Multiconfigurational perturbation theory: An efficient tool to predict magnetic coupling parameters in biradicals, molecular complexes and ionic insulators
Ref.: Journal of Physical Chemistry A 105, 11371-11378 (2001)

27. Authors: J. A. Aramburu, M. T. Barriuso, C. Sousa, C. de Graaf, M. Moreno, F. Illas
Title: Stability and optical properties of silver atoms in KCl
Ref.: Radiation Effects and Defects in Solids 154, 249-253 (2001)

28. Authors: R: Valiente, F. Rodríguez, J. A. Aramburu, M. Moreno, M. T. Barriuso, C. Sousa, C. de Graaf
Title: Optical spectroscopy of $(C_2H_5NH_3)_2CdCl_4$:Cu^{2+} under pressure: Study of Cu^{2+} local structure from theoretical calculations.
Ref.: International Journal of Quantum Chemistry 86, 239-244 (2002)

29. Authors: E. Ruiz, C. de Graaf, P. Alemany, S. Alvarez
Title: Further Theoretical Evidence for the Exceptionally Strong Ferromagnetic Coupling in Oxo-Bridged Cu(II) Dinuclear Complexes
Ref.: Journal of Physical Chemistry A 106, 4938-4941 (2002)

30. Authors: R. Valiente, F. Rodríguez, J. A. Aramburu, M. Moreno, M. T. Barriuso, C. Sousa, C. de Graaf
Title: Is it possible to use charge transfer bands to measure impurity-ligand distances? Experimental and theoretical results on Cu^{2+} doped $(C_2H_5NH_3)_2CdCl_4$
Ref.: High Pressure Research 22, 475-478 (2002)

31. Authors: C. de Graaf, I. de P. R. Moreira, F. Illas, O. Iglesias, A. Labarta
Title: Magnetic structure of Li_2CuO_2: From ab initio calculations to macroscopic simulations
Ref.: Physical Review B 66, 014448 (2002)

32. Authors: L. Hozoi, A. H. de Vries, A. B. van Oosten, R. Broer, J. Cabrero, C. de Graaf
Title: Theoretical characterization of the ground and optically excited states of α'-NaV_2O_5
Ref.: Physical Review Letters 89, 076407 (2002)

33. Authors: L. Hozoi, C. Presura, C. de Graaf, R. Broer
Title: Electronic structure of α'-NaV_2O_5: Wave-function-based embedded-cluster calculations
Ref.: Physical Review B 67, 035117 (2003)

34. Authors: C. J. Calzado, C. de Graaf, E. Bordas, R. Caballol, J. P. Malrieu
Title: Four spin cyclic exchange in spin ladder cuprates
Ref.: Physical Review B 67, 132409 (2003)

35. Authors: J. Cabrero, C. de Graaf, E. Bordas, R. Caballol, J. P. Malrieu
Title: Role of the coordination of the azido-bridge in the magnetic coupling in copper(II) binuclear complexes
Ref.: Chemistry, a European Journal 9, 2307-2315 (2003)

36. Authors: C. de Graaf, F. Illas, C. Sousa
Title: Quantum Chemical approach to excited states in Material Science
Ref.: in: Computational Materials Science, 167-195 (2003) – *book chapter*

37. Authors: N. Queralt, C. de Graaf, J. Cabrero, R. Caballol
Title: Ferrimagnetic coupling in oxamido-bridged Mn(II)Cu(II) compounds: a combined CASPT2 and DDCI study
Ref.: Molecular Physics 101, 2095-2102 (2003)

38. Authors: D. Taratiel, J. Cabrero, C. de Graaf, R. Caballol
Title: Magnetic coupling in oxalato-bridged hetero-bimetallic compounds: an ab initio study
Ref.: Polyhedron 22, 2409-2414 (2003)

39. Authors: F. Illas, D. Muñoz, C. de Graaf, I. de P. R. Moreira
Title: Unexpected role of Madelung potential in monoplanar high-Tc cuprate superconductors
Ref.: Chemical Physics Letters 379, 291-296 (2003)

40. Authors: C. de Graaf, L. Hozoi, R. Broer
Title: Magnetic interactions in calcium and sodium ladder vanadates
Ref.: Journal of Chemical Physics 120, 961-967 (2004)

41. Authors: C. Sousa, C. de Graaf, N. Lopez, N. M. Harrison, F. Illas
Title: Ab initio theory of magnetic interactions at surfaces
Ref.: Journal of Physics: Condensed Matter 16, 2557-2574 (2004)

42. Authors: D. Muñoz, C. de Graaf, F. Illas
Title: Putting Error Bars on the Ab Initio Theoretical Estimates of the Magnetic Coupling Constants: The Parent Compounds of Superconducting Cuprates as a Case Study
Ref.: Journal of Computational Chemistry 25, 1234-1241 (2004)

43. Authors: C. de Graaf, C. Sousa, R. Broer
Title: Ab initio study of the charge order and Zener polaron formation in half doped manganites
Ref.: Physical Review B 70, 235104 (2004)

44. Authors: E. Bordas, R. Caballol, C. de Graaf, J.-P. Malrieu
Title: Toward a variational treatment of the magnetic coupling between centers with elevated spin moments
Ref.: Chemical Physics 309, 259-269 (2005)

45. Authors: E. Bordas, C. de Graaf, R. Caballol, C. J. Calzado
Title: The electronic structure of $CaCu_2O_3$: Spin ladder versus one-dimensional spin chain
Ref.: Physical Review B 71, 045108 (2005)

46. Authors: E. Bordas, R. Caballol, C. de Graaf
Title: Ab initio study of the magnetic coupling in oxalato-bridged dinuclear Ni(II) complexes
Ref.: Journal of Molecular Structure: THEOCHEM 727, 173-179 (2005)

47. Authors: C. López, R. Costa, F. Illas, C. de Graaf, M. M. Turnbulll, C. P. Landee, E. Espinosa, I. Mata, E. Molins
Title: Magneto-structural correlations in binuclear copper(ii) compounds bridged by ferrocenecarboxylato(-1) and an hydroxo- or methoxo-ligands
Ref.: Dalton Transactions, pp. 2322-2330 (2005)

48. Authors: X. López, C. de Graaf, J. M. Maestre, M. Bénard, M.-M. Rohmer, C. Bo, J. M. Poblet
Title: Highly reduced polyoxometalates: Ab initio and DFT study of $[PMo_8V_4O_{40}(VO)_4]^{5-}$
Ref.: Journal of Chemical Theory and Computation 1, 856-861 (2005)

49. Authors: C. de Graaf, C. Sousa
Title: Assessing the zero-field splitting in magnetic molecules by wave function-based methods
Ref.: International Journal of Quantum Chemistry 106, 2470-2478 (2006)

50. Authors: A. Stoyanova, C. Sousa, C. de Graaf, R. Broer
Title: Hopping matrix elements from first-principles studies of overlapping fragments: Double exchange parameters in manganites
Ref.: International Journal of Quantum Chemistry 106, 2444-2457 (2006)

51. Authors: E. Bordas, C. de Graaf, R. Caballol, C. J. Calzado
Title: Accurate determination of the electronic structure parameters of the spin ladder compounds $SrCu_2O_3$, $Sr_2Cu_3O_5$ and $CaCu_2O_3$
Ref.: Theoretical Chemistry Accounts 116, 535-548 (2006)

52. Authors: R. Bastardis, N. Guihéry, C. de Graaf
Title: Ab initio study of the Zener polaron spectrum of half-doped manganites: Comparison of several model Hamiltonians
Ref.: Physical Review B 74, 014432 (2006)

53. Authors: A. Rodríguez-Fortea, C. de Graaf, J. M. Poblet
Title: Ab initio and DFT study of the exchange coupling in the highly reduced polyoxoanion $[PMo_{12}O_{40}(VO)_2]^{5-}$
Ref.: Chemical Physics Letters 428, 88-92 (2006)

54. Authors: A. Trueba, J. M. García-Lastra, C. de Graaf, P. García-Fernández, M. T. Barriuso, J. A. Aramburu, M. Moreno
Title: Jahn-Teller effect in Ag^{2+} doped KCl and NaCl: Is there any influence of the host lattice?
Ref.: Chemical Physics Letters 430, 51-55 (2006)

55. Authors: R. Bastardis, N. Guihéry, N. Suaud, C. de Graaf
Title: Competition between double exchange and purely magnetic Heisenberg models in mixed valence systems: Application to half doped manganites
Ref.: Journal of Chemical Physics 125, 194708 (2006)

56. Authors: L. Hozoi, A. H. de Vries, R. Broer, C. de Graaf, P. S. Bagus
Title: Ni 3s-hole states in NiO by non-orthogonal configuration interaction
Ref.: Chemical Physics 331, 178-185 (2006)

57. Authors: A. Sadoc, R. Broer, C. de Graaf
Title: Role of charge transfer configurations in $LaMnO_3$, $CaMnO_3$ and $CaFeO_3$
Ref.: Journal of Chemical Physics 126, 134709 (2007)

58. Authors: A. Sadoc, C. de Graaf, R. Broer
Title: Quantum chemical study of the ground state and the pressure-induced spin transition in $CaFeO_3$
Ref.: Physical Review B 75, 165116 (2007)

59. Authors: L. Hozoi, S. Nishimoto, C. de Graaf
Title: Renormalization of quasiparticle hopping integrals by spin interactions in layered copper oxides
Ref.: Physical Review B 75, 174505 (2007)

60. Authors: S. Romo, J. A. Fernández, J. M. Maestre, B. Keita, L. Nadjo, C. de Graaf, J. M. Poblet
Title: A DFT and ab initio study of electronic and electrochemistry properties of the tetranuclear sandwich complex $[Fe(III)_4(H_2O)_2(PW_9O_{34})_2]^{6-}$
Ref.: Inorganic Chemistry 46, 4022-4027 (2007)

61. Authors: J. A. Fernández, X. López, C. Bo, C. de Graaf, E. J. Baerends J. M. Poblet
Title: Polyoxometalates with internal cavities: redox activity, basicity and cation encapsulation in $[X^{n+}P_5W_{30}O_{110}]^{15-n-}$ Preyssler complexes, with X=Na^+, Ca^{2+}, Y^{3+}, La^{3+}, Ce^{3+} and Th^{4+}
Ref.: Journal of the American Chemical Society 129, 12244-12253 (2007)

62. Authors: R. Bastardis, N. Guihéry, C. de Graaf
Title: Microscopic origin of isotropic non-Heisenberg behavior in highly correlated systems
Ref.: Physical Review B 76, 132412 (2007)

63. Authors: E. Bordas, J. Cabrero, C. de Graaf, J. Igual, M. Reguero, R. Caballol
Title: The difference dedicated configuration interaction method: An accurate procedure to calculate energy transitions
Ref.: Afinidad 64, 154-162 (2007)

64. Authors: A. Stoyanova, C. de Graaf, R. Broer
Title: Many-electron bands in transition metal compounds
Ref.: in: Computation in modern science and engineering Vol. 2, 163-166 (2007) – *book chapter*, https://doi.org/10.1063/1.2836029

65. Authors: N. Queralt, D. Taratiel, C. de Graaf, R. Caballol, R. Cimiraglia, C. Angeli
Title: On the applicability of multireference second-order perturbation theory to study weak magnetic interactions in molecular complexes
Ref.: Journal of Computational Chemistry 29, 994-1003 (2008)

66. Authors: A. Sadoc, R. Broer, C. de Graaf
Title: CASSCF study of the relation between the Fe charge and the Mössbauer isomer shift
Ref.: Chemical Physics Letters 454, 196-200 (2008)

67. Authors: R. Bastardis, C. de Graaf, N. Guihéry
Title: Ab initio study of the CE magnetic phase in half-doped manganites: Purely magnetic versus double exchange description
Ref.: Physical Review B 77, 054426 (2008)

68. Authors: S. Romo, C. de Graaf, J. M. Poblet
Title: Mid-gap excitations in Anderson polyoxometalates
Ref.: Chemical Physics Letters 450, 391-395 (2008)

69. Authors: I. Negodaev, C. de Graaf, R. Caballol
Title: On the Heisenberg behaviour of magnetic coupling in the manganese dimer
Ref.: Chemical Physics Letters 458, 290-294 (2008)

