

Selected Publications

1. M. Grodzicki, J. Appel: Phonons and Superconducting p-state Pairing in Pd;
Physical Review **B20**, 3659-3669 (1979)
2. G. Amthauer, M. Grodzicki, S.S. Hafner, V. Marathe, A.X. Trautwein: Calculation of Hyperfine Parameters in Some Garnets;
Journal de Physique **C1**, 291-292 (1980)
3. M. Grodzicki: A Self-Consistent-Charge $X\alpha$ Method: I. Theory;
Journal of Physics B **13**, 2683-2691 (1980)
4. R. Bläs, M. Grodzicki, V. Marathe, A.X. Trautwein: A Self-Consistent-Charge $X\alpha$ Method: II. Application to Small Molecules;
Journal of Physics B **13**, 2693-2700 (1980)
5. M. Grodzicki, S. Lauer, A.X. Trautwein, A. Vera: Application of Molecular Orbital Calculations to Mössbauer and NMR Spectroscopy of Halogen Containing Compounds;
in: J. Stevens and G. Shenoy (eds.), *Mössbauer Spectroscopy and its Chemical Applications*;
ACS Advances in Chemistry Series **194**, 3-37 (1981)
6. H. Winkler, R. Eisberg, E. Alp, R. Rüffer, E. Gerdau, S. Lauer, A.X. Trautwein, M. Grodzicki, A. Vera: Pure Nuclear Reflexes and Combined Hyperfine Interactions in YIG;
Zeitschrift für Physik B **49**, 331-341 (1983)
7. A.X. Trautwein, R. Bläs, S. Lauer, M. Grodzicki, K.M. Hasselbach: Electronic Structure Theories, Computer Experiments, and Mössbauer Parameter;
in: P. Gülich, G.M. Kalvius (eds.), *Trends in Mössbauer Spectroscopy*, pp. 68-85, Mainz 1983
8. J. Avery, P.S. Larsen, M. Grodzicki: Measured Electron Density Distributions in Crystals as a Basis for Bandstructure Calculations;
in J.P. Dahl, J. Avery (eds.), *Local Density Approximations in Quantum Chemistry and Solid State Physics*, pp. 733-750, Plenum Press, New York and London, 1984
9. M. Grodzicki: The Calculation of Spectroscopic Data by the SCC- $X\alpha$ method;
in J.P. Dahl, J. Avery (eds.), *Local Density Approximations in Quantum Chemistry and Solid State Physics*, pp. 785-794, Plenum Press, New York and London, 1984
10. M. Grodzicki, H. Walther, S. Elbel: The Electronic Structures of the Group V Series ER_3 ($E = N, P, As, Sb$; $R = H, Hal$): An Intercomparison of Photoelectron Spectra and SCC- $X\alpha$ Calculations;
Zeitschrift für Naturforschung **39b**, 1319-1330 (1984)
11. S. Elbel, J. Kudnig, M. Grodzicki, H.J. Lempka: Photoelectron Spectra of Group V Compounds. The Elements: Sb_4 ;
Chemical Physics Letters **109**, 312-316 (1984)
12. M. Grodzicki: The Applicability of Point-Charge Approximations to the Calculation of Molecular Expectation Values;
Croatica Chemica Acta **57**, 1125-1144 (1984)
13. O. Zakhariyeva, H. Böse, H. Förster, W. Frede, M. Grodzicki: What Kind of Support for the Interpretation of Infrared Spectra can be Expected from Cluster MO Calculations on Zeolite Systems ?
