

## Publications

V. Kahlenberg, T. Manninger, L. Perfler, D. M. Többens: One-pot occurrence of two polymorphs of  $\text{Rb}_2\text{ScSi}_4\text{O}_{10}\text{F}$  and their structural, spectroscopic and computational characterization. *Journal of Solid State Chemistry* **220**, 79-90 (2014)

M. Pérez-Estébanez, J. Isasi-Marín, D. M. Többens, A. Rivera-Calzada, C. León: A systematic study of Nasicon-based  $\text{Li}_{1+x}\text{M}_x\text{Ti}_{2-x}(\text{PO}_4)_3$  (M: Cr, Al, Fe) by neutron diffraction and impedance spectroscopy. *Solid State Ionics* **266**, 1-8 (2014)

D. Schmidmair, V. Kahlenberg, L. Perfler, D. M. Többens: Structural, spectroscopic and computational studies on the monoclinic polymorph (form I) of potassium hydrogen disilicate ( $\text{KHSi}_2\text{O}_5$ ). *Mineralogical Magazine* **78(3)**, 609-622 (2014)

Anna Gaġor, Paweł Zajdel, Daniel Többens: The phase transitions in  $\text{CsFe}(\text{MoO}_4)_2$  triangular lattice antiferromagnet, neutron diffraction and high pressure studies. *Journal of Alloys and Compounds* **607**, 104–109 (2014)

C. Botta, V. Kahlenberg, C. Hejny, D.M. Többens, M. Bykov, S. van Smaalen: Structural investigations, high temperature behavior and phase transition of  $\text{Na}_6\text{Ca}_4(\text{SO}_4)_6\text{F}_2$ . *Mineralogy and Petrology* **108(4)**, 487-501 (2014)

B. Yan, A. Paul, K. Kumar, S. Kanun, M. Reehuis, A. Hoser, D. M. Többens, W. Schnelle, R. C. Williams, T. Lancaster, F. Xiao, J. S. Möller, St. J. Blundell, W. Hayes, C. Felser, M. Jansen: Lattice-site-specific spin-dynamics in double perovskite  $\text{Sr}_2\text{CoOsO}_6$ . *Physical Review Letters*, **112**, 147202 (2014)

V. Bon, I. Senkovska, D. Wallacher, D. M. Többens, I. Zizak, R. Feyerherm, U. Mueller, St. Kaskel: *In situ* observation of gating phenomena in the flexible porous coordination polymer  $\text{Zn}_2(\text{BPnDC})_2(\text{bpy})$  (SNU-9) in a combined diffraction and gas adsorption experiment. *Inorganic Chemistry*, **53(3)**, 1513-1520 (2014)

V. Sikolenko, V. V. Efimov, D. Többens, S. Schorr, C. Ritter, M. V. Bushinsky, I.O.Troyanchuk: Pressure effects on oxygen-deficient Ba-substituted cobaltites. *Powder Diffraction*, **28 S2**, 126-132 (2013)

I. O. Troyanchuk, M. V. Bushinsky, V. Sikolenko, V. Efimov, C. Ritter, T. Hansen, D. M. Többens: Pressure induced antiferromagnetic-ferromagnetic transition in  $\text{La}_{0.5}\text{Ba}_{0.5}\text{CoO}_{2.8}$  cobaltite. *European Physical Journal B*, **86**, 435(1-7) (2013)

A. K. Paul, M. Reehuis, V. Ksenofontov, B. Yan, A. Hoser, D. M. Többens, P. M. Abdala, P. Adler, M. Jansen, C. Felser: Lattice instability and competing spin structures in the double perovskite Mott insulator  $\text{Sr}_2\text{FeOsO}_6$ . *Physical Review Letters*, **111**, 167205-(1-5) (2013)

M. Wierzbicka-Wieczorek, D. M. Többens, U. Kolitsch, E. Tillmanns: Simultaneous presence of  $(\text{Si}_3\text{O}_{10})_{8-}$  and  $(\text{Si}_2\text{O}_7)_{6-}$  groups in new synthetic mixed sorosilicates:  $\text{BaY}_4(\text{Si}_2\text{O}_7)(\text{Si}_3\text{O}_{10})$  and isotopic compounds, studied by single-crystal X-ray diffraction, Raman spectroscopy and DFT calculations. *Journal of Solid State Chemistry*, **207**, 94-104 (2013)