70. Authors: R. Bastardis, N. Guihéry, C. de Graaf
Title: Isotropic non-Heisenberg terms in the magnetic coupling of transition metal complexes
Ref.: Journal of Chemical Physics 129, 104102 (2008)

71. Authors: B. Ordejón, C. de Graaf, C. Sousa
Title: Light-Induced Excited State Spin Trapping in Tetrazole-based Spin Crossover systems
Ref.: Journal of the American Chemical Society 130, 13961-13686 (2008)

72. Authors: R. Singh, C. de Graaf, E. Colacio, K. K. Rajak
Title: Mononuclear and binuclear iron(III) complexes incorporating N_4O_3 coordinating heptadentate ligand: Synthesis, structure and magnetic properties
Ref.: Polyhedron 27, 2751-2756 (2008)

73. Authors: A. Sadoc, C. de Graaf, R. Broer
Title: Embedded Cluster Approach: 3d Perovskite Oxides
Ref.: in: Encyclopedia of Materials: Science and Technology, pp. 1-6 (2008) – *book chapter*, doi.org/10.1016/B978-008043152-9.02188-6

74. Authors: D. Rubi, C. de Graaf, C. J. M. Daumont, D. Mannix, R. Broer, B. Noheda
Title: Ferromagnetism and increased ionicity in epitaxially grown $TbMnO_3$ films
Ref.: Physical Review B 79, 014416 (2009)

75. Authors: C. de Graaf, R. Caballol, S. Romo, J. M. Poblet
Title: *Ab initio* study of the singlet-triplet splitting in reduced polyoxometalates
Ref.: Theoretical Chemistry Accounts 123, 3-10 (2009)

76. Authors: M. Kepenekian, V. Robert, B. Le Guennic, C. de Graaf
Title: Energetics of $[Fe(NCH)_6]^{2+}$ via CASPT2 calculations: a spin-crossover perspective
Ref.: Journal of Computational Chemistry 30, 2327-2333 (2009)

77. Authors: R. Valencia, A. Rodríguez-Fortea, A. Clotet, C. de Graaf, M. N. Chaur, L. Echegoyen, J. M. Poblet
Title: Electronic Structure and Redox Properties of Metal Nitride Endohedral Fullerenes $M_3N@C_{2n}$ (M = Sc, Y, La and Gd; 2n = 80, 84, 88, 92, 96)
Ref.: Chemistry, a European Journal 15,10997-11009 (2009)

78. Authors: R. Maurice, R. Bastardis, C. de Graaf, N. Suaud, T. Mallah, N. Guihéry
Title: Universal theoretical approach to extract anisotropic spin Hamiltonians
Ref.: Journal of Chemical Theory and Computation 5, 2977-2984 (2009)

79. Authors: A. Domingo, M. A. Carvajal, C. de Graaf
Title: Spin-crossover in Fe(II) complexes: An *ab initio* study of the ligand σ donation
Ref.: International Journal of Quantum Chemistry 110, 331-337 (2010)

80. Authors: R. Maurice, R. Bastardis, C. de Graaf, N. Guihéry
Title: Rigorous extraction of the anisotropic multispin Hamiltonian in bimetallic complexes from the exact electronic Hamiltonian
Ref.: Journal of Chemical Theory and Computation 6, 55-65 (2010)

81. Authors: Z. Tabookht, X. López, C. de Graaf
Title: Analysis of the magnetic coupling in $M_3(dpa)_4Cl_2$ systems (M = Ni, Pd, Cu, Ag) by ab initio calculations
Ref.: Journal of Physical Chemistry A 114, 2028-2037 (2010)

82. Authors: C. de Graaf, X. López, J. L. Ramos, J. M. Poblet
Title: Ab Initio Study of the Antiferromagnetic Coupling in the Wheel-Shaped $[Cu_{20}Cl(OH)_{24}(H_2O)_{12}(P_8W_{48}O_{184})]^{25-}$ Anion
Ref.: Physical Chemistry Chemical Physics 12, 2716-2721 (2010)

83. Authors: C. de Graaf, C. Sousa
Title: Study of the Light-Induced Spin Crossover process of the $[Fe^{II}(bpy)_3]^{2+}$ complex
Ref.: Chemistry, a European Journal 16, 4550-4556 (2010)

84. Authors: R. Maurice, C. de Graaf, N. Guihéry
Title: Magnetic anisotropy in binuclear complexes in the weak-exchange limit: from the multi-spin to the giant-spin Hamiltonian
Ref.: Physical Review B 81, 214427 (2010)

85. Authors: M. A. Carvajal, M. Reguero, C. de Graaf
Title: On the mechanism of the photoinduced magnetism in copper octacyanomolybdates
Ref.: Chemical Communications 46, 5737-5739 (2010)

86. Authors: I. Negodaev, C. de Graaf, R. Caballol
Title: Extraction of magnetic coupling parameters in 2-dimensional magnetic honeycomb layers
Ref.: Journal of Physical Chemistry A 114, 7553-7560 (2010)

87. Authors: R. Maurice, C. de Graaf, N. Guihéry
Title: Magneto-structural relations from a combined ab initio and ligand field analysis for the non-intuitive zero-field splitting in Mn(III) complexes
Ref.: Journal of Chemical Physics 133, 084307 (2010)

88. Authors: R. Maurice, A. M. Pradipto, N. Guihéry, R. Broer, C. de Graaf
Title: Antisymmetric Magnetic Interactions in oxo-bridged Copper (II) Bimetallic Systems
Ref.: Journal of Chemical Theory and Computation 6, 3092-3101 (2010)

89. Authors: Z. Tabookht, X. López, M. Bénard, C. de Graaf
Title: Isotropic non-Heisenberg behavior in $M_3(dpa)_4Cl_2$ Extended Metal Atom Chains
Ref.: Journal of Physical Chemistry A 114, 12291-12298 (2010)

90. Authors: I. Negodaev, N. Queralt, R. Caballol, C. de Graaf
Title: Theoretical study of the magnetic exchange interaction in catena-μ-tris[oxalato(2-)-O^1,O^2;O^3,O^4]-dicopper complex with interlocked helical chains
Ref.: Chemical Physics 379, 109-115 (2011)

91. Authors: C. J. Calzado, C. Angeli, C. de Graaf, R. Caballol
Title: Analysis of the magnetic coupling in nitroxide organic biradicals
Ref.: Theoretical Chemistry Accounts 128, 505-529 (2011)

92. Authors: C. de Graaf, C. Sousa
Title: On the role of the metal-to-ligand charge transfer states in the light-induced spin crossover in $Fe^{II}(bpy)_3$
Ref.: International Journal of Quantum Chemistry 111, 3385-3393 (2011)

93. Authors: M. A. Carvajal, R. Caballol, C. de Graaf
Title: Insights on the photomagnetism in copper octacyanomolybdates
Ref.: Dalton Transactions 40 (*cover article*), 7295-7303 (2011)

94. Authors: I. Negodaev, C. de Graaf, R. Caballol, V. V. Lukov
Title: On the magnetic coupling in asymmetric bridged Cu(II) dinuclear complexes: The influence of substitutions on the carboxylato group
Ref.: Inorganica Chimica Acta 375, 166-172 (2011)

95. Authors: R. Maurice, K. Sivalingam, D. Ganyushin, N. Guihéry, C. de Graaf, F. Neese
Title: Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate
Ref.: Inorganic Chemistry 50, 6229-6236 (2011)

96. Authors: C. Angeli, C. J. Calzado, C. de Graaf, R. Caballol
Title: The electronic structure of Ullman's biradicals: an orthogonal Valence Bond interpretation
Ref.: Physical Chemistry Chemical Physics 13, 14617-14628 (2011)

97. Authors: Z. Tabookht, C. de Graaf, X. López
Title: Towards a Low-Spin Configuration in Extended Metal Atom Chains. Theoretical Study of Trimetallic Systems with 22 Metal Electrons
Ref.: Dalton Transactions 41, 498-504 (2012)

98. Authors: N. A. G. Bandeira, Z. Tabookht, C. de Graaf, X. López
Title: Simple vs. Composite Nature of the Magnetic Coupling in Copper and Nickel-based Metallic Chains. Over- and Underestimation of J
Ref.: Comptes rendus Chimie 15, 163-169 (2012)

99. Authors: A. M. Pradipto, R. Maurice, N. Guihéry, C. de Graaf, R. Broer
Title: First Principles Study of Magnetic Interactions in Cupric Oxide
Ref.: Physical Review B 85, 014409 (2012)

100. Authors: A. Domingo, A. Rodríguez-Fortea, C. de Graaf
Title: The absorption spectrum of cytosine tautomers: beyond the static approach
Ref.: Journal of Chemical Theory and Computation 8, 235-244 (2012)

101. Authors: Z. Tabookht, X. López, C. de Graaf, N. Guihéry, N. Suaud, N. Benamor
Title: Rationalization of the behavior of $M_2(CH_3CS_2)_4I$ (M = Ni, Pt) chains at room temperature from periodic DFT and ab initio cluster calculations
Ref.: Journal of Computational Chemistry, 33, 1748-1761 (2012)

102. Authors: A. Domingo, A. Rodríguez-Fortea, M. Swart, R. Broer, C. de Graaf
Title: Ab-initio absorption spectrum of NiO combining molecular dynamics with the embedded cluster approach in a discrete reaction field
Ref.: Physical Review B 85, 155143 (2012)

103. Authors: R. Maurice, A. M. Pradipto, C. de Graaf, R. Broer
Title: Magnetic Interactions in $LiCu_2O_2$: Single-Chain versus Double-Chain Couplings
Ref.: Physical Review B 86, 024411 (2012)

104. Authors: A. Domingo, M. A. Carvajal, C. de Graaf, K. Sivalingam, F. Neese, C. Angeli
Title: Metal-to-metal charge transfer transitions: Reliable excitation energies from ab initio calculations
Ref.: Theoretical Chemistry Accounts 131, 1264 (2012)

105. Authors: R. Ruamps, L. J. Batchelor, R. Maurice, N. Gogoi, P. Jiménez-Lozano, N. Guihéry, C. de Graaf, A.-L. Barra, J.-P. Sutter, T. Mallah
Title: Origin of the Magnetic Anisotropy in Ni(II) and Co(II) Heptacoordinate Complexes
Ref.: Chemistry, a European Journal 19, 950-956 (2013)

106. Authors: M. Pápai, G. Vankó, C. de Graaf, T. Rozgonyi
Title: Theoretical investigation of the electronic structure of Fe(II) complexes at spin-state transitions
Ref.: Journal of Chemical Theory and Computation 9, 509-519 (2013)

107. Authors: A. Domingo, M. Vérot, C. de Graaf, J. J. Novoa, F. Mota, V. Robert
Title: Short and Long-Range Effects Controlling Magnetic Interactions in Organic Radical-Based Materials
Ref.: Physical Chemistry Chemical Physics 15, 6982-6989 (2013)

108. Authors: J. Baltrusaitis, C. de Graaf, R. Broer, E. Patterson
Title: H_2S mediated thermal and photochemical methane activation
Ref.: ChemPhysChem 14, 3960-3970 (2013)

109. Authors: A. Rudavskyi, R. W. A. Havenith, R. Broer, C. de Graaf, C. Sousa
Title: Explanation of the site-specific spin crossover in $Fe(mtz)_6(BF_4)_2$
Ref.: Dalton Transactions 42 (*cover article*), 14702-14709 (2013)

110. Authors: C. Sousa, C. de Graaf, A. Rudavskyi, R. Broer, J. Tatchen, M. Etinski, C. M. Marian
Title: Ultrafast deactivation mechanism of the excited singlet in the light-induced spin crossover of $[Fe(bpy)_3]^{2+}$
Ref.: Chemistry, a European Journal 19, 17541-17551 (2013)

111. Authors: R. Maurice, C. de Graaf, N. Guihéry
Title: Theoretical determination of spin Hamiltonians with isotropic and anisotropic magnetic interactions in transition metal and lanthanide complexes
Ref.: Physical Chemistry Chemical Physics (perspective article) 15, 18784-18804 (2013)