Journal of Molecular Structure (THEOCHEM) **122**, 101-114 (1985)
14. S. Elbel, A. Blanck, H. Walther, M. Grodzicki: Bonding Modes in Analogous and Isoelectronic Group VB/VA Compounds $As(O)Cl_3$ and $Nb(O)Cl_3$;
JCS Faraday Transactions II **81**, 869-880 (1985)
15. M. Grodzicki: Theorie und Anwendungen der Self-Consistent-Charge- $X\alpha$ Methode;
Thesis of habilitation, Hamburg, 1985

16. S. Elbel, J. Kudnig, G. Rünger, M. Grodzicki: Comparison of the Electronic Structures of VOHal₃ and POHal₃ Analogues (Hal = F, Cl, Br) by UPS and SCC-X α Calculations; *Journal of Electron Spectroscopy and Related Phenomena* **37**, 329-339 (1986)
17. H. Förster, M. Grodzicki, O. Zakhariyeva: Application of Semiempirical MO calculations to the Interaction of Hydrocarbons with Zeolites; *Journal of Molecular Structure* **143**, 267-270 (1986)
18. M. Grodzicki, V. Männing, R. Bläs, A.X. Trautwein: A Comparative Theoretical Study of Compounds of the Heavy Main-Group Mössbauer Isotopes Sn to I; *Hyperfine Interactions* **29**, 1543-1546 (1986)
19. M. Grodzicki, A.X. Trautwein: Approximations in the Theoretical Interpretation of Mössbauer Spectra; *Hyperfine Interactions* **29**, 1547-1550 (1986)
20. M. Grodzicki: Das Prinzip Erfahrung – ein Mythos physikalischer Methodologie ? in: A. Bamme, W. Berger, E. Kotzmann (eds.), *Anything Goes – Science Everywhere ? Konturen von Wissenschaft heute*, pp. 135-216, Profil Verlag, München 1986
21. V. Männing, M. Grodzicki: Theoretical interpretation of Mössbauer spectra of ¹¹⁹Sn compounds; *Theoretica Chimica Acta* **70**, 189-202 (1986)
22. R. Bläs, E. Bill, S. Lauer, A.X. Trautwein, H. Winkler, M. Grodzicki, A. Kostikas: Molecular Orbital Theory and Mössbauer Spectroscopy: Electronic Structure Studies of Bioinorganic Iron Sulfur Clusters; in: A. Xavier (ed.), *Frontiers in Bioinorganic Chemistry*, pp. 515-536, Verlag Chemie, Weinheim 1986
23. M. Grodzicki, S. Elbel: The Electronic Structure of As₄S₄, S₄N₄ and Related Clusters: A Gas Phase UPS and SCC-X α MO Study; *Lecture Notes in Physics* **269**, 47-55 (1987)
24. O. Kühnholz, M. Grodzicki: Nickel Clusters as Surface Models for Adsorption; *Lecture Notes in Physics* **269**, 198-211 (1987)
25. M. Hütsch, M. Grodzicki: SCC-X α calculations on Small Titanium Compounds and TiO₂ Clusters; *Lecture Notes in Physics* **269**, 212-225 (1987)
26. M. Grodzicki: Calculation of Overlap Integrals over Slater Orbitals with Nearly Equal Exponents; *Croatica Chemica Acta* **60**, 263-268 (1987)
27. M. Grodzicki, S. Elbel: Electronic structure of analogous and isoelectronic main-group and transition metal compounds – a combined theoretical and experimental study; in: Z.B. Maksic (ed.), *Modelling of Structure and Properties of Molecules*, pp. 239-250, Ellis Horwood, Chichester 1987
28. M. Grodzicki, V. Männing, A.X. Trautwein, J.M. Friedt: Calibration of isomer shift and quadrupole coupling for ¹¹⁹Sn, ¹²⁷I and ¹²⁹I as derived from SCC-X α calculations and Mössbauer measurements; *Journal of Physics B* **20**, 5595-5625 (1987)
29. R. Bläs, J. Guillin, E.L. Bominaar, M. Grodzicki, V.R. Marathe, A.X. Trautwein: Spin-polarised SCC-X α calculations for electronic- and magnetic-structure properties of 2Fe-2S ferredoxin models; *Journal of Physics B* **20**, 5627-5637 (1987)
