Régis GAUTIER

Born in 1972
French citizenship

Professor at Ecole Nationale Supérieure de Chimie de Rennes (ENSCR)
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Education and research activities

2011	Visiting scientist, Department of Physics and Astronomy, University College London, UK (7 months)
2010	Professor, ENSCR
2005	Thesis Director Enabling Degree (University of Rennes 1)
1999-2010	Associate Professor, ENSCR
1998-99	Postdoctoral fellow, condensed matter theory group of Pr. O. K. Andersen, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
1995-98	PhD in Chemistry under the supervision of Dr. J.-F. Halet, LCSIM UMR CNRS 6511, University of Rennes 1.
1994-95	Master in Computational Chemistry, University of Rennes 1.

Research

Keywords: theoretical chemistry, solid-state chemistry, electronic structure, chemical bonding, structure-property relationships, computations of spectroscopic properties, transition metal clusters, thermoelectric materials

Director of 8 PhD Students, co-director of 4 PhD students, (co-)director of 14 master students

Author of
- 5 book chapters
- 102 publications in peer reviewed journals
- 8 invited conferences - 24 invited seminars – 37 orals in national & international meetings

2012-2017 Head of the *Inorganic Theoretical Chemistry* group (13 researchers + 2 engineers + 10 PhD students) of the *Institut des Sciences Chimiques de Rennes*, UMR CNRS 6226

2013-2018 Scientific Director of ENSCR (43 researchers, 10 engineers & technicians, 30 PhD Students, 7 postdocs, annual budget of 1.2 M€)

Collaborations

- K. Costuas, E. Furet, B. Fontaine, J.-F. Halet, J.-Y. Saillard, P. Gall, P. Gougeon, S. Cordier, Y. Molard, N. Audebrand, C. Boussard-Plédel, B. Bureau, L. Le Pollès, E. Le Fur, *Institut des Sciences Chimiques de Rennes - UMR 6226*
- J.-B. d'Espinose de Lacaillerie, *Laboratoire Physico-chimie des Polymères et Milieux Dispersés, UMR 7615, ESPCI, Paris*
- L. Delevoye, J. Trebosc, *Unité de Catalyse et Chimie du Solide, UMR 8181, Lille*
- F. Gascoin, E. Guilmeau, *CRISMAT, UMR 6508, Caen*
- B. Lenoir, C. Candolfi, *Institut Jean Lamour, UMR 7198, Nancy*
- C. J. Pickard, *Department of Physics & Astronomy, University College, London, UK*
- D. H. Gregory, *Department of Chemistry, University of Glasgow, UK*
- R. Riedel, *Department of Materials, TU Darmstadt, Germany*
- N. G. Naumov, *Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*
- D. Wee, *EWHA University, Seoul, South Corea*
- M. Fornari, *Central Michigan University, USA*
- T. Mori, *National Institute for Materials Science, Tsukuba, Japan*

List of publications

Book chapters

5 *Structural, Electronic, and Physical Properties of Solid-State Rare-Earth Boride Carbides*
V. Babizhetskyy, J. Bauer, R. Gautier, K. Hiebl, A. Simon, J.-F. Halet
Handbook on the Physics and Chemistry of Rare Earths, Eds. J.-C. G. Bünzli, V. K. Pecharsky, Elsevier, **2018**, 53, p. 145-269

4 *First-Principles Computation of NMR Parameters in Solid-State Chemistry*
J. Cuny, R. Gautier, J.-F. Halet
Handbook of Solid-State Chemistry, eds. R. Dronskowski, S. Kikkawa & A. Stein, Wiley-VCH, **2017**, 16, p. 607-646

3 *The Electronic Properties of Metal Borides and Borocarbides. Differences and Similarities*
S. Lassoued, R. Gautier, J.-F. Halet
Boron Rich Solids: Sensors, Ultra High Temperature Ceramics, Thermoelectrics, Armor, Eds. N. Orlovskaya, M. Lugovy, Springer Science and Business Media V. B., **2011**, p. 95-114

2 *The Contribution of Computational Methods to Transition Metal Cluster Chemistry*
R. Gautier, J.-F. Halet, J.-Y. Saillard
Computational Inorganic and Bioinorganic Chemistry, ed. E. I. Solomon, R. B. King, R. A. Scott, Wiley, Chichester, UK, **2009**, p. 433-452.