112. Authors: J.-P. Malrieu, R. Caballol, C. J. Calzado, C. de Graaf, N. Guihéry
Title: Magnetic interactions in molecules and highly correlated materials: Physical content, analytical derivation and rigorous extraction of magnetic Hamiltonians
Ref.: Chemical Reviews 114, 429-492 (2014) **Highly-cited paper**

113. Authors: S. Saureu, C. de Graaf
Title: On the role of solvent effects on the electronic transitions in Fe(II) and Ru(II) complexes
Ref.: Chemical Physics 428, 59-66 (2014)

114. Authors: C. de Graaf, M. Reguero
Title: Methods for describing open-shell systems: Following the trail of Rosa Caballol's research
Ref.: International Journal of Quantum Chemistry (invited review) 114, 481-492 (2014)

115. Authors: D. Barats-Damatov, L. J. W. Shimon, L. Weiner, R. Schreiber, P. Jiménez-Lozano, J. M. Poblet, C. de Graaf, R. Neumann
Title: A Dicobalt-μ-oxo Polyoxometalate Compound, $[(\alpha_2\text{-}P_2W_{17}O_{61}Co)_2O]^{14-}$, – A Potent Species for Water Oxidation, C–H Bond Activation and Oxygen Transfer
Ref.: Inorganic Chemistry 53, 1779-1787 (2014)

116. Authors: A. Ghisolfi, K. Yu. Manokhov, R. Pattacini, P. Braunstein, X. López, C. de Graaf, M. Speldrich, J. van Leusen, H. Schilder, P. Kögerler
Title: Comparative synthetic, magnetic and theoretical study of functional M_4Cl_4 cubane-type Co(II) and Ni(II) complexes
Ref.: Dalton Transaction 43, 7847-7859 (2014)

117. Authors: R. Ruamps, R. Maurice, C. de Graaf, N. Guihéry
Title: Interplay between local anisotropies in binuclear complexes
Ref.: Inorganic Chemistry 53, 4508-4516 (2014)

118. Authors: A. Rudavskyi, C. Sousa, C. de Graaf, R. W. A. Havenith, R. Broer
Title: Computational approach to the study of thermal spin crossover phenomena
Ref.: Journal of Chemical Physics 140, 184318 (2014)

119. Authors: M. Spivak, C. Angeli, C. J. Calzado, C. de Graaf
Title: Improving the calculation of magnetic coupling constants in MRPT methods
Ref.: Journal of Computational Chemistry 35, 1665-1671 (2014)

120. Authors: A. Domingo, C. Sousa, C. de Graaf
Title: The effect of thermal motion on the electron localization in metal-to-ligand charge transfer excitations in $[Fe(bpy)_3]^{2+}$
Ref.: Dalton Transactions 43, 17838-17846 (2014)

121. Authors: S. Farokhipoor, C. Magén, S. Venkatesan, J. Íñiguez, C. J. M. Daumont, D. Rubi, E. Snoeck, M. Mostovoy, C. de Graaf, A. Müller, M. Döblinger, C. Scheu, B. Noheda
Title: Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide
Ref.: Nature 515, 379-383 (2014)

122. Authors: G. Alcover-Fortuny, C. de Graaf, R. Caballol
Title: Spin-crossover in phenylazopyridine-functionalized Ni-porphyrin: trans-cis isomerization triggered by π-π interactions
Ref.: Physical Chemistry Chemical Physics 17,217-225 (2015)

123. Authors: A. Domingo, C. Angeli, C. de Graaf, V. Robert
Title: Electron reorganization triggered by electron transfer: the inter-valence charge transfer of a Fe^{3+}/Fe^{2+} bi-metallic complex
Ref.: Journal of Computational Chemistry 36, 861-869 (2015)

124. Authors: M. Álvarez-Moreno, C. de Graaf, N. López, F. Maseras, J. M. Poblet, C. Bo
Title: Managing the Computational Chemistry Big Data problem: the ioChem-BD platform
Ref.: Journal of Chemical Information and Modeling 55, 95-103 (2015)

125. Authors: N. Suaud, X. López, N. Ben Amor, N. A. G. Bandeira, C. de Graaf, J. M. Poblet
Title: Accuracy of Embedded Fragment Calculation for evaluating Electron Interactions in Mixed Valence Magnetic Systems: Study of 2e-reduced Lindqvist Polyoxometalates
Ref.: Journal of Chemical Theory and Computation 11, 550-559 (2015)

126. Authors: C. de Graaf, R. Broer
Title: Magnetic interactions in Molecules and Solids *(monograph)*
Ref.: Volume 2 of the Theoretical Chemistry and Computational Modeling series of textbooks for Master students, Springer (2015)

127. Authors: N. Guihéry, R. Ruamps, R. Maurice, C. de Graaf
Title: Synergy and destructive interferences between local magnetic anisotropies in binuclear complexes
Ref.: AIP Conference Proceedings 1702, 090015 (2015)

128. Authors: C. Sousa, C. de Graaf
Title: Ab Initio Wavefunction Approaches to Spin States
Ref.: in: Spin States in Biochemistry and Inorganic Chemistry, pp. 35-57, Wiley (2016) – *book chapter*

129. Authors: S. Saureu, C. de Graaf
Title: TD-DFT Study of the Light-induced Spin Crossover of Fe(III) Complexes
Ref.: Physical Chemistry Chemical Physics 18, 1233-1244 (2016)

130. Authors: G. Alcover-Fortuny, R. Caballol, K. Pierloot, C. de Graaf
Title: Role of the imide axial ligand in the spin and oxidation states of Mn corrole and corrolazine
Ref.: Inorganic Chemistry 55, 5274-5280 (2016)

131. Authors: R. Maurice, R. Broer, N. Guihéry, C. de Graaf
Title: Zero-field splitting in transition metal complexes: Ab initio calculations, effective Hamiltonians, model Hamiltonians, and crystal-field models
Ref.: in: Handbook of Relativistic Quantum Chemistry, Springer, dx.doi.org/10.1007/978-3-642-41611-8_37-1 (2016) – *book chapter*

132. Authors: C. Maxim, S. Saureu, C. de Graaf, S. Ferlay, M. W. Hosseini, V. Robert, C. Train
Title: Amidinium-containing 2D [MnCr] Bimetallic Oxalate-Based Networks: The Influence on Structure and Magnetism Explored by Combining Experience and Theory
Ref.: European Journal of Inorganic Chemistry 4185-4193 (2016)

133. Authors: V. Arcisauskaite, D. Fijan, M. Spivak, C. de Graaf, J. E. McGrady
Title: Biradical character in the ground state of $[Mn@Si_{12}]^+$: a DFT and CASPT2 study
Ref.: Physical Chemistry Chemical Physics 18, 24006-24014 (2016)

134. Authors: C. Ci, J. Carbó, R. Neumann, C. de Graaf, J. M. Poblet
Title: Photoreduction Mechanism of CO_2 to CO Catalyzed by a Rhenium(I)-Polyoxometalate Hybrid Compound
Ref.: ACS Catalysis 6, 6422-6428 (2016)

135. Authors: C. de Graaf, J. Schnack
Title: Ab initio modeling and calculations of magnetic properties
Ref.: in: Molecular Magnetic Materials, pp. 447-471, Wiley (2016) – *book chapter*

136. Authors: M. Spivak, K. D. Vogiatzis, C. J. Cramer, C. de Graaf, L. Gagliardi
Title: Quantum chemical characterization of single molecule magnets based on uranium
Ref.: Journal of Physical Chemistry A 121, 1726-1733 (2017)

137. Authors: M. Spivak, V. Arcisauskaite, X. López, J. E. McGrady, C. de Graaf
Title: A multiconfigurational approach to the electronic structure of trichromium extended metal atom chains
Ref.: Dalton Transactions 46, 6202-6211 (2017)

138. Authors: M. Spivak, V. Arcisauskaite, X. López, C. de Graaf
Title: Backbone flexibility of extended metal atom chains. Ab initio molecular dynamics for $Cr_3(dpa)_4X_2$ (X = NCS, CN, NO_3) in gas and crystalline phases
Ref.: Dalton Transactions 46, 15487-15493 (2017)

139. Authors: P. Kozłowski, A. Notario-Estévez, C. de Graaf, X. López, and K. Y. Monakhov
Title: Reconciling the valence state with magnetism in mixed-valent polyoxometalates: the case of a $VO_2F_2@V_{22}O_{54}$ cluster
Ref.: Physical Chemistry Chemical Physics 19, 29767-29771 (2017)

140. Authors: J. Casellas, G. Alcover-Fortuny, C. de Graaf, and M. Reguero
Title: Phenylazopyridine as switch in photochemical reactions. A detailed computational description of the mechanism of its photoisomerization
Ref.: Materials 10, 1342 (2017)

141. Authors: C. Sousa, C. de Graaf, A. Rudavskyi, R. Broer
Title: Theoretical Study of the Light-Induced Spin Crossover Mechanism in $[Fe(mtz)_6]^{2+}$ and $[Fe(phen)_3]^{2+}$
Ref.: Journal of Physical Chemistry A 121, 9720-9727 (2017)

142. Authors: C. Sousa, A. Domingo, C. de Graaf
Title: Effect of second-order spin-orbit coupling on the interaction between spin states in spin crossover systems
Ref.: Chemistry, a European Journal 24 (*cover article*), 5146-5152 (2018) **(Hot article)**

143. Authors: C. Sousa, M. Llunell, A. Domingo, C. de Graaf
Title: Theoretical evidence for the direct ^{3}MLCT-HS deactivation in the light-induced spin crossover of Fe(II)-polypyridyl complexes
Ref.: Physical Chemistry Chemical Physics 20, 2351-2355 (2018)

144. Authors: X. Zhang, Y. Wang, R. Morales-Martínez, J. Zhong, C. de Graaf, A. Rodríguez-Fortea, J. M. Poblet, L. Echegoyen, L. Feng, N. Chen
Title: $U_2@I_h(7)$-C_{80}: Crystallographic observation of a long-sought dimetallic actinide endohedral fullerene
Ref.: Journal of the American Chemical Society 140 *(cover article)*, 3907-3915 (2018)

145. Authors: G. Alcover-Fortuny, J. Wu, R. Caballol, C. de Graaf
Title: Quantum Chemical Study of the Interligand Electron Transfer in Ru Polypyridyl Complexes
Ref.: Journal of Physical Chemistry A 122, 1114-1123 (2018)

146. Authors: A. Notario-Estévez, P. Kozłowski, O. Linnenberg, C. de Graaf, X. López, and K. Y. Monakhov
Title: Decoding the role of encapsulated ions in the electronic and magnetic properties of mixed-valence polyoxovanadate capsules $\{X@V_{22}O_{54}\}$ ($X = ClO_4^-$, SCN^-, $VO_2F_2^-$): a combined theoretical approach
Ref.: Physical Chemistry Chemical Physics 20, 17847-17858 (2018)

147. Authors: T. Francese, J. Ribas-Arino, J. J. Novoa, R. W. A. Havenith, R. Broer, C. de Graaf, and M. Deumal
Title: The magnetic fingerprint of dithiazolyl-based molecule magnets
Ref.: Physical Chemistry Chemical Physics 20, 20406-20416 (2018)

148. Authors: O. Linnenberg, M. Moors, A. Notario-Estévez, X. López, C. de Graaf, S. Peter, C. Bäumer, R. Waser, and K-Y. Monakhov
Title: Addressing multiple resistive states of polyoxovanadates: Conductivity as a function of individual molecular redox states
Ref.: Journal of the American Chemical Society 140, 16635-16640 (2018)

149. Authors: C. Sousa, M. Alías, A. Domingo, and C. de Graaf
Title: Deactivation of excited states in transition metal complexes: Insight from computational chemistry
Ref.: Chemistry, a European Journal 25, 1152-1164 (2019), mini-review

150. Authors: G. Ielasia, G. Alcover, J. Casellas, C. de Graaf, G. Orellana, and M. Reguero
Title: Computer-aided design of short-lived phosphorescent Ru(II) polarity probes
Ref.: Dyes and Pigments 162, 168-176 (2019)

