

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

- 100 publications in peer reviewed journals

- 8 invited conferences - 24 invited seminars - 37 orals in national & international meetings

2012-2016 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, 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 Korea*
- 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

- 100 *Red-NIR luminescence of Mo₆ 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** en ligne
- 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 Ag₃Tl₂Mo₁₅Se₁₉*
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}yGa_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 ⁹³Nb 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 KLn₂CuS₆ (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 CuPb₁₈SbTe₂₀*
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 Mo₆ Cluster Cyanides and Mn²⁺, Mn³⁺ or Cd²⁺ 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}Mo₉Se₁₁*
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 CuCr₂S₄ 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 FeGa₃-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 Rb₂Mo₁₅Se₁₉.*
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 ScB₂C₂. 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 Mo₁₂ Cluster Compound Cs₂Mo₁₂Se₁₄: 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 CH₃NH₃PbX₃ (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 [Mo₆Br₆Br⁶]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 ⁹⁵Mo Nuclear Shielding and Chemical Shift of [Mo₆X₁₄]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 AMN₂ 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-Re₆ 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 Ag₂Tl₂Mo₉Se₁₁*
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_xMo₉Se₁₁ (3.41 ≤ x ≤ 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 AEMN₂*
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 Ta₆ Clusters in a Solid State Compound: Synthesis, Characterizations and Theoretical Investigations of Cs₂BaTa₆Br₁₅O₃*
A. Demont, O. Hernandez, E. Elkaïm, S. Paofai, 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 $K_4[Re_6Se^{I}_8(N_3)^{3-}_6] \cdot 4H_2O$; Luminescence, Redox and DFT Investigations of the $[Re_6Se^{I}_8(N_3)^{3-}_6]^{4-}$ 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 -VOPO₄: 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 *⁹⁵Mo 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 *VOPO₄·H₂O: 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 *⁹⁵Mo 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 ²³Na 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 *$Ag_{2.54}Ti_2Mo_{12}Se_{15}$: 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 ⁴⁵Sc 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 ⁹⁵Mo 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-1Mo12S14, Final Step of the Condensation of the Mo6LⁱL^a6 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 LaR4Mo36O52 (R = Dy, Er, Yb and Y) Containing Infinite Chains of Trans-edge-shared Mo6 Octahedra and Mo2 Pairs or/and Rectangular Mo4 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 [Re6S6Br6] and [Re6S5Br9] 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 RE15B6C20 (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 Mo6 Octahedral Clusters in a Chalcogenide Solid Solution: Synthesis, X-ray diffraction, EPR and DFT investigations of Cs3Mo6Mⁱ2-xSe^xP6.*
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 [VO2]⁺ 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
Inorg. Chem. **2007**, 46, 4935-4843.
- 39 *Crystal chemistry and electronic structure of the metallic ternary nitride, LiNiN.*
Z. Stoeva, B. Jäger, R. Gomez, S. Messaoudi, M. Ben Yahia, X. Rocquefelte, G. B. Hix, W. Wolf, J. J. Titman, R. Gautier, P. Herzog, D. H. Gregory
J. Am. Chem. Soc. **2007**, 129, 1912-1920.
- 38 *Chemical Bonding and Properties of EuPdGe and EuPtGe.*
X. Rocquefelte, R. Gautier, J.-F. Halet, R. Müllmann, C. Rosenbahn, B. D. Mosel, G. Kotzyba, R. Pöttgen
J. Solid State Chem. **2007**, 180, 533-540.
- 37 *Mo15S20 : First evidence of a new molybdenum cluster type in a metastable solid-state compound.*
D. Salloum, R. Gautier, M. Potel, P. Gougeon
Chem. Eur. J. **2006**, 12, 8513-8517.
- 36 *²³Na Multiple Quantum MAS NMR of the Perovskites NaNbO3 and NaTaO3.*
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