1 *Hexacapped Cubic Transition Metal Clusters and Derivatives: A Theoretical Approach.*
R. Gautier, J.-F. Halet, J.-Y. Saillard
Metal Clusters in Chemistry, ed. P. Braunstein, L. A. Oro, P. R. Raithby, VCH, **1999**, p. 1643-1663.

Articles

102 *Synthesis, Crystal and Electronic Structures, and Electrical Properties of the Fifth Member of the $Rb_2(Mo_9S_{11})(Mo_{6n}S_{6n+2})$ Series: $Rb_{10}Mo_{39}S_{43}$, an Atypical Reduced Molybdenum Sulfide Containing Mo_9 and Mo_{30} Clusters.*
P. Gougeon, P. Gall, A. Huguenot, R. Al Rahal Al Orabi, R. Gautier
***Inorg. Chem.* 2019**, 58, 15236-15245

101 *XBi_4S_7 (X = Mn, Fe): new cost-efficient layered n-type thermoelectric sulfides with ultralow thermal conductivity*
J-B. Labégorre, A. Virfeu, A. Bourhim, H. Willeman, T. Barbier, F. Appert, J. Juraszek, B. Malaman, A. Huguenot, R. Gautier, V. Nassif, P. Lemoine, C. Prestipino, E. Elkaim, L. Pautrot-d'Alençon, T. Le Mercier, A. Maignan, R. Al Rahal Al Orabi, E. Guilmeau
***Adv. Func. Mater.* 2019**, 29, 1904112

100 *Red-NIR luminescence of Mo_6 monolayered assembly directly anchored on Au(001)*
M. Kepenekian, Y. Molard, K. Costuas, P. Lemoine, R. Gautier, S. Ababou-Girard, B. Fabre, P. Turban, S. Cordier
***Mater. Horiz.* 2019** , 6, 1828-1833

99 *Enhanced Thermoelectric Performance through Crystal Field Engineering in Transition Metal Doped GeTe*
J. Shuai, X. Tan, Q. Guo, J. Xu, A. Gellé, R. Gautier, J.-F. Halet, F. Failamani, J. Jiang, T. Mori
***Mater. Today Phys.* 2019**, 9, 100094

98 *Electronic Band Structure and Transport Properties of the Cluster Compound $Ag_3Tl_2Mo_{15}Se_{19}$*
P. Gougeon, P. Gall, R. Al Rahal Al Orabi, B. Boucher, B. Fontaine, R. Gautier, A. Dauscher, C. Candolfi, B. Lenoir
***Inorg. Chem.* 2019**, 58, 5533-5542

97 *Realizing a Stable High Thermoelectric zT ~ 2 over a Broad Temperature Range in $Ge_{1-x-y}Ga_xSb_yTe$ via Band Engineering and Hybrid Flash-SPS Processing*
B. Srinivasan, A. Gellé, F. Gucci, C. Boussard-Pledel, B. Fontaine, R. Gautier, J.-F. Halet, M. J. Reece, B. Bureau
***Inorg. Chem. Front.* 2019**, 6, 63-73

96 *Computing ^{93}Nb NMR Parameters of Solid-State Niobates. The Geometry Matters.*
I. Saouli, S. Landron, B. Peric, A. Boutarfaia, C. Kouvatas, L. Le Pollès, J. Cuny, R. Gautier
***J. Struct. Chem.* 2019**, 60, 430-436

95 *Synthesis, Crystal Structure, and Liquid Exfoliation of Layered Lanthanide Sulfides KLn_2CuS_6(Ln = La, Ce, Pr, Nd, Sm)*
T. A. Pomelova, T. Y. Podlipskaya, N. V. Kuratieva, A. G. Cherkov, N. A. Nebogatikova, M. R. Ryzhikov, A. Huguenot, R. Gautier, N. G. Naumov
***Inorg. Chem.* 2018**, 57, 13594