V. A. Khomchenko, I. O. Troyanchuk, D. M. Többens, V. Sikolenko, J. A. Paixão: Composition- and temperature-driven structural transitions in  $\text{Bi}_{1-x}\text{Ca}_x\text{FeO}_3$  multiferroics: a neutron diffraction study. *Journal of Physics: Condensed Matter*, **25**, 135902 1-7 (2013)

H. Kojitani, D. M. Többens, M. Akaogi: High-pressure Raman spectroscopy, vibrational mode calculation and heat capacity calculation of calcium ferrite-type  $\text{MgAl}_2\text{O}_4$  and  $\text{CaAl}_2\text{O}_4$ . *American Mineralogist*, **98** (1), 197-206 (2013)

D. M. Többens, J. Glinneman, M. R. Chierotti, J. van de Streek, D. Sheptyakov: On the high-temperature phase of barbituric acid. *CrystEngComm* **14** (9), 3046-3055 (2012)

K. Ruschel, L. Nasdala, A. Kronz, J. M. Hanchar, D. M. Többens, R. Škoda, F. Finger, A. Möller: A Raman spectroscopic study on the structural disorder of monazite-(Ce). *Mineralogy and Petrology*, **105** (1), 45-55 (2012)

C. Hejny, R. Sagl, D. M. Többens, R. Miletich, M. Wildner, L. Nasdala, A. Ullrich, T. Balic-Zunic: Crystal-structure properties and the molecular nature of hydrostatically compressed realgar. *Physics and Chemistry of Minerals* **39**, 399-412 (2012)

E. V. Galuskin, F. Gfeller, V. B. Savelyeva, Th. Armbruster, B. Lazic, I. O. Galuskina, D. M. Többens, A. E. Zadov, P. Dzierzanowski, N. N. Pertsev, V. M. Gazeev: Pavlovskyite  $\text{Ca}_8(\text{SiO}_4)_2(\text{Si}_3\text{O}_{10})$  - a new mineral of altered silicate-carbonate xenoliths from the two Russian type localities: Birkhin massif, Baikal Lake area and Upper Chegem caldera, North Caucasus. *American Mineralogist* **97**, 503-512 (2012)

R. Kaindl, D. M. Többens, S. Penner, Th. Bielz, S. Soisuwan, B. Klötzer: Quantum mechanical calculations of the vibrational spectra of quartz and rutile-type  $\text{GeO}_2$ . *Physics and Chemistry of Minerals* **39** (1), 47-55 (2012)

D. M. Többens, V. Kahlenberg: Improved DFT calculation of Raman spectra of silicates. *Vibrational Spectroscopy* **56**, 265-272 (2011)

V. Kahlenberg, W. Wertl, D. M. Többens, H. Schottenberger: Structural Investigations and Thermal Behavior of  $(\text{EMIm})\text{Cr}(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$  [1-Ethyl-3-methylimidazolium Chromium (III) Dioxalate Dihydrate]. *Zeitschrift für Anorganische und Allgemeine Chemie* **637** (10), 1371-1377 (2011)

A. Lemmerer, J. Bernstein, U. J. Griesser, V. Kahlenberg, D. M. Többens, S. H. Lapidus, P. W. Stephens, C. Esterhuysen: A Tale of Two Polymorphic Pharmaceuticals: Pyrithyldione and Propyphenazone and their 1937 Co-crystal Patent. *Chemistry - A European Journal* **17**, 13455-13460 (2011)

R. Kaindl, D. M. Többens, U. Haefeker: Quantum-mechanical calculations of the Raman spectra of Mg- and Fe-cordierite. *American Mineralogist* **96**, 1568-1574 (2011)

St. C. Neumair, St. Vanicek, R. Kaindl, D. M. Többens, K. Wurst, H. Huppertz: High-pressure synthesis and crystal structure of the lithium borate HP-LiB<sub>3</sub>O<sub>5</sub>. *Journal of Solid State Chemistry* **184**, 2490–2497 (2011)

