Dr. rer. nat. habil. Michael Grodzicki

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 Xα 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 Xα 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. Gütlich, 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-Xα 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-Xα 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. Zakharieva, 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-Xα Methode;
    Thesis of habilitation, Hamburg, 1985

16. S. Elbel, J. Kudnig, G. Rünger, M. Grodzicki: Comparison of the Electronic Structures of $VOHal_3$ and $POHal_3$ Analogues (Hal = F, Cl, Br) by UPS and SCC-Xα Calculations; Journal of Electron Spectroscopy and Related Phenomena **37**, 329-339 (1986)

17. H. Förster, M. Grodzicki, O. Zakharieva: 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 ^{119}Sn 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 As_4S_4, S_4N_4 and Related Clusters: A Gas Phase UPS and SCC-Xα 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-Xα calculations on Small Titanium Compounds and TiO_2 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 ^{119}Sn, ^{127}I and ^{129}I as derived from SCC-Xα 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-Xα 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. Zakharieva: 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 CO_2 and N_2O 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-Xα 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-Xα 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-Xα 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 CuO_2 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 $FeI_2 \cdot [16]aneS_4$: 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 $[(Cl)Fe(IV)=O(TMP)^{\bullet}]$;
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 $[Fe^{III}(\mu\text{-N})Fe^{IV}]^{4+}$ (S=3/2) and $[Fe^{IV}(\mu\text{-N})Fe^{IV}]^{5+}$ (S=0) cores;
Chemistry - A European Journal **5**, 793-810 (1999)

62. H. Keutel, I. Käpplinger, E.-G. Jäger, M. Grodzicki, V. Schünemann, 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: Mössbauer 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: Mössbauer 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 α-Fe_2SiO_4 at moderate temperatures;
Physics and Chemistry of Minerals **29**, 112-121 (2002)

68. M. Grodzicki, G. Redhammer, G. Amthauer, V. Schünemann, 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 Mössbauer spectroscopy and electronic structure calculations; Physics and Chemistry of Minerals **30**, 280-292 (2003)

70. G. Amthauer, W. Lottermoser, G. Redhammer, M. Grodzicki: Mössbauer 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. Höche, P.A. van Aken, M. Grodzicki, F. Heyroth, R. Keding, R. Uecker: Electron energy-loss spectroscopy at incommensurately modulated crystalline and glassy $Ba_2TiGe_2O_8$;
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. Höche, 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 Mössbauer spectroscopy measurements of micas;
American Mineralogist **90**, 1540-1555 (2005)

75. T. Höche, 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. Mössbauer spectroscopic study of synthetic $(Mg_{0.5},Fe^{2+}_{0.5})_2SiO_4$ (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 $Sr_2TiSi_2O_8$;
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 $(CrCl_3)_3$;
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. Zherebetskyy, 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. Gütlich, 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;
Croatica 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}Mössbauer spectroscopic study of sogdianite: 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, α-Fe_2SiO_4: A reappraisal;
European Journal of Mineralogy **24**, 791-797 (2012)

96. D. Zherebetskyy, 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)

102. A. Benisek, E. Dachs, M. Grodzicki:
Vibrational entropy of disorder in Cu_3Au with different degrees of short-range order;
Physical Chemistry Chemical Physics **20** 19441-19446 (2018)

103. C.A. Geiger, M. Grodzicki, E. Dachs:
Magnetic behavior in garnets based on Neel temperature behavior;
American Mineralogist, **104** 1246-1255 (2019)

104. M. Grodzicki:
Physical Reality − Construction or Discovery ?
An Introduction to the Methodology and Aims of Physics,
333 pp., Springer, Heidelberg 2021
https://www.springer.com/in/book/9783030745783