94 *Effect of the Processing Route on the Thermoelectric Performance of Nanostructured $CuPb_{18}SbTe_{20}$*
B. Srinivasan, B. Fontaine, F. Gucci, V. Dorcet, T. Graves Saunders, M. Yu, F. Cheviré, C. Boussard-Pledel, J.-F. Halet, R. Gautier, M. J. Reece, B. Bureau
***Inorg. Chem.* 2018**, 57, 12976-12986

93 *Low Dimensional Solids based on Mo_6 Cluster Cyanides and Mn^{2+}, Mn^{3+} or Cd^{2+} Metal Ions: Crystal Chemistry, Magnetic and Optical Properties.*
G. Daigre, P. Lemoine, T.-D. Pham, V. Demange, R. Gautier, N. Naumov, A. Ledneva, M. Amela-Cortes, N. Dumait, N. Audebrand, S. Cordier
***CrystEngComm* 2018**, 20, 3396

92 *Influence of S and Te substitutions on the thermoelectric properties of the cluster compound $Ag_{3.8}Mo_9Se_{11}$*
P. Masschelein, C. Candolfi, A. Dauscher, C. Gendarme, R. Al Rahal Al Orabi, P. Gougeon, M. Potel, P. Gall, R. Gautier, B. Lenoir
***J. Alloys Compd.* 2018**, 739, 360-367.

91 *Impact of Coinage Metal Insertion on the Thermoelectric Properties of GeTe Solid-State Solutions*
B. Srinivasan, R. Gautier, F. Gucci, B. Fontaine, J.-F. Halet, F. Cheviré, C. Boussard-Pledel, M. J. Reece, B. Bureau
***J. Phys. Chem. C* 2018**, 122, 227-235

90 *Towards the Prediction of the Transport Properties of Cluster-Based Molybdenum Chalcogenides?*
R. Al Rahal Al Orabi B. Boucher, B. Fontaine, P. Gall, C. Candolfi, B. Lenoir, P. Gougeon, J.-F. Halet, R. Gautier
***J. Mater. Chem. C* 2017**, 5, 12097-12104

89 *Ultra-low Lattice Thermal Conductivity and Enhanced Thermoelectric Performance in SnTe:Ga Materials*
R. Al Rahal Al Orabi, J. Hwang, C.-C. Lin, R. Gautier, B. Fontaine, W. Kim, J.-S. Rhyee, D. Wee, M. Fornari
***Chem. Mater.* 2017**, 29, 612

88 *Sb Doping of Metallic $CuCr_2S_4$ as a Route to Highly Improved Thermoelectric Properties*
A. Ullah Khan, R. Al Rahal Al Orabi, A. Pakdel, J.-B. Vaney, B. Fontaine, R. Gautier, J.-F. Halet, S. Mitani, T. Mori
***Chem. Mater.* 2017**, *29*, 2988-2996.

87 *About Enhancement of the Thermoelectric Properties of $FeGa_3$-Type Structures with Group-6 Transition Metals: A Computational Exploration*
B. Boucher, R. Al Rahal Al Orabi, B. Fontaine, Y. Grin, R. Gautier, J.-F. Halet
***Inorg. Chem*. 2017**, *56*, 4229-4237.

86 *Synthesis, crystal structure and high-temperature transport properties of the new cluster compound $Rb_2Mo_{15}Se_{19}$.*
G. Daigre, P. Gougeon, P. Gall, R Gautier, O. Guillou, J.-B. Vaney, C. Candolfi, A. Dauscher, B. Lenoir
***J. Solid State Chem.* 2016**, 237, 1.

85 *Atom-Precise Organometallic Zinc Clusters*
H. Banh, K. Dilchert, C. Schulz, C. Gemel, R. W. Seidel, R. Gautier, S. Kahlal, J.-Y. Saillard, R. A. Fischer
***Angew. Chem. Int. Ed.* 2016**, 55, 3285

84 *The Coloring Problem in the Solid-State Metal Boride Carbide ScB_2C_2. A Theoretical Analysis*
S. Lassoued, B. Boucher, A. Boutarfaia, R. Gautier, J.-F. Halet
***Z. Naturforsch., B: J. Chem. Sci.* 2016**, 71, 593

83 *Cu Insertion Into the Mo_{12} Cluster Compound $Cs_2Mo_{12}Se_{14}$: Synthesis, Crystal and Electronic Structures, and Physical Properties*
R. Al Rahal Al Orabi, B. Fontaine, R. Gautier, P. Gougeon, P. Gall, Y. Bouyrie, A. Dauscher, C. Candolfi, B. Lenoir
***Inorg. Chem.* 2016**, 55, 6616