St. C. Neumair, St. Vanicek, R. Kaindl, D. Többens, Ch. Martineau, F. Taulelle, J. Senker, H. Huppertz: HP-KB<sub>3</sub>O<sub>5</sub> highlights the structural diversity of borates: corner-sharing BO<sub>3</sub>/BO<sub>4</sub> groups in combination with edge-sharing BO<sub>4</sub> tetrahedra. *European Journal of Inorganic Chemistry*, 4147-4152 (2011)

G. Laus, M. Hummel, D. M. Többens, Th. Gelbrich, V. Kahlenberg, K. Wurst, U. J. Griesser, H. Schottenberger: The 1:1 and 1:2 salts of 1,4-diazabicyclo[2.2.2]octane and bis(trifluoromethylsulfonyl)amine: thermal behaviour and polymorphism. *CrystEngComm* **13**, 5439-5446 (2011)

E. Arroyabe, R. Tessadri, D. M. Többens, V. Kahlenberg: Does K<sub>2</sub>CaSiO<sub>4</sub> exist? A phase-analytical study in the system K<sub>2</sub>O–CaO–SiO<sub>2</sub> with implications for the characterization of residual materials. *Journal of the American Ceramic Society* **94 (8)**, 2652-2655 (2011)

E. Arroyabe, F. Prechtel, D. M. Többens, R. Kaindl, V. Kahlenberg: K<sub>2</sub>Ca<sub>3</sub>Si<sub>3</sub>O<sub>10</sub>, a novel trisilicate: high-pressure synthesis, structural, spectroscopic and computational studies. *European Journal of Mineralogy* **23**, 425-435 (2011)

Th. Bielz, S. Soisuwan, R. Kaindl, R. Tessadri, D. M. Többens, B. Klötzer, S. Penner: A high-resolution diffraction and spectroscopic study of the low-temperature phase transformation of hexagonal to tetragonal GeO<sub>2</sub> with and without alkali hydroxide promotion. *The Journal of Physical Chemistry* **C115**, 9706-9712 (2011)

M. Bauer, D. M. Többens, E. Mayer, Th. Loerting: Pressure-amorphized cubic structure II clathrate hydrate: crystallization in slow motion. *Physical Chemistry Chemical Physics* **13**, 2167-2171 (2011)

R. Kaindl, D. M. Többens, V. Kahlenberg: DFT-aided interpretation of the Raman spectra of the polymorphic forms of Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>. *Journal of Raman Spectroscopy* **42**, 78-85 (2011)

V. Kahlenberg, D. Girtler, E. Arroyabe, R. Kaindl, D. M. Többens: Devitrite (Na<sub>2</sub>Ca<sub>3</sub>Si<sub>6</sub>O<sub>16</sub>) - structural, spectroscopic and computational investigations on a crystalline impurity phase in industrial soda-lime glasses. *Mineralogy and Petrology*, **100 (1-2)**, 1-9 (2010)

M. Bauer, K. Winkel, D. M. Toebbens, E. Mayer, Th. Loerting: Hexagonal ice transforms at high pressures and compression rates directly into “doubly metastable” ice phases. *The Journal of Chemical Physics* **131**, 224514 (1-8) (2009)