30. M. Grodzicki, H. Förster, R. Piffer, O. Zakhariyeva: Profitability of the Combined Application of MO-calculations and Vibrational Analysis on Intrazeolitic Sorption Complexes; *Catalysis Today* **3**, 75-82 (1988)
31. M. Grodzicki, O. Kühnholz: Theoretical Investigation of Adsorption of Water Dimers on a Ni(110) Surface; *Journal of Molecular Structure* **174**, 65-70 (1988)

32. M. Grodzicki, O. Zakharieva, H. Förster: Molecular Orbital Calculations and Normal Coordinate Analysis of CO₂ and N₂O in Zeolites;
Journal of Molecular Structure **175**, 195-201 (1988)
33. S. Elbel, M. Grodzicki, L. Pille, G. Rünger: Electronic Structures of Analogous and Isoelectronic Main-Group and Transition Metal Compounds – A Gas Phase UV-PES and Theoretical Study;
Journal of Molecular Structure **175**, 441-446 (1988)
34. M. Grodzicki, M. Wagner: Cluster molecular-orbital calculation on germanium adsorbed on Si(111) surfaces; Physical Review **B40**, 1110-1120 (1989)
35. O. Zakharieva, M. Grodzicki, H. Förster: SCC-X α calculations on Sorption Complexes of Nitrous Oxide Attached to Transition Metal Occupied Zeolite Clusters;
in: H. Karge, J. Weitkamp (eds.), *Zeolites as Catalysts, Sorbents and Detergent Builders*, pp. 575-584, Elsevier, Amsterdam 1989
36. St. Russ, M. Grodzicki: The Calculation of Core Binding Energy Shifts by the SCC-X α Method;
Physica Scripta **42**, 58-64 (1990)
37. M. Grodzicki, J.M. Seminario, P. Politzer: Conformation-dependent Effects of the Nitro Group upon some Strained Tertiary C-C Bonds;
Journal of Physical Chemistry **94**, 624-628 (1990)
38. M. Grodzicki: The Concept of the Chemical Bond in Solids;
in: Z.B. Maksic (ed.), *Theoretical Models of Chemical Bonding*, Vol. 2, pp. 417-452, Springer, Berlin etc. 1990
39. O. Zakharieva, H. Förster, H. Böse, M. Grodzicki: Study of the Geometry of Cyclopropane Adsorbed on a Calcium Ion in Zeolite A by SCC-X α calculations;
Journal of Molecular Structure **218**, 405-410 (1990)
40. M. Grodzicki, J.M. Seminario, P. Politzer: Computational analysis of some possible initial steps in the unimolecular thermal decomposition of 1,3-diazacyclobutane and its 1,3-dinitramine derivative;
Theoretica Chimica Acta **77**, 359-367 (1990)
41. J.M. Seminario, M. Grodzicki, P. Politzer: Application of Local Density Functional Theory to the Study of Chemical Reactions;
in: J.K.Labanowski, J.W.Andzelm (eds.), *Density Functional Theory Approaches to Chemistry*, pp. 419-425, Springer, Berlin etc. 1990
42. M. Grodzicki, J.M. Seminario, P. Politzer: Energy barriers of symmetry forbidden reactions: Local density functional calculations;
Journal of Chemical Physics **94**, 1668-1669 (1991)
43. D. Habibollahzadeh, M. Grodzicki, J.M. Seminario, P. Politzer: A Computational Study of the Concerted Triple Dissociation of 1,3,5-Triazacyclohexane and its 1,3,5-Trinitro Derivative (RDX);
Journal of Physical Chemistry **95**, 7699-7702 (1991)
44. D. Habibollahzadeh, J.S. Murray, M. Grodzicki, J.M. Seminario, P. Politzer: C-H Bond Dissociation of Acetylene: Local Density Functional Calculations;
International Journal of Quantum Chemistry **42**, 267-272 (1992)