82 *Multinuclear NMR as a tool for studying local order and dynamics in $CH_3NH_3PbX_3$ (X = Cl, Br, I) hybrid perovskites*
C. Roiland, G. Trippé-Allard, K. Jemli, B. Alonso, J.-C. Ameline, R. Gautier, T. Bataille, L. Le Pollès, E. Deleporte, J. Even, C. Katan
***Phys. Chem. Chem. Phys.* 2016**, 18, 27133

81 *Structural and Electronic Structures of Alkaline-Earth Transition Metal Oxynitride Perovskites*
E. Orisakwe, R. Marchal, B. Fontaine, R. Gautier, J.-F. Halet
***J. Ceram. Soc. Jpn.* 2016**, 124, 1056

80 *Combined theoretical and time-resolved photoluminescence investigations of $[Mo_6Br^i_8Br^a_6]^{2-}$ metal cluster units: evidence of dual emission*
K. Costuas,A. Garreau, A. Bulou, B. Fontaine, J. Cuny, R. Gautier, M. Mortier, Y. Molard, J.-L. Duvail, E. Faulques, S. Cordier
***Phys. Chem. Chem. Phys.* 2015**, *17*, 28574-28585

79 *Evaluation of ^{95}Mo Nuclear Shielding and Chemical Shift of $[Mo_6X_{14}]^{2-}$ Clusters in the Liquid Phase*
T. T. Nguyen, J. Jung, X. Trivelli, J. Trébosc, S. Cordier, Y. Molard, L. Le Pollès, C. J. Pickard, J. Cuny, R. Gautier
***Inorg. Chem.* 2015**, *54*, 7673

78 *Prediction of high thermoelectric potential in AMN_2 layered nitrides : electronic structure, phonons, and anharmonic effects*
R. Al Rahal Al Orabi, E. Orisakwe, D. Wee, B. Fontaine, R. Gautier, J.-F. Halet, M. Fornari
***J. Mater. Chem. A* 2015**, *3*, 9945.

77 *Supramolecular Frameworks Built up from Red-Phosphor-escent trans-Re_6 Cluster Building Blocks: One Pot Synthesis, Crystal Structures, and DFT Investigations*
R. El Osta, A. Demont, N. Audebrand, Y. Molard, T. T. Nguyen, R. Gautier, K. A. Brylev, Y. V. Mironov, N. G. Naumov, N. Kitamura, S. Cordier
***Z. Anorg. Allg. Chem.* 2015**, *641*, 1156

76 *On The Origin of The Differences in Structure Directing Properties of Polar Metal Oxyfluoride $[MO_xF_{6-x}]^{2-}$ (x = 1, 2) Building Units*
Ro. Gautier, R. Gautier, K. Chang, K. R. Poeppelmeier
***Inorg. Chem.* 2015**, 54, 1712-1719

75 *Analysis and Prediction of Stacking Sequences in Intercalated Lamellar Vanadium Phosphates*
Ro. Gautier, Y. Fourré, E. Furet, R. Gautier, E. Le Fur
***Eur. J. Inorg. Chem*. *2015**, 11, 1941*

74 *X-ray Characterization, Electronic Band Structure, and Thermoelectric Properties of the Cluster Compound $Ag_2Tl_2Mo_9Se_{11}$*
R. Al Rahal Al Orabi, P. Gougeon, P. Gall, B. Fontaine, R. Gautier, M. Colin, C. Candolfi, A. Dauscher, J. Hejtmanek, B. Malaman, B. Lenoir
***Inorg. Chem.* 2014**, 53, 11699–11709

73 *Comprehensive Study of the Low-Temperature Transport and Thermodynamic Properties of the Cluster Compounds $Ag_xMo_9Se_{11}$ ($3.41 \leq x \leq 3.78$)*
T. Zhou, M. Colin, C. Candolfi, C. Boulanger, A. Dauscher, E. Santava, J. Hejtmanek, P. Baranek, R. Al Rahal Al Orabi, M. Potel, B. Fontaine, P. Gougeon, R. Gautier, B. Lenoir
***Chem. Mater.* 2014**, 26, 4765−4775