151. Authors: M. Spivak, X. López, C. de Graaf
Title: Trends in the Bond Multiplicity of Cr_2, Cr_3 and Cr_2M (M = Zn, Ni, Fe, Mn) Complexes Extracted from Multiconfigurational Wave Functions
Ref.: Journal of Physical Chemistry A 123, 1538-1547 (2019)

152. Authors: A. Solé-Daura, A. Notario-Estévez, J. J. Carbó, J. M. Poblet, C. de Graaf, K. Y. Monakhov, X. López
Title: How does the Redox State of Polyoxovanadates Influence the Collective Behaviour in Solution? A Case Study with $[I@V_{18}O_{42}]^{q-}$ (q = 3, 5, 7, 11 and 13)
Ref.: Inorganic Chemistry , 58, 3881-3894 (2019)

153. Authors: J. Wu, C. Sousa, C. de Graaf
Title: The role of anharmonicity in the vibrational frequencies on the theoretical estimates of the thermal spin crossover temperature
Ref.: Magnetochemistry 5, 49 (2019)

154. Authors: M. Alías, N. Alkhaldi, M. Reguero, L. Ma, J. Zhang, C. de Graaf, M. N. Huda, W. Chen.
Title: Theoretical Studies on the energy structures and optical properties of Copper Cysteamine – A Novel Sensitizer
Ref.: Physical Chemistry Chemical Physics 21, 21084-21093 (2019)

155. Authors: X. Qi, S. Pillet, C. de Graaf, E.-E. Bendeif, P. Guionneau, M. Rouzières, V. Marvaud, O. Stefańczyk, M. Magott, D. Pinkowicz, C. Mathonière
Title: Photoinduced Mo@CN Bond Breakage in Octacyanomolybdate Leading to Spin Triplet Trapping
Ref.: Angewandte Chemie 59, 3117-3121 (2020)

156. Authors: T. P. Straatsma, R. Broer, S. Faraji, R. W. A. Havenith, L. E. Aguilar Suarez, R. K. Kathir, M. Wibowo, C. de Graaf
Title: GronOR: Massively Parallel and GPU-Accelerated Non-Orthogonal Configuration Interaction for Large Molecular Systems
Ref.: Journal of Chemical Physics 152, 064111 (2020)

157. Authors: R. K. Kathir, C. de Graaf, R. Broer, R. W. A. Havenith
Title: Reduced Common Molecular Orbital Basis for Nonorthogonal Configuration Interaction
Ref.: Journal of Chemical Theory and Computation 16, 2941-2951 (2020)

158. Authors: J. Wu, M. Alías, C. de Graaf
Title: Controlling the Lifetime of the Triplet MLCT State in Fe(II) Polypyridyl Complexes through Ligand Modification
Ref.: Inorganics 8, 16 (2020)

159.	Authors:	L. Luo, T. P. Straatsma, L. E. Aguilar Suarez, R. Broer, D. Bykov, E. F. D'Azevedo, S. S. Faraji, K. C. Gottiparthi, C. de Graaf, J. A. Harris, R. W. A. Havenith, H. J. Aa. Jensen, W. Joubert, R. K. Kathir, J. Larkin, Y. Li, D. I. Lyakh, O. E. B. Messer, M. R. Norman, J. C. Oefelein, R. Sankaran, A. F. Tillack, A. L. Barnes, L. Visscher, J. C. Wells, M. Wibowo
	Title:	Pre-exascale accelerated application development: the ORNL Summit experience
	Ref.:	IBM; J. Res. Dev. 64, 11 (2020)
160.	Authors:	F. Wang, H. Gao, C. de Graaf, J. M. Poblet, B. J. Campbell, A. Stroppa
	Title:	Switchable Rashba anisotropy in layered hybrid organic–inorganic perovskite by hybrid improper ferroelectricity
	Ref.:	npj Computational Materials 6, 183 (2020)
161.	Authors:	X. Li, Y. Roselló, Y.-R. Yao, J. Zhuang, X. Zhang, A. Rodríguez-Fortea, C. de Graaf, L. Echegoyen, J. M. Poblet, N. Chen
	Title:	$U_2N@I_h(7)$-C_{80}: fullerene cage encapsulating an unsymmetrical U(IV)=N=U(V) cluster
	Ref.:	Chemical Science 12, 282-292 (2021)
162.	Authors:	F. Wang, R. Neumann, C. de Graaf, J. M. Poblet
	Title:	Photoreduction Mechanism of CO_2 to CO Catalyzed by a Three Component Hybrid Construct with a Bimetallic Rhenium Catalyst
	Ref.:	ACS Catalysis 11, 1495-1504 (2021)
163.	Authors:	F. Wang, Z. Lang, L. Yan, A. Stroppa, J. M. Poblet, C. de Graaf
	Title:	Density Functional Theory Analysis of Single-molecule Ferroelectricity in Preyssler-type Polyoxometalates
	Ref.:	APL Materials 9, 021109 (2021)
164.	Authors:	J. Zhuang, R. Morales-Martínez, J. Zhang, Y. Wang, Y.-R. Yao, C. Pei, A. Rodríguez-Fortea, S. Wang, L. Echegoyen, C. de Graaf, J. M. Poblet, N. Chen
	Title:	Characterization of a strong covalent Th^{3+}-Th^{3+} bond inside an $I_h(7)$-C_{80} fullerene cage
	Ref.:	Nature Communications 12, 2372 (2021)
165.	Authors:	L. E. Aguilar-Suarez, C. de Graaf, S. Faraji
	Title:	Influence of the crystal packing in singlet fission: one step beyond the gas phase approximation
	Ref.:	Physical Chemistry Chemical Physics 23, 14164-14177 (2021)
166.	Authors:	A. Notario-Estévez, X. López, C. de Graaf
	Title:	Computational study of the staircase molecular conductivity of polyoxovanadates adsorbed on Au(111)
	Ref.:	Dalton Transactions 50, 5540-5551 (2021)
167.	Authors:	M. Spivak, C. de Graaf, V. Arcisauskaite, X. López
	Title:	Gating the Conductance of Extended Metal Atom Chains: a Computational Analysis of $Ru_3(dpa)_4(NCS)_2$ and $[Ru_3(npa)_4(NCS)_2]$
	Ref.:	Physical Chemistry Chemical Physics 23, 14836-14844 (2021)

168. Authors: M. Moors, J. Warneke, X. López, C. de Graaf, B. Abel, K. Y. Monakhov
Title: Insights from Adsorption and Electron Modification Studies of Polyoxometalates on Surfaces for Molecular Memory Applications
Ref.: Accounts of Chemical Research 54, 3377-3389 (2021)

169. Authors: M. Alías-Rodríguez, C. de Graaf, M. Huix-Rotllant
Title: Ultrafast intersystem crossing in xanthone from wavepacket dynamics
Ref.: Journal of the American Chemical Society 143, 21474-21477 (2021)

170. Authors: D. Azaiza-Dabbah, C. Vogt, F. Wang, A. Masip-Sánchez, C. de Graaf, J. M. Poblet, E. Haviv, R. Neumann
Title: Molecular Transition Metal Oxide Electrocatalysts for the Reversible Carbon Dioxide-Carbon Monoxide Transformation
Ref.: Angewandte Chemie 61, e202112915 (2022)

171. Authors: A. Wojciechowska, C. de Graaf, T. Rojek, M. Jerzykiewicz, M. Malik, A. Gagor, M. Duczmal
Title: A rare diiodo-L-tyrosine copper(II) complexes – Crystal and molecular structure of materials stabilized by weak interactions
Ref.: Polyhedron 219, 115780 (2022)

172. Authors: A. Sánchez-Mansilla, C. Sousa, R. K. Kathir, R. Broer, T. P. Straatsma, C. de Graaf
Title: On the role of dynamic electron correlation in non- orthogonal configuration interaction with fragments
Ref.: Physical Chemistry Chemical Physics 24, 11931-11944 (2022)

173. Authors: T. P. Straatsma, R. Broer, A. Sánchez-Mansilla, C. Sousa, C. de Graaf
Title: GronOR: Scalable and Accelerated Non-Orthogonal Configuration Interaction for Molecular Fragment Wave Functions
Ref.: Journal of Chemical Theory and Computation 18, 3549-3565 (2022)

174. Authors: M. Alías-Rodríguez, M. Huix-Rotllant, C. de Graaf
Title: Quantum dynamics simulations of the thermal and light-induced high-spin to low-spin relaxation in $Fe(bpy)_3$ and $Fe(mtz)_6$
Ref.: Faraday Discussions 237, 93-107 (2022)

175. Authors: C. de Graaf, R. Broer, T. P. Straatsma
Title: Non-Orthogonal Configuration Interaction for Fragments
Ref.: in: Comprehensive Computational Chemistry, Major Reference Works, doi:10.1016/B978-0-12-821978-2.00056-8 (2023) – *book chapter*

176. Authors: T. P. Straatsma, R. Broer, C. de Graaf
Title: Tutorial for Non-Orthogonal Configuration Interaction Fragment Studies using GronOR
Ref.: in: Comprehensive Computational Chemistry, Major Reference Works, doi:10.1016/B978-0-12-821978-2.00060-X (2023)– *book chapter*

177. Authors: G. Li Manni, I. F. Galván, A. Alavi, F. Aleotti, F. Aquilante, J. Autschbach, D. Avagliano, A. Baiardi, J. J. Bao, S. Battaglia, L. Birnoschi, A. Blanco-González, S. I. Bokarev, R. Broer, R. Cacciari, P. B. Calio, R. K. Carlson, R. C. Couto, L. Cerdán, L. F. Chibotaru, N. F. Chilton, J. R. Church, I. Conti, S. Coriani, J. Cúellar-Zuquin, R. E. Daoud, N. Dattani, P. Decleva, C. de Graaf, M. Delcey, L. De Vico, W. Dobrautz, S. S. Dong, R. Feng, N. Ferré, M. Filatov, L. Gagliardi, M. Garavelli, L. González, Y. Guan, M. Guo, M. R. Hennefarth, M. R. Hermes, C. E. Hoyer, M. Huix-Rotllant, V. K. Jaiswal, A. Kaiser, D. S. Kaliakin, M. Khamesian, D. S. King, V. Kochetov, M. Krośnicki, A. A. Kumaar, E. D. Larsson, S. Lehtola, M. B. Lepetit, H. Lischka, P. López Ríos, M. Lundberg, D. Ma, S. Mai, P. Marquetand, I. C. D. Merritt, F. Montorsi, M. Mörchen, A. Nenov, V. H. A. Nguyen, Y. Nishimoto, M. S. Oakley, M. Olivucci, M. Oppel, D. Padula, R. Pandharkar, Q. M. Phung, F. Plasser, G. Raggi, E. Rebolini, M. Reiher, I. Rivalta, D. Roca-Sanjuán, T. Romig, A. A. Safari, A. Sánchez-Mansilla, A. M. Sand, I. Schapiro, T. R. Scott, J. Segarra-Martí, F. Segatta, D.-C. Sergentu, P. Sharma, R. Shepard, Y. Shu, J. K. Staab, T. P. Straatsma, L. K. Sørensen, B. N. C. Tenorio, D. G. Truhlar, L. Ungur, M. Vacher, V. Veryazov, T. A. Voß, O. Weser, D. Wu, X. Yang, D. Yarkony, C. Zhou, J. P. Zobel, R. Lindh

Title: The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry

Ref.: Journal of Chemical Theory and Computation 19, 6933-6991 (2023).

---

178. Authors: A. Moreno-Vicente, Y. Roselló, N. Chen, L. Echegoyen, P. W. Dunk, A. Rodríguez-Fortea, C. de Graaf, J. M. Poblet

Title: Are U-U Bonds Inside Fullerenes Really Unwilling Bonds?