- E. Arroyabe, R. Kaindl, D.M. Töbrens, V. Kahlenberg: Synthesis, crystal structure, and vibrational spectroscopy of  $\text{K}_2\text{Ca}_4\text{Si}_8\text{O}_{21}$  - an unusual single layer silicate containing Q2 and Q3 units. *Inorganic Chemistry* **48** (24), 11929-11934 (2009)
- E. Arroyabe, R. Kaindl, D. M. Töbrens, V. Kahlenberg:  $\text{K}_2\text{Ca}_6\text{Si}_4\text{O}_{15}$  - structural and spectroscopical studies on a mixed tetrahedral–octahedral framework. *Journal of Solid State Chemistry* **182** (12), 3254-3261 (2009)
- B. Peplinski, A. N. Fitch, A. Evans, R. M. Ibberson, D. M. Töbrens, L. M. D. Cranswick, I. Dörfel, F. Emmerling, R. Matschat: Structural characterization of a coarse-grained transparent silicon carbide powder by a combination of powder diffraction techniques. *Zeitschrift für Kristallographie Supplement* **30** (Proceedings of EPDIC 11), 61-66 (2009)
- D. M. Töbrens, V. Kahlenberg, R. Kaindl, B. Sartory, J. Konzett:  $\text{Na}_{8.25}\text{Y}_{1.25}\text{Si}_6\text{O}_{18}$  and its family of *zwölfer* ring silicates. *Zeitschrift für Kristallographie* **223** (6), 389-398 (2008)
- D. M. Töbrens, M. Hummel, R. Kaindl, H. Schottenberger, V. Kahlenberg: Novel linear acetylpentanedionato complexes for metal-organic framework construction. *CrystEngComm* **10**, 327-334 (2008)
- D. Braun, D. Töbrens, V. Kahlenberg, J. Ludescher, U. Griesser: Structural and thermodynamic features of crystal polymorphs of R-cinacalcet hydrochloride. *Crystal Growth & Design* **8** (11), 4109-4119 (2008)
- H. Gamari-Seale, I. O. Troyanchuk, A. P. Sazonov, K. L. Stefanopoulos, D. M. Töbrens: Structure and magnetic order in  $\text{La}_{0.7}\text{Ca}_{0.3}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_3$  and  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_3$  perovskites. *Physica B: Physics of Condensed Matter* **403** (17), 2924-2929 (2008)
- D. Gournis, A. Lappas, M. A. Karakassides, D. Töbrens, A. Moukarika: A neutron diffraction study of alkali cation migration in montmorillonites. *Physics and Chemistry of Minerals* **35**, 49-58 (2008)
- V. Kahlenberg, R. Tessadri, D. M. Töbrens, W. Wertl, A. Rössler:  $\text{Mg}[\text{ZnPO}_4(\text{H}_2\text{O})]_2 \cdot 10\text{H}_2\text{O}$  - a layered hydrous zinc phosphate retrieved from an industrial filter cake residual. *Zeitschrift für anorganische und allgemeine Chemie* **634**, 1181-1186 (2008)
- V. Kahlenberg, W. Wertl, D. M. Töbrens, R. Kaindl, P. Schuster, H. Schottenberger: Rietveld analysis and Raman spectroscopic investigations on  $\alpha\text{-Y}_2\text{Si}_2\text{O}_7$ . *Zeitschrift für anorganische und allgemeine Chemie* **634**, 1166-1172 (2008)
- D. M. Töbrens, V. Kahlenberg, Ch. Gspan, G. Kothleitner: Atomic and domain structure of the low temperature phase of barium metagermanate ( $\text{BaGeO}_3$ ). *Acta Crystallographica B* **62**, 1002-1009 (2006)