72 *Theoretical Study on the Structural, Electronic and Physical Properties of Layered Alkaline-Earth-Group-4 Transition-Metal Nitrides $AEMN_2$*
E. Orisakwe, B. Fontaine, D. H. Gregory, R. Gautier, J.-F. Halet
***RSC Adv.* 2014**, 4, 31981–31987

71 *Thermotropic Luminescent Clustomesogen Showing a Nematic Phase: a Combination of Experiments and Molecular Simulation Tools*
M. A. Cortes, F. Dorson, M. Prévôt, A. Ghoufi, B. Fontaine, R. Gautier, F. Goujon, V. Cîrcu, C. Mériadec, F. Artzner, H. Folliot, S. Cordier, Y. Molard
***Chem. Eur. J.* 2014**, 20, 8561 – 8565

70 *Solid-State NMR/NQR and First-Principles Study of Two Niobium Halide Cluster Compounds*
B. Perić, R. Gautier, C. J. Pickard, M. Bosiočić, M. S. Grbić, M. Požek
***Solid State Nucl. Magn. Reson.* 2014**, 59-60, 20-30

69 *Unprecedented Electron-Poor Octahedral Ta_6 Clusters in a Solid State Compound: Synthesis, Characterizations and Theoretical Investigations of $Cs_2BaTa_6Br_{15}O_3$*
A. Demont, O. Hernandez, E. Elkaïm, S. Paofaï, C. Prestipino, N. Naumov, B. Fontaine, R. Gautier, S. Cordier
***Chem. Eur. J.* 2013**, 19, 12711-12719.

68 *Synthesis and Crystal Structure of the azide $K_4[Re_6Se^i_8(N_3)^a_6]\cdot 4H_2O$; Luminescence, Redox and DFT Investigations of the $[Re_6Se^i_8(N_3)^a_6]^{4-}$ Cluster Unit*
A. Gandubert, K. A. Brylev, T. T. Nguyen, N. G. Naumov, N. Kitamura, Y. Molard, R. Gautier, S. Cordier
***Z. Allg. Anorg. Chem.* 2013**, 639, 1756-1762.

67 *DFT-assisted Structure Determination of α_1- and α_2-$VOPO_4$: New Insights into the Understanding of the Catalytic Performances of Vanadium Phosphates*
Ro. Gautier, R. Gautier, O. Hernandez, N. Audebrand, T. Bataille, C. Roiland, E. Elkaïm, L. Le Pollès, E. Furet, E. Le Fur
***Dalton Trans.* 2013**, 8124-8131.

66 *Synthesis, crystal and electronic structures and magnetic properties of $Li_2SnMo_3O_8$: a novel reduced molybdenum oxide containing Mo_3O_{13} cluster units*
P. Gall, R. Al Rahal Al Orabi, T. Guizouarn, J. Cuny, B. Fontaine, R. Gautier, P. Gougeon
***J. Solid State Chem.* 2013**, 201, 312-316.

65 *Theoretical analysis of the structure and bonding in electron-rich edge-bridged octahedral tungsten chloride clusters*
N. Nebbache, B. Fontaine, H.-J. Meyer, R. Gautier, J.-F. Halet
***Solid State Sci.* 2013**, 19, 150-155.

64 *^{95}Mo Solid-State Nuclear Magnetic Resonance Spectroscopy and Quantum Simulations: Synergetic Tools for the Study of Molybdenum Cluster Materials*
J. Cuny, S. Cordier, C. Perrin, C. J. Pickard, L. Delevoye, J. Trebosc, Z. Gan, L. Le Pollès, R. Gautier
***Inorg. Chem.* 2013**, 52, 617-627.