45. P. Politzer, J.E. Huheey, J.S. Murray, M. Grodzicki: Electronegativity and the concept of charge capacity; Journal of Molecular Structure (THEOCHEM) **259**, 99-120 (1992)
46. J. Appel, M. Grodzicki, F. Paulsen: Bond-charge repulsion and hole superconductivity in the atomic representation of the CuO₂ plane;
Physical Review **B47**, 2812-2820 (1993)
47. H. Paulsen, X.-Q. Ding, M. Grodzicki, Ch. Butzlaff, A.X. Trautwein, R. Hartung, K. Wieghardt: Spectroscopic and theoretical studies on a three-iron cluster with linear arrangement;
Chemical Physics **184**, 149-162 (1994)

48. O. Zakharieva, D. Paneva, M. Grodzicki: NCA and MO calculations on normal and deuterated pyrroles; *Journal of Molecular Structure* **348**, 115-118 (1995)
49. T. Gog, P. Schotters, J. Falta, G. Materlik, M. Grodzicki: The lattice position of Fe in Fe-doped LiNbO_3 ; *Journal of Physics Condensed Matter* **7**, 6971-6980 (1995)
50. H. Paulsen, M. Kröckel, M. Grodzicki, E. Bill, A.X. Trautwein, G.J. Leigh, J. Silver: Structure of $\text{FeI}_2 \cdot [16]\text{aneS}_4$: Square-Planar or Octahedral Iron Coordination ? *Inorganic Chemistry* **34**, 6244-6249 (1995)
51. W.O. Koch, A. Barbieri, M. Grodzicki, V. Schünemann, A.X. Trautwein, H.-J. Krüger: Eight-Coordinate Iron(II) and Iron(III) Complexes in Distorted Dodecahedral FeN_8 Environment: Synthesis and Structure of Bis(2,11-diaza[3,3](2,6)pyridinophane) Iron Complexes; *Angewandte Chemie* **108**, 484-486 (1996)
52. M. Kröckel, M. Grodzicki, V. Papaefthymiou, A.X. Trautwein, A. Kostikas: Tuning of electron delocalization in polynuclear mixed-valence clusters by super-exchange and double exchange; *Journal of Biological Inorganic Chemistry* **1**, 173-176 (1996)
53. O. Zakharieva, M. Grodzicki, A.X. Trautwein, C. Veeger, I.M.C.M. Rietjens: Molecular orbital study of the hydroxylation of benzene and monofluorobenzene catalyzed by iron-oxo porphyrin π cation radical complexes; *Journal of Biological Inorganic Chemistry* **1**, 192-204 (1996)
54. J.R. Polam, J.L. Wright, K.A. Christensen, F.A. Walker, H. Flint, H. Winkler, M. Grodzicki, A.X. Trautwein: Valence Electron Cloud Asymmetry from Two Points of View: A Correlation between Mössbauer Quadrupole Splittings and ^{57}Fe NMR Chemical Shifts of Diamagnetic Iron(II) Porphyrinates; *Journal of the American Chemical Society* **118**, 5272-5276 (1996)
55. I.M.C.M. Rietjens, A.M. Osman, C. Veeger, O. Zakharieva, J. Antony, M. Grodzicki, A.X. Trautwein: On the role of the axial ligand in heme-based peroxidase- and P450-type catalysis; *Journal of Biological Inorganic Chemistry* **1**, 372-376 (1996)
56. H. Paulsen, M. Müther, M. Grodzicki, A.X. Trautwein, E. Bill: Complementary Mössbauer, EPR and theoretical studies of the exchange-coupled oxoferryl porphyrin cation radical system $[(\text{Cl})\text{Fe}(\text{IV})=\text{O}(\text{TMP})^\bullet]$; *Bulletin Societe Chimie France* **133**, 703-710 (1996)
57. J. Antony, M. Grodzicki, A.X. Trautwein: Local density functional study of oxo-iron(IV) porphyrin complexes and their one-electron oxidized derivatives. Axial ligand effects; *Journal of Physical Chemistry A* **101**, 2692-2701 (1997)
58. M. Grodzicki, H. Flint, H. Winkler, F.A. Walker, A.X. Trautwein: Electronic structure, porphyrin core distortion and fluxional behavior of bis-ligated low-spin iron(II) porphyrinates; *Journal of Physical Chemistry A* **101**, 4202-4207 (1997)