Ref.: Journal of the American Chemical Society 145, 6710-6718 (2023)

---

179. Authors: A. Moreno-Vicente, M. Alías-Rodríguez, P. W. Dunk, C. de Graaf, J. M. Poblet, A. Rodríguez- Fortea

Title: Highly oxidized U(VI) within the smallest fullerene: gas-phase synthesis and computational study of boron-doped U@C_{27}B

Ref.: Inorganic Chemistry Frontiers 20, 908-914 (2023)

---

180. Authors: X. López, T. P. Straatsma, A. Sánchez-Mansilla, and C. de Graaf

Title: Non-orthogonal Configuration Interaction Study on the Effect of Thermal Distortions on the Singlet Fission Process in Photoexcited Pure and B,N-Doped Pentacene Crystals

Ref.: Journal of Physical Chemistry C 127, 16249-16258 (2023)

---

181. Authors: C. Sousa, A. Sánchez-Mansilla, R. Broer, T. P. Straatsma, C. de Graaf

Title: A Nonorthogonal Configuration Interaction Approach to Singlet Fission in Perylenediimide Compounds

Ref.: Journal of Physical Chemistry A 127, 9944-9958 (2023), *Roland Lindh Festschrift*

182. Authors:	Y. Yan, L. Abella, R. Sun, Y.-H. Fang, Y. Roselló, Y. Shen, A. Rodríguez-Fortea, C. de Graaf, Q. Meng, Y.-R. Yao, L. Echegoyen, B.-W. Wang, S. Gao, J. M. Poblet, N. Chen
Title:	Actinide-lanthanide single electron metal-metal bond formed in mixed-valence dimetallofullerenes
Ref.:	Nature Communications 14, 6637 (2023)
183. Authors:	X. López, A. Sánchez-Mansilla, C. Sousa, T. P. Straatsma, R. Broer, C. de Graaf
Title:	Comparison of Computational Strategies for the Calculation of the Electronic Coupling in Intermolecular Energy and Electron Transport Processes
Ref.:	Journal of Physical Chemistry A 127, 10717-10731 (2023), *Roland Lindh Festschrift*

Development of scientific software

- Co-author of the Quantum Chemistry program MOLCAS 5, used by more than 400 research groups world-wide. Reference: MOLCAS Version 5, K. Andersson, M. Barysz, A. Bernhardsson, M. R. A. Blomberg, D. L. Cooper, T. Fleig, M. P. Fülscher, C. de Graaf, B. A. Hess, G. Karlström, R. Lindh, P.-Å. Malmqvist, P. Neogrády, J. Olsen, B. O. Roos, B. Schimmelpfennig, M. Schütz, L. Seijo, L. Serrano-Andrés, P. E. M. Siegbahn, J. Stålring, T. Thorsteinsson, V. Veryazov, P.-O. Widmark, Lund University, Sweden (2000).
- Main developer of the massively parallel and GPU-accelerated non-orthogonal configuration interaction code GronOR (2019-). Webpages: gitlab.com/gronor/gronor and www.gronor.org
- Developer of the Quantum Chemistry program OpenMolcas (2021-).
  Webpage: https://gitlab.com/Molcas/OpenMolcas

Participation in public R+D Projects

Title of the project:	TMR activity "Marie Curie research training grants"- Magnetic Interactions in low-dimensional Heisenberg systems
Financed by:	European Union
Participating entities:	University of Barcelona
Duration:	from: 01/07/1998 until: 30/09/2001
Amount of subvention:	105.184,00 €
Researcher-in-chief:	Francesc Illas Riera and Coen de Graaf
Participating scientists:	2
Title of the project:	Theoretical study of magnetic materials "Acción Integrada Hispano–Francesa 2000HF-0030"
Financed by:	Spanish Ministry of Science and Technology (MCYT)
Participating entities:	Universitat Rovira i Virgili (Tarragona, Spain) and Paul Sabatier University (Toulouse, France)
Duration:	from: 01/07/2001 until: 31/12/2002
Amount of subvention:	10.277,31 €
Researcher-in-chief:	Rosa Caballol Lorenzo and Jean-Paul Malrieu
Participating scientists:	6
Title of the project:	Support to consolidated research groups within the framework "Pla de Recerca de Catalunya", of the "Generalitat de Catalunya". SGR01-00315.
Financed by:	Interdepartmental Commission of Research and Technological Innovation (CIRIT)
Participating entities:	Universitat Rovira i Virgili (Tarragona, Spain)
Duration:	from: 01/01/2002 until: 31/12/2005
Amount of subvention:	42.070,85 €
Researcher-in-chief:	Rosa Caballol Lorenzo
Participating scientists:	17
Title of the project:	"Estudi teòric de materials amb propietats electròniques rellevants", support to the cooperation and mobility with the CNRS of the "Direcció General de Recerca de la Generalitat de Catalunya." Ref. PICS2001-13 *(Theoretical study of materials with relevant electronic properties)*
Financed by:	DGR-DURSI, Generalitat de Catalunya
Participating entities:	Universitat Rovira i Virgili (Tarragona, Spain), University of Barcelona and Paul Sabatier University (Toulouse, France)
Duration:	from: 01/01/2002 until: 31/12/2004
Amount of subvention:	18.217,21 €(for 2002 and 2003)
Researcher-in-chief:	Rosa Caballol Lorenzo and Jean-Paul Malrieu
Participating scientists:	6

Title of the project:	"Predicción ab initio de parámetros derivados de la estructura electrónica en química de materiales. Un punto de partida para la simulación no empírica de propiedades macroscópicas." Ref. BQU2002-04029-C02-02 *(Ab initio prediction of electronic structure parameters in Materials Chemistry. A starting point for the non-empirical simulation of macroscopic properties.)*
Financed by:	Spanish Ministry of Science and Technology (MCYT)
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2002 until: 2005
Amount of subvention:	108.000,00 €
Researcher-in-chief:	Rosa Caballol Lorenzo
Participating scientists:	9
Title of the project:	"Tractament ab initio del magnetisme i de fenòmens relacionats d'òxids de metalls de transició." Integrated Actions 2002-2003. Ref. ACI2002-15 and ACI2003-7 *(Ab initio treatment of magnetism and related phenomena of transition metal oxides)*
Financed by:	DURSI, Generalitat de Catalunya
Participating entities:	Universitat Rovira i Virgili and Material Science Center (Groningen, The Netherlands).
Duration:	from: 01/01/2003 until: 31/12/2004
Amount of subvention:	7.000 €
Researcher-in-chief:	Coen de Graaf
Participating scientists:	6
Title of the project:	"Understanding and prediction of magnetic properties in molecules and solids." COST Action D26/0006/02
Financed by:	European Union (DG 12)
Participating entities:	Universitat Rovira i Virgili (Tarragona, Spain), University of Barcelona, Paul Sabatier University (Toulouse, France), Material Science Center (Groningen, The Netherlands), University of Torino (Italy), Universidad de Sevilla (Spain), Ruhr Universität (Bochum, Germany), Imperial College (London, United Kingdom)
Duration:	from: 01/01/2002 until: 31/12/2005
Researcher-in-chief:	Francesc Illas Riera (Universitat de Barcelona)
Title of the project:	"A meta-laboratory for code integration in ab-initio methods" COST Action D23/0006/01
Financed by:	European Union (DG 12)
Participating entities:	CINECA of Bologna (Italia), Universitat Rovira i Virgili (Tarragona, Spain), Paul Sabatier University (Toulouse, Francia), University of Ferrera (Italy), Universidad de Valencia (Spain), Eötvös Loránd University (Hungria)
Duration:	from: 01/01/2002 until: 31/12/2005
Researcher-in-chief:	Elda Rossi (CINECA)

Title of the project:	"Xarxa temàtica en Química Teòrica" Ref. 2002XT0007, *(Thematic network in Theoretical Chemistry)*, renewed from the beginning
Financed by:	Interdepartmental Commission of Research and Technological Innovation (CIRIT), Generalitat de Catalunya
Participating entities:	Several Catalan universitites and CSIC (Superior council of research and science)
Duration:	from: 01/01/2003 until: 31/12/2004
Amount of subvention:	9.000 €
Researcher-in-chief:	Miquel Duran (Universitat de Girona, Spain)
Title of the project:	"Red de Excelencia en Química Teórica y Computacional" Ref. BQU2001-5037-E *(Network of Excellence in Theoretical and Computational Chemistry)*
Financed by:	Spanish Ministry of Science and Technology (MCYT)
Participating entities:	18 Spanish universities that signed the interuniversity agreement for the pre-doctoral course in Theoretical and Computational Chemistry
Duration:	from: 01/01/2003 until: 31/12/2004
Amount of subvention:	12.000 €
Researcher-in-chief:	Manuel Yáñez Montero (Universidad Autónoma of Madrid)
Title of the project:	"Red de Excelencia en Magnetismo Molecular" Ref. MAT2001-5408-E *(Network of Excellence in molecular magnetism)*
Financed by:	Spanish Ministry of Science and Technology (MCYT)
Duration:	from: 01/01/2003 until: 31/12/2004
Amount of subvention:	34.000 €
Researcher-in-chief:	Eugenio Coronado (Instituto de Ciencia Molecular, Universidad de Valencia)
Title of the project:	"Modelización ab initio a escala molecular, nanoscópica y macroscópica de materiales de interés tecnológico, Ayudas a la Investigación." Ref. CTQU2005-08459-C02-02/BQU *(Ab initio modelization at the molecular, nanoscopic and macroscopic scale of materials of technological interest.)*
Financed by:	Spanish Ministry of Science and Technology (MCYT)
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2005 until: 2008
Amount of subvention:	79.000 €
Researcher-in-chief:	Rosa Caballol Lorenzo
Participating scientists:	9

Title of the project:	Support to consolidated research groups within the framework "Pla de Recerca de Catalunya", of the "Generalitat de Catalunya". 2005SGR-00104.
Financed by:	General Research Direction (DGR)
Participating entities:	Universitat Rovira i Virgili (Tarragona, Spain)
Duration:	from: 01/01/2005 until: 31/12/2008
Amount of subvention:	43.200 €
Researcher-in-chief:	Rosa Caballol Lorenzo
Participating scientists:	17
Title of the project:	"Descripción ab initio de los estados excitados en materiales moleculares y extendidos" Ref. CTQ2008-06644-C02-01 *(Ab initio description of excited states in molecular and extended materials)*
Financed by:	Spanish Ministry of Science and Technology (MCYT)
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2009 until: 2011
Amount of subvention:	95.469 €
Researcher-in-chief:	Coen de Graaf
Participating scientists:	8
Title of the project:	Grupo consolidado (Generalitat) Ref. 2009SGR462
Financed by:	General Research Direction (DGR)
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2009 until: 2013
Amount of subvention:	48.800 €
Researcher-in-chief:	Josep Maria Poblet
Participating scientists:	19
Title of the project:	"Descripción ab initio de procesos fotoinducidos en complejos de metales de transición y compuestos orgánicos" Ref. CTQ2011-23140 *(Ab initio description of photoinduced processes in transition metal complexes and organic compounds)*
Financed by:	Spanish Ministry of Science and Innovation
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2012 until: 2014
Amount of subvention:	96.800 € + one PhD grant
Researcher-in-chief:	Coen de Graaf
Participating scientists:	8
Title of the project:	"Equipamiento informático para cálculo intensivo" Ref. UNRV10-4E-1133 *(Computer cluster for high-performance computing)*
Financed by:	Spanish Ministry of Science and Innovation (FEDER program)
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 01-01-2012 until: 31-12-2012
Amount of subvention:	174.999,95 €
Researcher-in-chief:	Josep M. Poblet, Coen de Graaf, Allan Mackie, Josep Bonet, Ildefonso Cuesta, Roger Guimerà
Participating scientists:	6

