

# Thomas Malcherek

## List of Publications by Year in descending order

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68

papers

1,118

citations

394421

19

h-index

434195

31

g-index

78

all docs

78

docs citations

78

times ranked

1243

citing authors

#	ARTICLE	IF	CITATIONS
1	Fehrite, $MgCu_4(SO_4)_2(OH)_6 \cdot 6H_2O$ , the magnesium analogue of ktenasite from the Casualidad mine near Baños de Alhamilla, Almeria, Spain. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2021, 197, 1-10.	0.3	3
2	Perrierite-(Ce) from the Laacher See tephra, Eifel, Germany, and the modular character of the chevkinitie group of minerals. <i>Physics and Chemistry of Minerals</i> , 2021, 48, 1.	0.8	1
3	Nondestructive determination of the amphibole crystalchemical formulae by Raman spectroscopy: One step closer. <i>Journal of Raman Spectroscopy</i> , 2020, 51, 1530-1548.	2.5	20
4	The modulated low-temperature structure of malayaite, $CaSnOSiO_4$ . <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 316-321.	1.1	1
5	The atacamite family of minerals – a testbed for quantum spin liquids. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 519-526.	1.1	13
6	Radiation-damaged zircon under high pressures. <i>Physics and Chemistry of Minerals</i> , 2018, 45, 981-993.	0.8	20
7	Phase transitions of titanite $CaTiSiO_5$ from density functional perturbation theory. <i>Physical Review Materials</i> , 2018, 2, .	2.4	24
8	Vondechenite, a new hydrous calcium copper chloride hydroxide, from the Bellerberg, East-Eifel volcanic area, Germany. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2018, 195, 79-86.	0.3	3
9	Structural and compositional variations of basic Cu(II) chlorides in the herbertsmithite and gillardite structure field. <i>Mineralogical Magazine</i> , 2017, 81, 123-134.	1.4	3
10	Composition–thermal expandability relations and oxidation processes in tourmaline studied by in situ Raman spectroscopy. <i>Physics and Chemistry of Minerals</i> , 2017, 44, 735-748.	0.8	9
11	Erazoite, a new copper tin sulfide from the El Guanaco gold deposit, Antofagasta Province, Chile. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2017, 194, 91-96.	0.3	0
12	Structural phase transitions of clinoatacamite and the dynamic Jahn–Teller effect. <i>Physics and Chemistry of Minerals</i> , 2017, 44, 307-321.	0.8	13
13	Exploring the potential of Raman spectroscopy for crystallochemical analyses of complex hydrous silicates: II. Tourmalines. <i>American Mineralogist</i> , 2016, 101, 970-985.	1.9	61
14	Influence of the octahedral cationic-site occupancies on the framework vibrations of Li-free tourmalines, with implications for estimating temperature and oxygen fugacity in host rocks. <i>American Mineralogist</i> , 2016, 101, 2554-2563.	1.9	19
15	Vanackerite, a new lead cadmium arsenate of the apatite supergroup from Tsumeb, Namibia. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2016, 193, .	0.3	4
16	Crystal structure of Cr-bearing $Mg_3BeAl_8O_{16}$ , a new polytype of magnesiotaaffeite-2N <sup>22S</sup> . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016, 72, 1060-1063.	0.5	2
17	Crystal structures of new potassium silicates and aluminosilicates of Sm, Tb, Gd, and Yb and their relation to the armstrongite ( $CaZr(Si_6O_{15}) \cdot 3H_2O$ ) structure. <i>Journal of Solid State Chemistry</i> , 2015, 227, 196-203.	2.9	7
18	Cayalsite-(Y), a new rare-earth calcium aluminium fluorosilicate with OD character. <i>European Journal of Mineralogy</i> , 2015, 27, 683-694.	1.3	0