59. O. Zakharieva, M. Grodzicki, A.X. Trautwein, C. Veeger, I.M.C.M. Rietjens: Molecular orbital study of porphyrin-substrate interactions in cytochrome P450 catalysed aromatic hydroxylation of substituted anilines; *Biophysical Chemistry* **73**, 189-203 (1998)
60. T. Wolenski, M. Grodzicki, J. Appel: Helical spin-density wave in V_{2-y}O_3 ; *Physical Review B* **58**, 303-308 (1998)
61. T. Jüstel, M. Müller, T. Weyhermüller, C. Kressl, E. Bill, P. Hildebrandt, M. Lengen, M. Grodzicki, A.X. Trautwein, B. Nuber, K. Wieghardt: The molecular and electronic structure of symmetrically and asymmetrically coordinated, non-heme iron complexes containing $[\text{Fe}^{III}(\mu\text{-N})\text{Fe}^{IV}]^{4+}$ ($S=3/2$) and $[\text{Fe}^{IV}(\mu\text{-N})\text{Fe}^{IV}]^{5+}$ ($S=0$) cores; *Chemistry - A European Journal* **5**, 793-810 (1999)

62. H. Keutel, I. K  pplinger, E.-G. J  ger, M. Grodzicki, V. Sch  nemann, A.X. Trautwein: Structural, magnetic and electronic properties of a pentacoordinated intermediate-spin ($S=3/2$) iron(III) complex with a macrocyclic $[N_4]^{2-}$ ligand; *Inorganic Chemistry* **38**, 2320-2327 (1999)
63. M. Grodzicki: Dichtefunktionaltheorie; Essay in: *Lexikon der Physik*, Vol.2, pp.18-22; Spektrum Verlag, Heidelberg 1999
64. A. Lougear, A.X. Trautwein, M. Grodzicki, C. Bertoldi, K.Steiner, G. Amthauer: M  ssbauer and molecular orbital study of chlorites; *Physics and Chemistry of Minerals* **27**, 258-269 (2000)
65. M. Grodzicki, G. Amthauer: Electronic and magnetic structure of vivianite: cluster molecular orbital calculations; *Physics and Chemistry of Minerals* **27**, 694-702 (2000)
66. M. Grodzicki, S. Heuss-Assbichler, G. Amthauer: M  ssbauer investigations and molecular orbital calculations on epidote; *Physics and Chemistry of Minerals* **28**, 675-681 (2001)
67. W. Lottermoser, K. Steiner, M. Grodzicki, K. Jiang, G. Scharfetter, J.W. Bats, G. Redhammer, W. Treutmann, S. Hosoya, G. Amthauer: The electric field gradient in synthetic fayalite $\alpha\text{-Fe}_2\text{SiO}_4$ at moderate temperatures; *Physics and Chemistry of Minerals* **29**, 112-121 (2002)
68. M. Grodzicki, G. Redhammer, G. Amthauer, V. Sch  nemann, A.X. Trautwein, B. Velickov, P. Schmid-Beurmann: Electronic structure of Fe-bearing lazulites; *American Mineralogist* **88**, 481-488 (2003)
69. C.A. Geiger, M. Grodzicki, G. Amthauer: The crystal chemistry and Fe^{II} -site properties of aluminosilicate garnet solid solutions as revealed by M  ssbauer spectroscopy and electronic structure calculations; *Physics and Chemistry of Minerals* **30**, 280-292 (2003)
70. G. Amthauer, W. Lottermoser, G. Redhammer, M. Grodzicki: M  ssbauer spectroscopy: basic principles; in: E. Libowitzky and A. Beran (eds.), *Spectroscopic methods in mineralogy*, EMU notes in mineralogy, vol. 6, 345-367 (2004)
71. T. H  che, P.A. van Aken, M. Grodzicki, F. Heyroth, R. Keding, R. Uecker: Electron energy-loss spectroscopy at incommensurately modulated crystalline and glassy $\text{Ba}_2\text{TiGe}_2\text{O}_8$; *Philosophical Magazine* **84**, 3117-3132 (2004)