Title of the project:	Solvation Dynamics: The very first steps (proposal number L662)
Financed by:	Linac Coherent Light Source (LCLS) at Stanford University (USA)
Participating entities:	European XFEL (Hamburg), Lund University (Sweden), University of Denmark, KFKI Research Institute (Budapest, Hungary), ESRF (Grenoble, France), SwissFel (Villigen, Switzerland), Universitat Rovira i Virgili (Tarragona, Spain), Ecole Normale Superieur, Paris
Duration:	January 2013
Amount of subvention:	48 hours of beam time at LCLS
Researcher-in-chief	Christian Bressler, European XFEL, Hamburg (Germany)
Participating scientists:	24
Title of the project:	Solvation dynamics - the very first steps
Financed by:	Barcelona Supercomputing Center
Participating entities:	Universtitat Rovira i Virgili
Duration:	from July 2013 until: September 2013
Amount of subvention:	200000 CPU hours on MareNostrum
Researcher-in-chief	Coen de Graaf
Participating scientists:	4
Title of the project:	"Dinámica de estados excitados: estudio teórico de reactividad y spin crossover inducidos por irradiación" CTQ2014-51938-P *(Dynamics in the excited state: A theoretical study of photo-induced reactivity and spin crossover)*
Financed by:	Spanish Administration
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2015 until: 2018
Amount of subvention:	94.380 € + one PhD grant
Researcher-in-chief:	Coen de Graaf
Participating scientists:	5
Title of the project:	Nonorthogonal configuration interaction for the study of electron and excitation transfer
Financed by:	Shell-NWO/FOM programme"Computational sciences for energy research" (Dutch organization for scientific research)
Participating entities:	University of Groningen, Universitat Rovira i Virgili
Duration:	from: 16 April 2016 until: 15 April 2021
Amount of subvention:	256000 €
Researcher-in-chief:	Ria Broer
Participating scientists:	3

Title of the project:	Cost Action: Explicit control over spin states in technology and biochemistry (CM1305)
Financed by:	European Union
Participating entities:	Research groups in 26 European countries
Duration:	from: 2014 until: 2019
Researcher-in-chief:	M. Swart (University of Girona)
Participating scientists:	145

Title of the project:	Managing the Computational Chemistry Big Data problem: the ioChem-BD platform
Financed by:	ValChem2016 program of the "Xarxa de Referència en Química Teòrica i Computacional (XRQTC)"
Participating entities:	Universitat Rovira i Virgili / Institut Catalana d'Investigació en Química (ICIQ)
Duration:	from: May 2016 until: December 2016
Amount of subvention:	6600 €
Researcher-in-chief:	Coen de Graaf
Participating scientists:	5

Title of the project:	"Materiales multifuncionales: Control de la interdependencia entre interacciones magnéticas, conductividad y reactividad de estados excitados" CTQ2017-83566-P *(Multifunctional materials: Control of the interplay between magnetic interactions, conductivity and excited state reactivity)*
Financed by:	Spanish Administration
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2018 until: 2020
Amount of subvention:	72.600 €
Researcher-in-chief:	Coen de Graaf
Participating scientists:	3.5

Title of the project:	Martí-Franquès COFUND Fellowships, 2018MFP-COFUND-20-22
Financed by:	Universitat Rovira i Virgili and European Union
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2019 until: 2021
Amount of subvention:	one PhD grant
Researcher-in-chief:	Josep Maria Poblet and Coen de Graaf
Participating scientists:	3

Title of the project:	"Transferencia intermolecular de energía y electrones mediante interacción de configuraciones no ortogonales" PID2020-113187GB-I00 *(Intermolecular energy and electron transfer by non-orthogonal configuration interaction)*
Financed by:	Spanish ministry of Science and Innovation
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2022 until: 2024
Amount of subvention:	90.000 €
Researcher-in-chief:	Coen de Graaf
Participating scientists:	2.5
Title of the project:	INCITE 2022, CHM154: Intermolecular energy and electron transfer by non-orthogonal configuration interaction
Financed by:	Department of Energy, US Government
Participating entities:	Universitat Rovira i Virgili, University of Groningen, Oak Ridge National Laboratory, Universitat de Barcelona
Duration:	from: 2022 until: 2023
Amount of subvention:	1.080.000 Summit node hours and 170.000 Frontier node hours (world's leading high-performance computing facilities)
Researcher-in-chief:	Coen de Graaf
Participating scientists:	8
Title of the project:	PRACE, pra129: Intermolecular energy and electron transfer by non-orthogonal configuration interaction
Financed by:	European Union
Participating entities:	Universitat Rovira i Virgili, University of Groningen, Oak Ridge National Laboratory, Universitat de Barcelona
Duration:	from: October 2021 until: September 2022
Amount of subvention:	245.000 Juwels-Booster node hours (Europe's leading high-performance computing facility in 2021)
Researcher-in-chief:	Coen de Graaf
Participating scientists:	8

Title of the project:	EuroHPC-Extreme : Intermolecular energy and electron transfer by non-orthogonal configuration interaction
Financed by:	European Union
Participating entities:	Universitat Rovira i Virgili, University of Groningen, Oak Ridge National Laboratory, Universitat de Barcelona
Duration:	from: August 2023 until: July 2024
Amount of subvention:	670.000 Leonardo node hours (Europe's leading high-performance computing facility in 2023)
Researcher-in-chief:	Coen de Graaf
Participating scientists:	8
Title of the project:	"Ajuts per donar suport a l'activitat científica dels grups de recerca de Catalunya (2021-SGR00110): Grup de Química Quántica de la Universitat Rovira i Virgili" (*Support to the scientific activity of the Catalan research groups: Quantum Chemistry group of the URV*)
Financed by:	Generalitat de Catalunya
Participating entities:	Universitat Rovira i Virgili
Duration:	from: 2023 until: 2025
Amount of subvention:	40.000 €
Researcher-in-chief:	Coen de Graaf
Participating scientists:	25
Title of the project:	INCITE 2024, CHM154: Intermolecular energy and electron transfer by non-orthogonal configuration interaction
Financed by:	Department of Energy, US Government
Participating entities:	Universitat Rovira i Virgili, University of Groningen, Oak Ridge National Laboratory, Universitat de Barcelona
Duration:	from: 2024 until: 2026
Amount of subvention:	800.000 Frontier node hours per year (world's leading high-performance computing facility)
Researcher-in-chief:	Coen de Graaf
Participating scientists:	9

Stays in international research centres

Centre:	University of Groningen, The Netherlands
Duration:	from: September 1993 until: December 1997 (4 years and 4 months)
Subject:	Local excitations and magnetism in late transition metal oxides
Key:	Ph. D. Thesis
Centre:	University of Barcelona, Spain
Duration:	from: October 1995 until: December 1995 (2 months)
Subject:	Magnetic coupling in Nickel Oxide
Key:	Pre-doctoral stay
Centre:	University of Barcelona, Spain
Duration:	from: February 1997 until: April 1997 (3 months)
Subject:	Many centre interactions in the magnetic coupling constant
Key:	Pre-doctoral stay
Centre:	Universidad Autónoma de Madrid, Spain
Duration:	March 1997 (2 weeks)
Subject:	Implementation of model potentials in non-orthogonal CI methods
Key:	Invited stay
Centre:	University of Barcelona, Spain
Duration:	from: June 1998 until: September 2000 (2 years and 3 months)
Subject:	Magnetic interactions in low-dimensional Heisenberg systems
Key:	Post-doctoral stay
Centre:	University of Lund, Sweden
Duration:	January 1999 (1 week)
Subject:	Implementation of visualization software in MOLCAS
Key:	Invited stay
Centre:	University of Milano, Italy
Duration:	July 2000 (2 weeks)
Subject:	Spectroscopy of peroxi radicals in silica
Key:	Post-doctoral stay
Centre:	Universitat Rovira i Virgili (Tarragona, Spain)
Duration:	from: October 2000 until: November 2001 (1 year and 1 month)
Subject:	Theoretical study of the electronic structure of transition metal compounds
Key:	Post-doctoral stay
Centre:	University of Groningen, The Netherlands
Duration:	from: June 2003 until: September 2003 (3 months)
Subject:	Charge and orbital ordering in half-doped manganites
Key:	Post-doctoral stay
Centre:	University of Groningen, The Netherlands
Duration:	July 2005 (1 month)
Subject:	Covalent interactions in hexagonal manganites
Key:	Post-doctoral stay

Invited talks

1.	Title: :	C. de Graaf, R. Broer, W. C. Nieuwpoort, P. S. Bagus
	Title:	On the role of relaxed charge transfer excitations: Ni-3s hole states in NiO
	Conference:	European program for Human Capital and Mobility: access to large scale computer facilities, Barcelona, Spain, 1995
2.	Authors:	C. de Graaf
	Title:	On the magnetic coupling in NiO
	Conference:	Invited stay at the 'Max-Planck –Institut für Physik komplexer Systeme', Dresden, Germany, 1996
3.	Authors:	C. de Graaf, R. Broer, W. C. Nieuwpoort
	Title:	d-d Transitions in CoO, La_2CuO_4 and La_2NiO_4
	Conference:	International Conference on Quantum Chemistry in Material Sciences, Paterswolde, The Netherlands, 1997
4.	Authors:	C. de Graaf, R. Broer, W. C. Nieuwpoort
	Title:	Comparison of the Superexchange interaction in NiO and NiO(100)
	Conference:	European program for Human Capital and Mobility: access to large scale computer facilities, Barcelona, Spain, 1997
5.	Authors:	C. de Graaf
	Title:	On the role of relaxed charge-transfer excitations: Ni-3s hole states in NiO
	Conference:	Invited stay at the Department of Applied Chemical Physics of the Universidad Autónoma de Madrid, Spain, 1997
6.	Authors:	C. de Graaf
	Title:	Magnetic coupling in low-dimensional Heisenberg systems
	Conference:	Invited stay at the Theoretical Chemistry Department of the University of Lund, Sweden, 1999
7.	Authors:	C. de Graaf, F. Illas, I. de P. R. Moreira, R. L. Martin
	Title:	Magnetic coupling in low-dimensional Heisenberg systems
	Conference:	Invited stay at the Material Science Centre of the University of Groningen, The Netherlands, 1999
8.	Authors:	C. de Graaf
	Title:	Magnetic interactions and spectroscopy of defects by cluster model calculations
	Conference:	Invited stay at the Material Science Centre of the University of Groningen, The Netherlands, 2000
9.	Authors:	C. de Graaf
	Title:	Acoplamiento magnético en compuestos de estado sólido: Interpretación y predicción teórica
	Conference:	Invited talk at the "Centre de Recerca en Quimica Teòrica", Parc Científic de Barcelona, University of Barcelona, Spain, 2001

10.	Authors:	C. de Graaf
	Title:	Acoplamiento magnético en compuestos de estado sólido: Interpretación y predicción teórica (plenary lecture)
	Conference:	27ème congrès des Chimistes Théoriciens d'Expression Latine, Toulouse, France, 2001
11.	Authors:	C. de Graaf, C. Sousa, I. de P. R. Moreira, F. Illas
	Title:	Multiconfigurational perturbation theory, an efficient tool to predict magnetic coupling parameters in biradicals, molecular complexes and ionic insulators
	Conference:	CECAM-ESF workshop "Electronic Structure Approaches to the Magnetic Behavior of Molecular-based Materials: From the Molecule to the Solid", Lyon, France, 2002
12.	Authors:	C. de Graaf
	Title:	Magnetic interactions with ab initio methods: Interpretation and accurate predictions
	Conference:	7^{th} FIGIPS meeting on Inorganic Chemistry, Lisboa, Portugal, 2003
13.	Authors:	C. de Graaf, C. Sousa, R. Broer
	Title:	Ab initio embedded cluster calculations on manganites
	Conference:	Stay at the Material Science Centre of the University of Groningen, The Netherlands, 2003
14.	Authors:	C. de Graaf, E. Bordas, D. Taratiel, N. Queralt, R. Caballol
	Title:	In search of non-Heisenberg behaviour in ferrimagnetic molecular complexes
	Conference:	Joint COST meeting (D23-D26) on orbital localisation, Siena, Italy, 2004
15.	Authors:	C. de Graaf
	Title:	An exploration of the possibilities of wave function based methods in the study of the electronic structure of polyoxometalates
	Conference:	CECAM-ESF Workshop "Electronic Structure of Polyoxometalates: Interplay between Experiment and Theory", Lyon, France (2005)
16.	Authors:	C. de Graaf
	Title:	Ab initio determination of electronic structure parameters in transition metal oxides
	Conference:	Invited stay at the "Max Planck Institut für Physik komplexer Systeme", Dresden, Germany (2006)
17.	Authors:	C. de Graaf
	Title:	non-Heisenberg behaviour in magnetic molecules
	Conference:	CECAM workshop on Models and Theory for Molecular Magnetism, Lyon, France (2006)
18.	Authors:	C. de Graaf
	Title:	Multireference second-order perturbation theory – CASPT2
	Conference:	Jujols III conference on magnetism, Alenyà, France (2007)