- D. M. Többens: Calculating the peak shape of axially focusing powder diffractometers. *Zeitschrift für Kristallographie Supplement* **23** (Proceedings of EPDIC 9), 255-260 (2006)
- D. M. Többens, R. Kaindl, V. Kahlenberg, H. Schottenberger, M. Hummel: The homoleptic square-antiprismatic chelate tetrakis (3-acetyl-2,4-pentanedionato)zirconium (IV): A promising coordination motif for tetrahedral metal-organic frameworks. *Crystal Growth & Design* **6** (2), 1720-1725 (2006)
- B. Peplinski, D. M. Toebbens, W. Kockelmann, R. Ibberson: Estimates of the uncertainty of lattice parameters refined from neutron powder diffraction data. *Zeitschrift für Kristallographie Supplement* **23** (Proceedings of EPDIC 9), 21-26 (2006)
- I. V. Golosovsky, I. Mirebeau, G. André, M. Tovar, D. M. Többens, D. A. Kurdyukov, Yu. A. Kumzerov: Magnetic phase transition in a nanostructured antiferromagnet CoO embedded in porous glass. *Physics of the Solid State* **48** (11), 2130-2133 (2006), translation of *Fizika Tverdogo Tela* **48** (11), 2010-2013 (2006)
- V. Kahlenberg, R. Kaindl, D. M. Többens: Synthesis, Rietveld analysis and solid state Raman spectroscopy of  $K_4SrSi_3O_9$ . *Zeitschrift für anorganische und allgemeine Chemie* **632**, 2037-2042 (2006)
- M. M. Guenter, M. Lerch, H. Boysen, D. Toebbens, E. Suard, C. Baetz: Combined neutron and synchrotron X-ray diffraction study of Sr/Mg-doped lanthanum gallates up to high temperatures. *Journal of Physics and Chemistry of Solids* **67** (8), 1754-1768 (2006)
- J. Khalil-Allafi, W. W. Schmahl, D. M. Toebbens: Space group and crystal structure of the R-phase in binary NiTi shape memory alloys. *Acta Materialia* **54** (12), 3171-3175 (2006)
- V. Kahlenberg, R. Kaindl, D. M. Többens: The crystal structure of the interrupted framework silicate  $K_{9.6}Ca_{1.2}Si_{12}O_{30}$  determined from laboratory X-ray diffraction data. *Journal of Solid State Chemistry* **179**, 1948-1956 (2006)
- R. Gilles, D. Mukherji, M. Hoelzel, P. Strunz, D. M. Toebbens, B. Barbier: Neutron and X-ray diffraction measurements on micro- and nano-sized precipitates embedded in a Ni-based superalloy and after their extraction from the alloy. *Acta Materialia* **54** (5), 1307-1316 (2006)
- G. Laus, V. Kahlenberg, D. M. Többens, R. K. R. Jetti, U. J. Griesser, J. Schütz, E. Kristeva, K. Wurst, H. Schottenberger: Lattice architecture and hydrogen-bonding networks of N-aminoazolium and N,N'-diaminoazolium chlorides. *Crystal Growth & Design* **6** (2), 404-410 (2006)
- M. Hoelzel, D. Del Genovese, R. Gilles, D. Mukherji, D. M. Toebbens, J. Roesler, H. Fuess: Phase analysis and lattice mismatches in superalloys DT706 and Inconel 706. *Physica B: Physics of Condensed Matter* **385**, 594-596 (2006)