63 *Structural, electronic and magnetic properties of layered REB_2C compounds (RE=Dy, Tm, Lu).*
V. Babizhetskyy, A. Simon, C. Hoch, K. Hiebl, L. Le Pollès, R. Gautier, J.-F. Halet
***J. Solid State Chem.* 2012**, 191, 121-128

62 *$Sc_{0.43(2)}Rb_2Mo_{15}S_{19}$, a partially Sc-filled variant of $Rb_2Mo_{15}S_{19}$.*
P. Gougeon, R. Al Rahal Al Orabi, R. Gautier, M. Potel
***Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* 2012** C68, i25-i28

61 *Synthesis, Crystal and Electronic Structures and Thermoelectrical Properties of the Novel Cluster Compound $Ag_3In_2Mo_{15}Se_{19}$.*
P. Gougeon, P. Gall, R. Al Rahal Al Orabi, B. Fontaine, R. Gautier, M. Potel, T. Zhou, B. Lenoir, M. Colin, C. Candolfi, A. Dauscher
***Chem. Mater.* 2012**, 24, 2899–2908

60 *$VOPO_4\cdot H_2O$: A Stacking Faults Structure Studied by X-ray Powder Diffraction and DFT-D Calculations.*
Ro. Gautier, N. Audebrand, E. Furet, R. Gautier, E. Le Fur
***Inorg. Chem.* 2011**, 50, 4378–4383

59 *High Temperature Experimental and Theoretical Study of Magnetic Interactions in Diamond and Pseudo-Diamond Frameworks Built up from Hexanuclear Tantalum Clusters.*
B. Peric, S. Cordier, J.Cuny, R. Gautier, T. Guizouarn, P. Planinic
***Chem. Eur. J.* 2011**, 17, 6263–6271.

58 *New Members of Ternary Rare-Earth Metal Boride Carbides Containing Finite Boron-Carbon Chains: $RE_{25}B_{14}C_{26}$ (RE = Pr, Nd) and $Nd_{25}B_{12}C_{28}$.*
V. Babizhetskyy, H. Mattausch, A. Simon, R. Gautier, J.-F. Halet
***J. Solid State Chem.* 2011**, 184, 1671-1681

57 *Octahedral Niobium Cluster-Based Solid State Halides and Oxyhalides: Effects of the Cluster Condensation via Oxygen Ligand on Electronic and Magnetic Properties.*
B. Fontaine, S. Cordier, R.Gautier, F.Gulo, J.-F. Halet, B. Perić, C.Perrin
***New J. Chem.* 2011**, 35, 2245-2252

56 *^{95}Mo Nuclear Magnetic Resonance Parameters of Molybdenum Hexacarbonyl from Density Functional Theory: Appraisal of Computational and Geometrical Parameters.*
J. Cuny, K. Sykina, B. Fontaine, L. Le Pollès, C. J. Pickard, R. Gautier
***Phys. Chem. Chem. Phys.* 2011**, 13, 19471-19479

55 *Synthesis, Crystal and Electronic Structures, and Magnetic Properties of the $LiR_9Mo_{16}O_{35}$ (R = La, Ce, Pr, and Nd) Compounds Containing the Original Cluster $Mo_{16}O_{36}$.*
P. Gougeon, P. Gall, J. Cuny, R. Gautier, L. Le Pollès, L. Delevoye, J. Trébosc
***Chem. Eur. J.* 2011**, 17, 13806-13813

54 *A new combined approach to investigate stacking faults in lamellar compounds.*
Ro. Gautier, E. Furet, R. Gautier, N. Audebrand, E. Le Fur
***Z. Kristallogr. Proc.* 2011**, 1, 49-54

53 *Electric Field Gradient Calculations in paramagnetic compounds using the PAW approach. Application to ^{23}Na NMR in layered vanadium phosphates.*
J. Cuny, J. Yates, R. Gautier, E. Furet, E. Le Fur, L. Le Pollès
***Magn. Reson. Chem.* 2010**, 48, S171-S175

52 *$Ag_{2.54}Tl_2Mo_{12}Se_{15}$: a new structure type containing Mo_6 and Mo_9 clusters.*
P. Gougeon, P. Gall, R. Gautier, M. Potel
***Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* 2010**, C66, i67-i70

51 *Improving sensitivity and resolution of MQMAS spectra: a ^{45}Sc case study of scandium sulphate pentahydrate.*
C. V. Chandran, J. Cuny, R. Gautier, L. Le Pollès, C. J Pickard, T. Braüniger
***J. Magn. Reson.* 2010**, 203, 226-235.