72. R.J. Evans, D.G.Rancourt, M. Grodzicki: Hyperfine electric field gradients and local distortion environments of octahedrally co-ordinated Fe^{2+} ; *American Mineralogist* **90**, 187-198 (2005)
73. T. H  che, F. Heyroth, M. Grodzicki, P.A. van Aken: Coordination of transition-metals in glasses from high-resolution electron energy-loss spectroscopy; *physica status solidi(a)* **202**, 2355-2360 (2005)
74. R.J. Evans, D.G.Rancourt, M. Grodzicki: Hyperfine electric field gradient tensors at Fe^{2+} sites in octahedral layers: Towards understanding oriented single-crystal M  ssbauer spectroscopy measurements of micas; *American Mineralogist* **90**, 1540-1555 (2005)
75. T. H  che, M. Grodzicki, F. Heyroth, P.A. van Aken: Assessment of transition-metal coordination in glasses by electron energy-loss spectroscopy; *Physical Review B* **72**, 205111:1-6 (2005)
76. M. Morozov, C. Brinkmann, M. Grodzicki, W. Lottermoser, G. Tippelt, G. Amthauer, H. Kroll: Octahedral cation partitioning in Mg,Fe^{2+} -olivine. M  ssbauer spectroscopic study of synthetic $(\text{Mg}_{0.5}\text{Fe}_{0.5}^{2+})_2\text{SiO}_4$ (Fa_{50}); *Hyperfine Interactions* **166**, 573-578 (2005)

77. T. Höche, F. Schrempel, M. Grodzicki, P.A. van Aken, F. Heyroth: Experimental assessment of structural differences between amorphous and amorphized matter; *Chemistry of Materials* **18**, 5351-5354 (2006)
78. S.U. Weber, M. Grodzicki, C.A. Geiger, W. Lottermoser, G. Tippelt, G. Redhammer, M. Bernroider, G. Amthauer: ^{57}Fe -Mössbauer measurements and electronic structure calculations on natural lawsonites; *Physics and Chemistry of Minerals* **34**, 1-9 (2007)
79. T. Höche, M. Grodzicki, F. Heyroth, R. Uecker, P.A. van Aken: Manifestation of incommensurate structural modulations in the Ti- $L_{2,3}$ electron energy-loss near-edge structure of $\text{Sr}_2\text{TiSi}_2\text{O}_8$; *Philosophical Magazine Letters* **87**, 431-439 (2007)
80. H. Dittrich, A. Bieniok, U. Brendel, M. Grodzicki, D. Topa: Sulfosalts – A new class of compound semiconductors for photovoltaic applications; *Thin Solid Films* **515**, 5745-5750 (2007)
81. E. Dachs, C.A. Geiger, V.v. Seckendorff, M. Grodzicki: A low-temperature calorimetric study of synthetic forsterite-fayalite (Mg_2SiO_4 - Fe_2SiO_4) solid solutions; *Journal of Chemical Thermodynamics* **39**, 906-933 (2007)
82. S.U. Weber, M. Grodzicki, W. Lottermoser, G. Redhammer, G. Tippelt, J. Ponahlo, G. Amthauer: ^{57}Fe -Mössbauer spectroscopy, X-ray single-crystal diffractometry, and electronic structure calculations on natural alexandrite; *Physics and Chemistry of Minerals* **34**, 507-515 (2007)
83. S. Lebernegg, G. Amthauer, M. Grodzicki: Single-centre MO theory of transition metal complexes; *Journal of Physics B* **41**, 035102:1-7 (2008)
84. S.U. Weber, M. Grodzicki, W. Lottermoser, G. Redhammer, D. Topa, G. Tippelt, G. Amthauer: ^{57}Fe -Mössbauer spectroscopy, X-ray single-crystal diffractometry, and electronic structure calculations on natural sinhalites; *Physics and Chemistry of Minerals* **36**, 259-269 (2009)
85. S. Lebernegg, G. Amthauer, M. Grodzicki: The d-Hamiltonian - a new approach for evaluating optical spectra of transition metal complexes; *Journal of Molecular Structure*, **924-926** 473-476 (2009)
86. S. Lebernegg, M. Grodzicki:
Anwendung und Grenzen der Kristallfeldtheorie;
88 pp., VDM Verlag Dr. Müller, 2009
87. M. Grodzicki, G. Redhammer, M. Reissner, W. Steiner, G. Amthauer: Electronic and magnetic structure of pyroxenes I. Hedenbergite; *Physics and Chemistry of Minerals* **37**, 11-23 (2010)
88. M. Grodzicki, B. Mallick, A.-V. Mudring:
Electronic and magnetic structure of $(\text{CrCl}_3)_3$;
Journal of Physics Conf. Series **200**, 032020 (2010)
89. S. Lebernegg, G. Amthauer, M. Grodzicki:
Magneto-structural correlations in double-bridged Cu(II)-dimers;
Journal of Physics Conf. Series **200**, 032039 (2010)
90. D. Zhrebetsky, G. Amthauer, M. Grodzicki:
Electronic and magnetic structure of pyroxenes II. Orthoferrosilite;
Physics and Chemistry of Minerals **37**, 455-464 (2010)
91. M. Grodzicki, S. Lebernegg:
Computation and Interpretation of Mössbauer Parameters of Fe-bearing Compounds; in: P. Gülich, E. Bill, A.X. Trautwein, *Mössbauer Spectroscopy and Transition Metal Chemistry*, Springer, Berlin etc. 2011

92. S. Lebernegg, G. Amthauer, M. Grodzicki:
An analytical approach for calculating transfer integrals in superexchange coupled dimers;
Croatia Chemica Acta **84**, 39-52 (2011)
93. W. Lottermoser, G. Redhammer, S.U. Weber, F.J. Litterst, G. Tippelt, S. Dlugosz, H. Bank,
G. Amthauer, M. Grodzicki:
The electric field gradient in natural iron-doped chrysoberyl Al_2BeO_4 and sinhalite
 MgAlBO_4 single crystals;
Physics and Chemistry of Minerals **38**, 787-799 (2011)
94. C.A. Geiger, M. Grodzicki:
A ^{57}Fe Mössbauer spectroscopic study of sodianite: an example of a symmetric electric field
gradient around Fe^{3+} ;
Physics and Chemistry of Minerals **39**, 73-78 (2012)
95. W. Lottermoser, S.U. Weber, M. Grodzicki, A. Kirfel, G. Amthauer:
A semi-quantitative approach to derive the electric field gradient applied to synthetic fayalite,
 $\alpha\text{-Fe}_2\text{SiO}_4$: A reappraisal;
European Journal of Mineralogy **24**, 791-797 (2012)
96. D. Zhrebetsky, S. Lebernegg, G. Amthauer, M. Grodzicki:
Magnetic structure of almandine;
Physics and Chemistry of Minerals **39**, 351-361 (2012)
97. A. Katerinopoulou, M. Grodzicki, G. Tippelt, G. Amthauer:
Mössbauer spectroscopy and molecular orbital calculations on iron bearing omphacite;
Mineralogy and Petrology **107**, 281-287 (2013)
98. W. Lottermoser, K. Steiner, G. Scharfetter, S.U. Weber, M. Grodzicki, A. Kirfel, G. Amthauer:
Application of a Difference Electron Nanoscope (DEN) - a computer hard- and software to display
3D electron densities and magnetical structures based on spectroscopic and diffractometric data;
Crystal Research and Technology **49**, 14-20 (2014)
99. E. Dachs, C.A. Geiger, A. Benisek, M. Grodzicki:
Thermodynamic mixing properties and behavior of almandine-spessartine solid solutions;
Geochimica and Cosmochimica Acta, **125**, 210-224 (2014)
100. M. Grodzicki:
Physikalische Wirklichkeit – Konstruktion oder Entdeckung ?
Eine Einführung in die Methoden und Ziele der Physik,
528 pp., Living Edition, Pöllauberg-Hainault-Atascadero 2015
101. A. Benisek, E. Dachs, M. Grodzicki:
First principles investigation of the lattice vibrations in the alkali feldspar solid solution;
Physics and Chemistry of Minerals **42** 243-249 (2015)