- D. M. Többens, V. Kahlenberg, R. Kaindl: Characterization and ab-initio XRPD structure determination of a novel silicate with *vierer* single chains: The crystal structure of NaYSi<sub>2</sub>O<sub>6</sub>. *Inorganic Chemistry* **44**, 9554-9560 (2005)
- A. Krimmel, Z. Seidov, G. G. Guseinov, A. I. Najafov, H.-A. Krug von Nidda, A. Loidl, D. M. Többens: Crystal structure and magnetic properties of the spinel compound Fe<sub>0.76</sub>In<sub>2.17</sub>S<sub>4</sub>. *Journal of Physics: Condensed Matter* **17**, 3611-3618 (2005)
- R. Chemnitzer, G. Auffermann, D. M. Többens, R. Kniep: (Sr<sub>2</sub>N)H: On the redox-intercalation of hydrogen into Sr<sub>2</sub>N. *Zeitschrift für Anorganische und Allgemeine Chemie* **631**, 1813-1817 (2005)
- I. Mastoraki, A. Lappas, J. Giapintzakis, D. Többens, J. Hernández-Velasco: Relations of crystal structure to magnetic properties in the quasi-one-dimensional compound PbNi<sub>1.88</sub>Mg<sub>0.12</sub>V<sub>2</sub>O<sub>8</sub>. *Journal of Solid State Chemistry* **177**, 2404-2414 (2004)
- Th. Lonkai, D. G. Tomuta, U. Amann, J. Ihringer, R. W. A. Hendrikx, D. M. Többens, J. A. Mydosh: Development of the high temperature phase of hexagonal manganites. *Physical Review B* **69**, 134108 1-10 (2004)
- J. Khalil-Allafi, W. W. Schmahl, M. Wagner, H. Sitepu, D. M. Többens, G. Eggeler: The influence of temperature on lattice parameters of coexisting phases in NiTi shape memory alloys – a neutron diffraction study. *Materials Science and Engineering A* **378**, 161-164 (2004)
- O. Pritula, L. Smrcök, D. M. Többens, V. Langer: X-ray and neutron Rietveld quantitative phase analysis of industrial Portland cement clinkers. *Powder Diffraction* **19-3**, 232-239 (2004)
- K. Zagorodniy, V. Shivanyuk, D. Toebbens, S. Danilkin, V. Gavriljuk: Hydrogen-caused phase transformations, relaxation and hysteretic phenomena in fcc alloys Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> and Fe<sub>50</sub>Ni<sub>50</sub>. *Scripta Materialia* **50**, 12, 1467-1470 (2004)
- V. V. Efimov, S. S. Khasanov, B. N. Mavrin, N. N. Novikova, A. V. Shilnikov, A. I. Burkhanov, V. V. Sikolenko, A. Sternberg, S. I. Tiutiunnikov, D. M. Többens, V. A. Yakovlev: Structure and lattice dynamics in PLZT 8/65/35 ceramics irradiated by high-current pulsed electron beam. *Ferroelectrics* **302**, [573]/327-[579]/333 (2004)
- V. V. Sikolenko, A. P. Sazonov, I. O. Troyanchuk, D. Többens, U. Zimmermann, E. V. Pomjakushina, H. Szymczak: Magnetic properties of La<sub>1-x</sub>Sr<sub>x</sub>CoO<sub>3</sub> ( $x = 0.15$  and  $0.3$ ). *Journal of Physics: Condensed Matter* **16-41**, 7313-7320 (2004)
- M. Hoelzel, S. Danilkin, H. Ehrenberg, D. M. Toebbens, T. Udovic, H. Fuess, H. Wipf: Effects of high-pressure hydrogen charging on the structure of austenitic stainless steels. *Materials Science and Engineering A* **384**, 255-261 (2004)

- P. Sittner, D. Neov, P. Lukas, D. M. Toebbens: Neutron diffraction studies of the stress effect on texture transformations in NiTi shape memory alloys. *Journal of Neutron Research* **12**, 1-3, 15-20 (2004)
- O. Troyanchuk, A. P. Sazonov, H. Szymczak, D. M. Többens, H. Gamari-Seale: Phase Separation in  $\text{La}_{2-x}\text{A}_x\text{CoMnO}_6$  (A = Ca and Sr) perovskites. *Journal of Experimental and Theoretical Physics* (translation of *Žurnal èksperimental'noj i teoretičeskoj fiziki*) **99** (2), 363-369 (2004)
- P. Šittner, V. Novák, P. Lukáš, D. Neov, D. M. Toebbens: In-situ neutron diffraction studies of martensitic transformations in NiTi. *Journal de Physique IV* **112**, 2, 709-712 (2003)
- H. Sitepu, W. W. Schmahl, G. Eggeler, J. Khalil Allafi, D. M. Többens: A neutron diffraction study of the martensitic transformations in aged Ni-rich NiTi alloys. *Journal de Physique IV* **112**, 643-646 (2003)
- D. M. Többens, M. Tovar: Peak shape at the axially focusing E9 powder diffractometer - theoretical and experimental description. *Applied Physics A. Material Science & Processing A* **74**, 136-138 (2002)
- D. M. Toebbens: Asymmetry from axially focusing monochromators. *Acta Crystallographica A* **58** [Supplement], C356 (2002)
- H. Sitepu, W. W. Schmahl, J. K. Allafi, G. Eggeler, A. Dlouhy, D. M. Toebbens, M. Tovar: Neutron diffraction phase analysis during thermal cycling of a Ni-rich NiTi shape memory alloy using the Rietveld method. *Scripta Materialia* **46**, 543-548 (2002)
- H. Sitepu, W. W. Schmahl, J. Khalil Allafi, G. Eggeler, T. Reinecke, H. G. Brokmeier, M. Tovar, D. M. Többens: Texture and quantitative phase analysis of aged Ni-rich NiTi using x-ray and neutron diffractions. *Material Science Forum* **394-395**, 237-240 (2002)
- J. Baszyński, T. Toliński, B. Idzikowski, D. M. Többens, A. Hoser: Structural effects of grinding on  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  ceramic studied by neutron diffraction. *Journal of Alloys and Compounds* **345**, 210-213 (2002)
- H. Boysen, M. Lerch, R. Gilles, B. Krimmer, D. M. Többens: Structure and ionic conductivity in doped  $\text{LaGaO}_3$ . *Applied Physics A. Material Science & Processing A* **74**, 966-968 (2002)
- G. Brunauer, F. Frey, H. Boysen, H. Schneider, P. Fischer, Th. Hansen, D. Többens, H. Ehrenberg: Neutron diffraction study up to  $1600^\circ$  of 3:2 mullite. *Applied Physics A. Material Science & Processing A* **74**, 986-988 (2002)
- R. Gilles, D. Mukherji, D. M. Többens, P. Strunz, B. Barbier, J. Rösler, H. Fuess: Neutron-, X-ray- and electron diffraction measurements for the determination of  $\gamma/\gamma'$  lattice misfit in Ni-base superalloys. *Applied Physics A. Material Science & Processing A* **74**, 1446-1448 (2002)