19.	Authors:	C. de Graaf, B. Ordejón, C. Sousa
	Title:	Light-Induced Excited State Spin Trapping in Tetrazole-based Spin Crossover systems (keynote lecture)
	Conference:	EUCO-CC7, Venice, Italy (2008)
20.	Authors:	C. de Graaf, B. Ordejón, C. Sousa
	Title:	Light-Induced Excited State Spin Trapping in Tetrazole-based Spin Crossover systems
	Conference:	Invited stay at the Department of Physical Chemistry, University of Geneva, Switzerland (2008)
21.	Authors:	C. de Graaf, C. Sousa
	Title:	Quantum Chemical study of spin crossover phenomena in Fe^{II} complexes
	Conference:	Invited stay at the European XFEL, Hamburg, Germany (2010)
22.	Authors:	C. de Graaf
	Title:	Derivation of effective Hamiltonians for further insight in the electronic structure of $M_2(dta)_4I$ (M=Ni,Pt)
	Conference:	CFCAM Workshop on Density Functional Theory and Wave Function Theory for Molecular Magnetism, Toulouse, France (2011)
23.	Authors:	C. de Graaf, C. Sousa
	Title:	Quantum chemical study of spin crossover phenomena in Fe^{II} complexes
	Conference:	Invited stay at the KFKI Research Institute for Particle and Nuclear Physics, Budapest, Hungary (2011)
24.	Authors:	C. de Graaf, M. A. Carvajal, M. Reguero, R. Caballol
	Title:	Light induced magnetism in copper octacyanomolybdates
	Conference:	Ninth triennial congress of the world association of theoretical and computational chemists (WATOC-2011), Santiago de Compostella, Spain (2011)
25.	Authors:	C. de Graaf, C. Sousa
	Title:	Ultrafast deactivation mechanism of the excited singlet in the light induced spin crossover of $[Fe(bipy)_3]^{2+}$
	Conference:	Spin states in biochemistry and inorganic chemistry, Zaragoza, Spain (2012)
26.	Authors:	C. de Graaf, C. Sousa
	Title:	Ultrafast deactivation mechanism of the excited singlet in the light induced spin crossover of $[Fe(bipy)_3]^{2+}$
	Conference:	48th Symposium on Theoretical Chemistry, Karlsruhe, Germany (2012)
27.	Authors:	C. de Graaf, C. Sousa
	Title:	The photocycle of light-induced spin crossover: A quantum chemical perspective
	Conference:	European XFEL Science Lecture Series on femtochemistry, Hamburg, Germany (2012)

28.	Authors:	C. de Graaf, C. Sousa
	Title:	The photocycle of light-induced spin crossover: A quantum chemical perspective
	Conference:	Invited stay at SwissFEL Photonics, Paul Scherrer Institute, Villigen, Switzerland (2014)
29.	Authors:	C. de Graaf, R. Broer
	Title:	Magnetic Interactions in molecules and solids
	Conference:	Jujols VIII, international workshop on Theoretical approaches of Molecular Magnetism, Bages, France (2015)
30.	Authors:	C. de Graaf
	Title:	Transition metals
	Conference:	Workshop on Computation of Electronic Excited States, Donosti, Spain (2015)
31.	Authors:	G. Alcover, S. Saureu, R. Caballol, C. de Graaf
	Title:	Spin crossover and intersystem crossing rates in complexes with Fe(III), Ru(II) and Ni(II) ions
	Conference:	Invited lecture in the lecture series of the Fédération des Sciences Chimiques, Marseille, France (2016)
32.	Authors:	C. de Graaf. C. Sousa, R. Broer
	Title:	Theoretical study of the deactivation of the excited singlet state in Fe(II) and Ru(II) SCO complexes
	Conference:	3rd Bordeaux Olivier Kahn Discussions, Bordeaux, France (2017)
33.	Authors:	C. Sousa, A. Domingo, C. de Graaf
	Title:	Second-order spin-orbit coupling in SCO systems
	Conference:	Invited stay at ICMCB (*Institute for condensed matter chemistry*), Bordeaux, France (2017)
34.	Authors:	C. de Graaf, C. Sousa, A. Domingo
	Title:	Second-order spin-orbit coupling through effective Hamiltonian theory
	Conference:	6th Molcas developer's workshop, Leuven, Belgium (2018)
35.	Authors:	C. Sousa, M. Alías, A. Domingo, C. de Graaf
	Title:	Second-order spin-orbit coupling through effective Hamiltonian theory
	Conference:	Theoretical Studies of Magnetic Systems: Methodological Developments and Applications, Toulouse, France (2018)
36.	Authors:	C. de Graaf
	Title:	Theoretical insights into molecular magnetism induced by light
	Conference:	Multidisciplinary seminar program of the ETSEQ-URV, Tarragona, Spain (2018)
37.	Authors:	C. de Graaf
	Title:	Multiconfigurational electronic structure methods applied to spin anisotropy and excited state deactivation
	Conference:	Theoretical methods in molecular spintronics, Donostia, Spain (2018)

38.	Authors:	C. de Graaf
	Title:	Multiconfigurational electronic structure methods applied to spin anisotropy and excited state deactivation
	Conference:	American Physical Society March meeting, Boston, USA (2019)
39.	Authors:	R. Morales, A. Moreno, C. de Graaf, T. Rodríguez-Fortea, L. Echegoyen, N. Chen, J.-M. Poblet
	Title:	Uranium-Uranium bonds in fullerenes
	Conference:	Fifth Quantum BioInorganic Conference (QBIC-V), Marseille, France (2019)
40.	Authors:	R. Broer, T. Straatsma, R. W. A. Havenith, S. Faraji, C. de Graaf, M. Wibowo, M. Izquierdo, L. Aguilar Suarez, R. K. Kathir
	Title:	GronOR: A program for non-orthogonal configuration interaction
	Conference:	Computation and understanding in quantum molecular science, Toulouse, France (2019)
41.	Authors:	M. Alías, C. de Graaf
	Title:	Theoretical study of reverse-LIESST in Fe(II) complexes
	Conference:	5th Bordeaux Olivier Kahn Discussions, on-line, organized by ICMCB, Bordeaux, France (2020)
42.	Authors:	C. de Graaf
	Title:	Non-orthogonal CI in GronOR, interfaced to OpenMolcas
	Conference:	8th Molcas developer's workshop, on-line, organized by the Max Planck Institute Stuttgart, Germany (2020)
43.	Authors:	A. Notario-Estévez, X. López, C. de Graaf
	Title:	Staircase conductivity of polyoxo- vanadates adsorbed on Au(111) - a computational study
	Conference:	RES (Spanish network of supercomputers) user meeting, on-line, organized by the Barcelona Supercomputer Centre (2020)
44.	Authors:	C. de Graaf
	Title:	GronOR, a massively parallel and GPU accelerated program for Non-Orthogonal Configuration Interaction with Fragments
	Conference:	National Center for Computational Sciences meeting (Oak Ridge, USA), on-line (2021)
45.	Authors:	C. de Graaf
	Title:	Non-orthogonal configuration interaction in GronOR
	Conference:	Pacifichem2021, organized by the Chemical Society of Japan, on-line (2021)
46.	Authors:	C. de Graaf
	Title:	From papain to Q-Force
	Conference:	CTC Symposium 2022, organized by the computational chemistry division of the Royal Netherlands Chemical Society (CTC-KNCV) on-line (2022)

47.	Authors:	C. de Graaf
	Title:	Magnetic exchange interactions with non-orthogonal configuration interaction
	Conference:	Jujols X, international workshop on Theoretical approaches of Molecular Magnetism, Erguy, France (2022)
48.	Authors:	C. de Graaf, A. Mansilla-Sánchez, R. Broer, C. Sousa, T. P. Straatsma
	Title:	Non-orthogonal configuration interaction: conceptual and computational aspects
	Conference:	WATOC-2022, Vancouver, Canada (2022)
49.	Authors:	C. de Graaf
	Title:	GronOR, a massively parallel and GPU accelerated program for Non-Orthogonal Configuration Interaction
	Conference:	Modern Trends in Molecular Magnetism 3, Kharagpur, India, on-line (2022)
50.	Authors:	C. de Graaf
	Title:	GronOR, a massively parallel and GPU accelerated program for Non-Orthogonal Configuration Interaction
	Conference:	13th Symposium of the Accelerated Data Analytics and Computing Institute (ADAC), Paris, France (2023)

Oral contributions to conferences

1.	Authors:	C. de Graaf, B. Ordejón, C. Sousa
	Title:	Ab initio study of light-induced excited spin state trapping in tetrazole-based spin crossover complexes
	Conference:	Electronic Structure: Principles and Applications (ESPA 2008), Palma de Mallorca, Spain (2008)
2.	Authors:	C. de Graaf, C. Sousa
	Title:	Ab initio study of light-induced excited spin state trapping in $Fe^{II}(bipy)_3$ and $Fe^{II}(pap)_3$
	Conference:	Jujols-IV conference on magnetism, Groningen, the Netherlands (2009)
3.	Authors:	C. de Graaf, C. Sousa
	Title:	Study of light-induced spin crossover in Fe^{II}-tris-bipyridine and $Fe^{II}(tetrazole)_6$
	Conference:	MOLMAT 2010, Montpellier, France (2010)
4.	Authors:	C. de Graaf, A. Domingo, A. Rodríguez-Fortea, M. Swart, R. Broer
	Title:	Effect of thermal motion of spectroscopic properties of NiO
	Conference:	Electronic Structure: Principles and Applications (ESPA 2012), Barcelona, Spain (2012)
5.	Authors:	C. de Graaf
	Title:	Magnetic interactions near the domain walls in TbMnO3 thin films
	Conference:	Mini symposium on electronic structure of strongly correlated systems, University of Groningen, Netherlands (2013)
6.	Authors:	M. Àlvarez-Moreno, C. de Graaf, N. López, F. Maseras, J. M. Poblet, C. Bo
	Title:	ioChem-BD: Managing the BigData of Computational Chemistry
	Conference:	Fourth ECOSTBio scientific workshop, Prague (2016)
7.	Authors:	M. Spivak, X. López,C. de Graaf
	Title:	Trichromium extended metal atom chains from a multiconfigurational perspective
	Conference:	Farewell symposium Ria Broer, Groningen, Netherlands (2017)
8.	Authors:	R. Havenith, K. Kathir, C. de Graaf, R. Broer, S. Farji
	Title:	Non-orthogonal configuration interaction for the study of electron and excitation transfer
	Conference:	Physics@Veldhoven, Netherlands (2018)
9.	Authors:	C. de Graaf
	Title:	Second-order spin-orbit coupling in SCO systems
	Conference:	Invited stay at ICMCB (Institute for condensed matter chemistry), Bordeaux, France (2018)
10.	Authors:	C. de Graaf, C. Sousa, A. Domingo
	Title:	Effect of second-order spin-orbit coupling on the interaction between spin-states in spin-crossover compounds
	Conference:	Final scientific ECOSTBio scientific meeting, Berlin, Germany (2018)

11.	Authors:	A. Notario-Estévez, X. López, C. de Graaf, P. Kozłowski, O. Linnenberg, K. Y. Monakhov
	Title:	$X@V_{22}O_{54}$: How many valence electrons and where are they?
	Conference:	1st 2018 Berendsen symposium, Groningen, Netherlands (2018)
12.	Authors:	C. de Graaf, J. Wu, M. Alías-Rodríguez
	Title:	Controlling the lifetime of excited states in Fe(II) complexes by ligand modifications
	Conference:	PhD Symposium, Groningen, Netherlands (2019)
13.	Authors:	C. de Graaf
	Title:	Intermolecular energy and electron transfer through non-orthogonal configuration interaction
	Conference:	European Conference of Theoretical and Computational Chemistry, online. (2021)
14.	Authors:	C. de Graaf
	Title:	GronOR: A massively parallel and GPU-accelerated program for non-orthogonal configuration interaction
	Conference:	ESPA 2022, Vigo, Spain (2022)
15.	Authors:	C. de Graaf
	Title:	"Interacció de configuracions no-ortogonals per a la transferència d'excitons i el bescanvi magnètic" *(Non-orthogonal configuration interaction for exciton transfer and magnetic exchange)*
	Conference:	Reunió de Química Teòrica i Computacional, Barcelona (2023)