50 *Rings and chains in solid-state metal borides and borocarbides. The electron count matters.*
S. Lassoued, R. Gautier, A. Boutarfaia, J.-F. Halet
***J. Organomet. Chem.* 2010**, 695, 987-993.

49 *DFT Calculations of ^{95}Mo NMR Parameters in Solid-State Compounds.*
J. Cuny, E. Furet, R. Gautier, L. Le Pollès, C. J. Pickard, J.-B. d'Espinose de Lacaillerie
***ChemPhysChem* 2009**, 10, 3320-3329.

48 *Synthesis, Electronic & Crystal Structures, & Physical Studies of the Superconductor $Cs_{\sim 1}Mo_{12}S_{14}$, Final Step of the Condensation of the $Mo_6L^i_8L^a_6$ Unit.*
P. Gougeon, D. Salloum, J. Cuny, L. Le Pollès, M. Le Floch, R. Gautier, M. Potel.
***Inorg. Chem.* 2009**, 48, 8337-8341.

47 *Synthesis, Crystal and Electronic Structures of the Novel Compounds $LaR_4Mo_{36}O_{52}$ (R = Dy, Er, Yb and Y) Containing Infinite Chains of Trans-edge-shared Mo_6 Octahedra and Mo_2 Pairs or/and Rectangular Mo_4 Clusters with Triple Mo-Mo Bonds.*
N. Barrier, B. Fontaine, S. Pierrefixe, R. Gautier, P. Gougeon.
***Inorg. Chem.* 2009**, 48, 3848-3856.

46 *Cations Insertion in Molybdenum Cluster Compounds. Electronic Structure and Electrochemical Study Using Cavity Microelectrode.*
S. Bouazza, D. Salloum, R. Gautier, P. Gougeon, M. Potel, D. Hauchard
***J. Cluster Sci.* 2009**, 20, 133-143.

45 *Isomery of $[Re_6S_6Br_8]$ and $[Re_6S_5Br_9]$ Units in a Rhenium Cluster Thiobromide: Experimental and Theoretical Approaches.*
B. Fontaine, R. Gautier, G. Pilet, S. Cordier, C. Perrin, A. Perrin, Y. V. Mironov
***J. Cluster Sci.* 2009**, 20, 145-151.

44 *DFT Calculations of Quadrupolar Solid State NMR Properties. Some Examples in Solid-State Inorganic Chemistry.*
J. Cuny, S. Messaoudi, V. Alonzo, E. Furet, J.-F. Halet, E. Le Fur, S. E. Ashbrook, C. J. Pickard, R. Gautier, L. Le Pollès.
***J. Comput. Chem.* 2008**, 29, 2279-2887.

43 *New examples of ternary rare-earth metal boride carbides containing finite boron-carbon chains: The crystal and electronic structure of $RE_{15}B_6C_{20}$ (RE = Pr, Nd).*
V. Babizhetskyy, H. Mattausch, A. Simon,K. Hiebl, M. Ben Yahia, R. Gautier, J.-F. Halet
***J. Solid State Chem.* 2008**, 181, 1882-1890.

42 *Can Undoped Calcium Tetraboride Exist? An Answer from the Comparison of their DFT Electronic Structure with that of Rare-Earth Metal Tetraborides.*
M. Ben Yahia, O. Reckeweg, R. Gautier, J. Bauer, T. Schleid, J.-F. Halet, J.-Y. Saillard.
***Inorg. Chem.* 2008**, 47, 6137-6143.

41 *Unusual Coexistence of Magnetic and Nonmagnetic Mo_6 Octahedral Clusters in a Chalcohalide Solid Solution: Synthesis, X-ray diffraction, EPR and DFT investigations of $Cs_3Mo_6I^i_6I^i_{2-x}Se^i_xI^a_6$.*
K. Kirakci, S. Cordier, A. Shames, B. Fontaine, O. Hernandez, E. Furet, J.-F. Halet, R. Gautier, C. Perrin
***Chem. Eur. J.* 2007**, 13, 9608-9616

40 *Structure and Stability of $[VO_2]^+$ in Aqueous Solution: A Car-Parrinello and Static Ab Initio Study.*
A. Sadoc, S. Messaoudi, E. Furet, R. Gautier, E. Le Fur, L. Le Pollès, J.-Y. Pivan
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