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19	Polarization Dependent High Energy Resolution X-ray Absorption Study of Dicesium Uranyl Tetrachloride. <i>Inorganic Chemistry</i> , 2015, 54, 174-182.	4.0	41
20	A temperature-induced reversible transformation between paratacamite and herbertsmithite. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 33-48.	0.8	22
21	TEMPERATURE-INDUCED $P_{21}C_{13}TO_2C_2C_1$ PHASE TRANSITION IN PARTIALLY AMORPHOUS (METAMICT) TITANITE REVEALED BY RAMAN SPECTROSCOPY. <i>Canadian Mineralogist</i> , 2014, 52, 587-587.	1.0	0
22	Highly Distorted Uranyl Ion Coordination and One/Two-Dimensional Structural Relationship in the $Ba_2[UO_2(TO_4)_2]$ ( $T = P, As$ ) System: An Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2014, 53, 7650-7660.	4.0	18
23	Galloplumbogummite from Tsumeb, Namibia, a new member of the alunite group with tetravalent charge balance. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2014, 191, 301-309.	0.3	3
24	The keyite crystal structure, revisited. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2013, 228, .	0.8	4
25	The new mineral erikapohlite, $Cu_3(Zn,Cu,Mg)4Ca_2(AsO_4)_6 \cdot 2H_2O$ , the Ca-dominant analogue of keyite, from Tsumeb, Namibia. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2013, 190, 319-325.	0.3	5
26	The crystal structure of creaseyite: a disordered, nanoporous lead iron copper aluminosilicate. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2013, 228, 134-139.	0.8	0
27	High Structural Complexity of Potassium Uranyl Borates Derived from High-Temperature/High-Pressure Reactions. <i>Inorganic Chemistry</i> , 2013, 52, 5110-5118.	4.0	32
28	$K[AsW_2O_9]$ , the first member of the arsenate-tungsten bronze family: Synthesis, structure, spectroscopic and non-linear optical properties. <i>Journal of Solid State Chemistry</i> , 2013, 204, 59-63.	2.9	41
29	Novel Fundamental Building Blocks and Site Dependent Isomorphism in the First Actinide Borophosphates. <i>Inorganic Chemistry</i> , 2013, 52, 7881-7888.	4.0	10
30	Atelisite-(Y), a new rare earth defect silicate of the KDP structure type. <i>European Journal of Mineralogy</i> , 2012, 24, 1053-1060.	1.3	4
31	Rich Coordination of $Nd^{3+}$ in $Mg_{2Nd_{13}}(BO_3)_8(SiO_4)_4(OH)_4$ Derived from High-Pressure/High-Temperature Conditions. <i>Inorganic Chemistry</i> , 2012, 51, 3941-3943.		
32	Complex clover cross-sectioned nanotubules exist in the structure of the first uranium borate phosphate. <i>Chemical Communications</i> , 2012, 48, 3479.	4.1	25
33	Structural anisotropy and annealing-induced nanoscale atomic rearrangements in metamict titanite. <i>American Mineralogist</i> , 2012, 97, 1354-1365.	1.9	17
34	Synthesis of Uranium Materials under Extreme Conditions: $UO_2[B_3Al_4O_11(OH)]$ , a Complex 3D Aluminoborate. <i>Chemistry - A European Journal</i> , 2012, 18, 4166-4169.	3.3	15
35	Micro-Raman study of copper hydroxychlorides and other corrosion products of bronze samples mimicking archaeological coins. <i>Analytical and Bioanalytical Chemistry</i> , 2012, 402, 1451-1457.	3.7	52
36	Anatacamite from La Vendida mine, Sierra Gorda, Atacama desert, Chile: a triclinic polymorph of $Cu_2(OH)_3Cl$ . <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2010, 187, 307-312.	0.3	8