- M. Pissas, G. Kallias, M. Hofmann, D. M. Többens: Crystal and magnetic structure of the  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  compound ( $x=0.8, 0.85$ ). *Physical Review B* **65**, 064413 1-9 (2002)
- D. Sangaa, A. Balagurov, G. Batdemberel, D. Chultem, H. Fuess, D. Toebbens: X-ray and neutron diffraction studies of the dinosaur and modern animal bones from the Gobi desert, Mongolia. *Acta Crystallographica A* **58** [Supplement], C356 (2002)
- D. M. Többens, W. Depmeier: The intermediate phase of strontium chromate aluminate sodalite. *Zeitschrift für Kristallographie* **216**, 611-615 (2001)
- D. M. Többens, W. Depmeier: Superstructure of strontium chromate aluminate sodalite at low temperatures. *Zeitschrift für Kristallographie* **216**, 506-590 (2001)
- D. M. Többens, N. Stüßer: E9: The new high-resolution neutron powder diffractometer at BENSCH. *Neutron News* **12.3**, 28-32 (2001)
- D. M. Többens, N. Stüßer, K. Knorr, H. M. Mayer, G. Lampert: E9: The new high-resolution neutron powder diffractometer at the Berlin Neutron Scattering Center. *Materials Science Forum* **378-381**, 288-293 (2001)
- I. Maksimov, D. Baabe, H. H. Klauss, F. J. Litterst, R. Feyerherm, D. M. Többens, A. Matsushita, S. Süllow: Structure and magnetic order in  $\text{Fe}_{2+x}\text{V}_{1-x}\text{Al}$ . *Journal of Physics: Condensed Matter* **13**, 5487-5501 (2001)
- S. Baran, M. Hofmann, G. Lampert, N. Stüsser, A. Szytula, D. Többens, P. Smeibidl, K. Kausche: Neutron diffraction studies of the magnetic structures of  $\text{HoAuGe}$  and  $\text{ErAuGe}$ . *Journal of magnetism and magnetic materials* **236**, 293-301 (2001)
- D. M. Többens, W. Depmeier: Intermediate phases in the Ca-rich part of the system  $(\text{Ca}_{1-x}\text{Sr}_x)_8[\text{Al}_{12}\text{O}_{24}](\text{WO}_4)_2$ . *Zeitschrift für Kristallographie* **213**, 522-531 (1998)
- D. M. Többens: Untersuchungen zu Struktur und Phasenumwandlungen von Kristallen der Aluminatsodalithgruppe. *Dissertation, Universität Kiel* (1998)
- D. Többens: Al-Si-Ordnung in Na-Nephelinen der Zusammensetzung  $\text{Na}_{8-a}\text{Al}_{8-a}\text{Si}_{8+a}\text{O}_{32}$  mit  $a=0$  bis  $a=2$ . *Diplomarbeit, Universität Münster* (1994)