Master supervision

1. Co-direction with R. Broer of the Master in Theoretical Chemistry by Michel Geleijns
   Title: Theoretical study of local electronic transitions in the NiO(100) surface
   Centre: University of Groningen, The Netherlands (1997)

2. Co-direction with N. Guihéry of the Master Thesis in Chemistry by Rémi Maurice
   Title: Anisotropy parameters in mono- and dinuclear systems through CASSCF/ CASPT2/RASSI calculations
   Centre: Université Paul Sabatier, Toulouse, France (Defended June 2008)

3. Master Thesis in Theoretical and Computational Chemistry by Alex Domingo
   Title: Electronic absorption spectrum of Nickel Oxide
   Centre: Universitat Rovira i Virgili, Tarragona (Defended September 2008)

4. Master Thesis in Theoretical and Computational Chemistry by Alejandro Jiménez
   Title: DFT and multiconfigurational study of the two-state-reactivity of the reaction $FeO^+ + H_2 \rightarrow Fe^+ + H_2O$
   Centre: Universitat Rovira i Virgili, Tarragona (Defended September 2011)

5. Master Thesis in Theoretical and Computational Chemistry by Sergi Saureu
   Title: Theoretical study of the solvent effects on electronic states of $[Fe(phen)_3]^{2+}$
   Centre: Universitat Rovira i Virgili, Tarragona (Defended September 2012)

6. Co-direction with R. Caballol of Master Thesis in Theoretical and Computational Chemistry by Gerard Alcover
   Title: Theoretical study of the magnetic bistability of the Ni-tetrakis(pentafluorophenyl)-porphyrin complex
   Centre: Universitat Rovira i Virgili, Tarragona (Defended September 2012)

7. Erasmus Mundus Master Thesis in Theoretical Chemistry and Computational Modelling by Cecilia Gómez
   Title: Spin Crossover in Co(III) imido complexes
   Centre: University of Groningen, the Netherlands (Defended June 2016)

8. Erasmus Mundus Master Thesis in Theoretical Chemistry and Computational Modelling by Jinggang Lan
   Title: Absorption of cubane-type tetranuclear Ni(II) complexes with thioether-functionalized ligands on Au(111)
   Centre: University of Groningen, the Netherlands (Defended June 2016)

9. Master Thesis in Synthesis, Catalysis and Molecular Modelling by Marc Alías
   Title: Light-induced *trans-cis* isomerization of azobenzene studied with CASSCF molecular dynamics
   Centre: University Rovira i Virgili (Defended June 2017)

10. Master Thesis in Synthesis, Catalysis and Molecular Modelling by Sateesh Babu Alapati
    Title: Emission properties of $Ac@C_{82}$ ($Ac = U^{3+}$,Th^{4+})
    Centre: University Rovira i Virgili (Defended July 2019)

11. Erasmus Mundus Master Thesis in Theoretical Chemistry and Computational Modelling
    by Ionut Stan
    Title: Redox properties of Polyoxometale sandwich compounds
    Centre: University Rovira i Virgili (Started January 2024)

Ph. D. supervision

1. Co-direction with prof. dr. R. Caballol of the Ph D Thesis of Esther Bordas
   Title: Ab initio determination of electronic structure parameters in transition metal oxides
   Centre: Universitat Rovira i Virgili, Tarragona (defended January 2005)

2. Co-direction with prof. R. Broer of the Ph. D. Thesis of Aymeric Sadoc
   Title: Charge disproportionation in transition metal oxides
   Centre: University of Groningen, The Netherlands (defended May 2008)

3. Co-direction with prof. J. M. Poblet of the PhD Thesis of Susana Romo
   Title: Theoretical study of the spectroscopic and electrochemical properties of polioxometalates with group VI-IX transition metals
   Centre: Universitat Rovira i Virgili, Tarragona (defended April 2009)

4. Co-direction with prof. R.Caballol of the Ph. D. Thesis of Núria Queralt
   Title: Study of the magnetic coupling in heterometallic complexes with oxamido, oxamato, thioxalato and analogous bridging ligands
   Centre: Universitat Rovira i Virgili, Tarragona (defended May 2010)

5. Co-direction with prof. R.Caballol of the Ph. D. Thesis of Igor Negodaev
   Title: Theoretical determination of magnetic susceptibility of paramagnetic systems based on ab initio electronic structure parameters
   Centre: Universitat Rovira i Virgili, Tarragona (defended February 2011)

6. Co-direction with prof. N. Guihéry of the Ph. D. Thesis of Rémi Maurice
   Title: Zero-Field Anisotropic Spin Hamiltonians in First-row Transition Metal Complexes: Theory, Models and Applications
   Centre: Université Paul Sabatier, Toulouse, France/ Universitat Rovira i Virgili (defended June 2011)

7. Direction of the Ph. D. Thesis of Alex Domingo
   Title: Theoretical description of electronic excitations in extended systems: beyond the static material model
   Centre: Universitat Rovira i Virgili, Tarragona (defended November 2011)

8. Co-direction with Dr. X. Lopéz of the Ph. D. Thesis of Zahra Tabookht
   Title: Theoretical study of magnetic and conducting properties of transition metal nanowires
   Centre: Universitat Rovira i Virgili, Tarragona (defended December 2011)

9. Co-direction with prof. R. Broer of the Ph. D. Thesis of Abdul Muizz Pradipto
   Title: Local interactions in magnetic and ferroelectric materials: magnetic and vibronic couplings
   Centre: University of Groningen, The Netherlands (defended June 2013)

10. Direction of the Ph. D. Thesis of Sergi Saureu
    Title: From mononuclear to binuclear: magnetic interactions in transition metal complexes
    Centre: Universitat Rovira i Virgili, Tarragona (defended in May 2016)

11. Co-direction with prof. R. Caballol of the Ph. D. Thesis of Gerard Alcover
    Title: Spin-Crossover Beyond the Traditional Fe(II) Complexes: Ab Initio Study of Spin State Stability in Complexes with Mn, Ni and Ru
    Centre: Universitat Rovira i Virgili, Tarragona (defended September 2016)

12. Co-direction with Dr. X. López of the Ph. D. Thesis of Mariano Spivak
    Title: Electronic structure calculations on Extended Metal Atom Chains. Insights on structural, magnetic and transport properties
    Centre: Universitat Rovira i Virgili, Tarragona (defended January 2017)

13. Direction of the Ph. D. Thesis of Jianfang Wu
    Title: Controlling the light induced magnetism in Ru en Fe complexes via ligand modifications
    Centre: Universitat Rovira i Virgili, Tarragona (Defended February 2020)

14. Co-direction with X. López of the Ph. D. Thesis of Almudena Notario
    Title: Interplay of the oxidation state and the conductivity of polyoxovanadates
    Centre: Universitat Rovira i Virgili, Tarragona (Defended February 2021)

15. Direction of the Ph. D. Thesis of Marc Alías
    Title: Excited state dynamics of spin crossover complexes
    Centre: Universitat Rovira i Virgili, Tarragona (defended May 2021)

16. Co-direction with R. Havenith of the Ph. D. Thesis of R. K. Kathir
    Title: Non-orthogonal Configuration Interaction for the study of electron and excitation transfer
    Centre: University of Groningen, The Netherlands (defended January 2022)

17. Co-direction with J. M. Poblet of the Ph. D. Thesis of Fei Weng
    Title: Activation of small molecules catalysed by polyoxometales (EU-COFUND grant)
    Centre: Universitat Rovira i Virgili, Tarragona (defended July 2022)

18. Direction of the Ph. D. Thesis of Aitor Sánchez Mansilla
    Title: GronOR: A program for non-orthogonal configuration interaction
    Centre: Universitat Rovira i Virgili, Tarragona (started November 2019)

Post Doc supervision

1. Post-Doc of Belen Ordejón (with dr. C. Sousa, Universitat de Barcelona)
    Title: Ab initio study of the light induced spin transition in Fe(II) complexes
    Centre: Universitat Rovira i Virgili (2007)

2. Post-Doc of Nuno Bandeira (with prof. J. M. Poblet, Universitat Rovira i Virgili)
    Title: Singlet-triplet gap in doubly reduced polyoxometallates
    Centre: Universitat Rovira i Virgili (2010)

Teaching experience

1. Problems in *Atomic structure and chemical bonding*, University of Groningen, The Netherlands, Academic years 1995-1998.
2. Theory and problems in *Theory of the chemical structure and reactivity*, Universitat Rovira i Virgili (Tarragona, Spain), Academic years 2000-2004.
3. Pre-doctoral course on *Multiconfigurational Quantum Chemistry* with prof. dr. B. O. Roos, organized by the Universitat Rovira i Virgili within the mark of the Spanish inter-university doctorate in theoretical and computational chemistry (2004).
4. Theory and problems in *Computational Chemistry*, Universitat Rovira i Virgili (Tarragona, Spain), Academic years 2005-2012
5. Pre-doctoral course on *Accurate determination of electronic structure parameters of magnetic systems with ab initio wave function based methods*, Summerschool in Theoretical and Computational Chemistry of Catalonia (June 2007)
6. Supervision of various "*Treballs Experimental*" (research project for undergraduate Chemistry students), Universitat Rovira i Virgili (2006-2010)
7. Supervision of the research project "*Beca de collaboració, iniciació a la recerca*" (Grant for collaboration, introduction to research), financed by the "Dept. Química Física i Inorgànica", Universitat Rovira i Virgili (Oct. 2008-Febr. 2009).
8. *Advanced Electronic Structure Methods* in the European Master in Computational Chemistry, Groningen, the Netherlands (2009); Porto, Portugal (2010,2016); Valencia, Spain (2011,2017,2023); Perugia, Italy (2018); Madrid, Spain (2019), on-line (2020), Toulouse (2021)
9. *Theoretical methods for determining electronic and molecular structure* in the Master in Synthesis, Catalysis and Molecular Design, Universitat Rovira i Virgili, Tarrgona (2013-2021)
10. *Magnetic Interactions in extended systems* in the EMTCCM School on Theoretical Solid State Chemistry, Zaragoza, Madrid (Spain) and on-line (2015-2021)
11. *Excited states – Transition metals* in the Summerschool on the Computation of electronic excited states in molecules, aggregates, nanoclusters, nanoparticles, polymers and solids, Donostia, Spain (2015)
12. *Magnetic Interactions in Molecules and Solids* in the European Master in Theoretical Chemistry and Computational Modelling, Groningen, the Netherlands (2015)
13. Supervision of several "*Treball fi de Grau*" (bachelor projects) in the Chemistry bachelor program of the Universitat Rovira i Virgili (Tarragona, Spain), Academic years 2011-
14. Theory and problems in *Quantum Physics* in the bachelor program "Mathematical and Physical Engineering", Universitat Rovira i Virgili (Tarragona, Spain), Academic years 2022-

Academic responsibilities

1.	Member of the "*Consell de Direcció*" (daily board) of the Departament de Química Física i Inorgànica, Universitat Rovira i Virgili (2007-2011).
2.	Responsable of the ISO-9001 Quality System of the Quantum Chemistry Group, Universitat Rovira i Virgili (2007-2012)
3.	Group leader of the Quantum Chemistry Group, Universitat Rovira i Virgili (2022-)

Organization of conferences and Summerschools

1.	Title:	Jujols IX, international workshop on theoretical approaches of molecular magnetism
	Place:	Tortosa, Spain
	Date:	May 2017
2.	Title:	XXXIII annual meeting of the Reference Network of Theoretical and Computational Chemistry in Catalonia (XRQTC)
	Place	Tarragona, Spain
	Date:	July 2017
3.	Title:	Summer School on Non-Orthogonal Configuration Interaction and its Parallel and GPU Accelerated Implementation
	Place	online
	Date:	May 2022
4.	Title:	ESPA 2024 (conference co-chair)
	Place	Tarragona, Spain
	Date:	June 2024