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37	The crystal structure of Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> : symmetry mode analysis of the ferroelectric phase. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 205401.	1.8	18
38	Chemical mixing and Raman hard-mode spectroscopy in ferroelastic lead phosphate-arsenate: local symmetry splitting and multiscaling behaviour. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s275-s275.	0.3	0
39	Y <sub>4</sub> H <sub>8</sub> Si <sub>3</sub> O <sub>16</sub> : a naturally occurring defect silicate of the KDP structure type. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s187-s187.	0.3	0
40	The new mineral stetindite, CeSiO <sub>4</sub> , a cerium end-member of the zircon group. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2009, 186, 195-200.	0.3	18
41	First Mixed Alkaline Uranyl Molybdates: Synthesis and Crystal Structures of CsNa <sub>3</sub> [(UO <sub>2</sub> ) <sub>4</sub> O <sub>4</sub> (Mo <sub>2</sub> O <sub>8</sub> )] and Cs <sub>2</sub> Na <sub>8</sub> [(UO <sub>2</sub> ) <sub>8</sub> O <sub>8</sub> (Mo <sub>5</sub> O <sub>20</sub> )]. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009, 635, 1231-1235.	1.2	9
42	Structures of the pseudo-trigonal polymorphs of Cu <sub>2</sub> (OH) <sub>3</sub> Cl. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 334-341.	1.8	29
43	RASTGUI- a free software package for reciprocal space mapping. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s236-s237.	0.3	0
44	Ferroelectric ordering of Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> . <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s204-s205.	0.3	0
45	Crystal chemistry of anhydrous Li uranyl phosphates and arsenates. I. Polymorphism and structure topology: Synthesis and crystal structures of $\hat{1}\pm$ -Li <sub>2</sub> [(UO <sub>2</sub> )(PO <sub>4</sub> )], $\hat{1}\pm$ -Li <sub>2</sub> [(UO <sub>2</sub> )(AsO <sub>4</sub> )], $\hat{1}^2$ -Li <sub>2</sub> [(UO <sub>2</sub> )(AsO <sub>4</sub> )] and Li <sub>2</sub> [(UO <sub>2</sub> ) <sub>3</sub> (P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> ]. <i>Journal of Solid State Chemistry</i> , 2008, 181, 3010-3015.	2.9	20
46	Structure and stability of Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> and Cd <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> explored by ab initio calculations. <i>Physical Review B</i> , 2008, 78, .	3.2	43
47	Sanromanite, Na <sub>2</sub> CaPb <sub>3</sub> (CO <sub>3</sub> ) <sub>5</sub> , from the Santa Rosa mine, Atacama desert, Chile, a new mineral of the burbankite group. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2007, 183, 117-121.	0.3	0
48	The crystal structure of Li <sub>4</sub> [(UO <sub>2</sub> ) <sub>2</sub> (W <sub>2</sub> O <sub>10</sub> )] and crystal chemistry of Li uranyl tungstates. <i>Zeitschrift Fur Kristallographie</i> , 2007, 222, 391-395.	1.1	12
49	Haydeeite, Cu <sub>3</sub> Mg(OH)6Cl <sub>2</sub> , a new mineral from the Haydee mine, Salar Grande, Atacama desert, Chile. <i>Neues Jahrbuch Fur Mineralogie, Abhandlungen</i> , 2007, 184, 39-43.	0.3	10
50	One-Dimensional Array of Two- and Three-Center Cation- $\cdots$ Cation Bonds in the Structure of Li <sub>4</sub> [(UO <sub>2</sub> ) <sub>10</sub> O <sub>10</sub> (Mo <sub>2</sub> O <sub>8</sub> )]. <i>Inorganic Chemistry</i> , 2007, 46, 8442-8444.	4.0	58
51	Cu <sub>3</sub> MgCl <sub>2</sub> (OH) <sub>6</sub> and the bond-valence parameters of the OH $\cdots$ Cl bond. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 157-160.	1.8	27
52	A structural phase transition in NaTaOGeO <sub>4</sub> and its relation to phase transitions in titanite. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 545-550.	1.8	6
53	Tuning of Inter- versus Intrachain Magnetic Interactions in Cyano-Bridged Ni <sup>II</sup> /M <sup>III</sup> (M = Cr, Fe, Co) Chain Complexes. <i>Inorganic Chemistry</i> , 2006, 45, 7722-7735.	4.0	32
54	Encapsulation of Cyanometalates by a Tris-macroyclic Ligand Tricopper(II) Complex: Syntheses, Structural Variation, and Magnetic Exchange Coupling Pathways. <i>Chemistry - A European Journal</i> , 2006, 12, 737-748.	3.3	30

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55	The structure of SrTiOGGeO <sub>4</sub> and its solid solution with CaTiOGGeO <sub>4</sub> . Physics and Chemistry of Minerals, 2005, 32, 531-545.	0.8	4
56	Temperature and composition dependence of structural phase transitions in Ca(TixZr1-x)OGeO <sub>4</sub> . American Mineralogist, 2005, 90, 687-694.	1.9	11
57	A high-temperature diffraction study of the solid solution CaTiOSiO <sub>4</sub> -CaTiOGGeO <sub>4</sub> . American Mineralogist, 2005, 90, 1325-1334.	1.9	8
58	CaZrGeO <sub>5</sub> and the triclinic instability of the titanite structure type. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	4
59	Structure and phase transitions of CaTaOAlO <sub>4</sub> . Journal of Applied Crystallography, 2004, 37, 117-122.	4.5	4
60	Isomorphy of structural phase transitions in LiTaOSiO <sub>4</sub> , LiTaOGGeO <sub>4</sub> and titanite, CaTiOSiO <sub>4</sub> . Journal of Solid State Chemistry, 2004, 177, 3254-3262.	2.9	9
61	Metamictization and recrystallization of titanite: An infrared spectroscopic study. American Mineralogist, 2002, 87, 882-890.	1.9	28
62	"Early partial melting" in annealed natural cordierites. European Journal of Mineralogy, 2002, 14, 879-890.	1.3	3
63	Structure and phase transitions of LiTaOGGeO <sub>4</sub> . Acta Crystallographica Section B: Structural Science, 2002, 58, 607-612.	1.8	9
64	Structural properties of ferromagnesian cordierites. American Mineralogist, 2001, 86, 66-79.	1.9	38
65	Strain modulation around inclusions in an annealed natural cordierite. European Journal of Mineralogy, 2001, 13, 921-928.	1.3	2
66	Diffuse scattering anisotropy and the P21/aâ†"A2/aphase transition in titanite, CaTiOSiO <sub>4</sub> . Journal of Applied Crystallography, 2001, 34, 108-113.	4.5	43
67	Localized defects in radiation-damaged zircon. Acta Crystallographica Section B: Structural Science, 2000, 56, 947-952.	1.8	53
68	Autocorrelation analysis of infrared spectra from minerals. European Journal of Mineralogy, 2000, 12, 503-519.	1.3	102