

Peter Kroll

List of Publications by Year in descending order

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142
papers

5,902
citations

94269

37
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76769

74
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157
all docs

157
docs citations

157
times ranked

6400
citing authors

#	ARTICLE	IF	CITATIONS
1	Melem (2,5,8-Triamino-tri-s-triazine), an Important Intermediate during Condensation of Melamine Rings to Graphitic Carbon Nitride: Synthesis, Structure Determination by X-ray Powder Diffractometry, Solid-State NMR, and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2003, 125, 10288-10300.	6.6	954
2	Tri-s-triazine derivatives. Part I. From trichloro-tri-s-triazine to graphitic C ₃ N ₄ structures Part II: Alkalicymelurates M ₃ [C ₆ N ₇ O ₃], M = Li, Na, K, Rb, Cs, manuscript in preparation.. <i>New Journal of Chemistry</i> , 2002, 26, 508-512.	1.4	614
3	Synthesis of cubic silicon nitride. <i>Nature</i> , 1999, 400, 340-342.	13.7	613
4	High-pressure chemistry of nitride-based materials. <i>Chemical Society Reviews</i> , 2006, 35, 987.	18.7	200
5	Hafnium Nitride with Thorium Phosphide Structure: Physical Properties and an Assessment of the Hf-N, Zr-N, and Ti-N Phase Diagrams at High Pressures and Temperatures. <i>Physical Review Letters</i> , 2003, 90, 125501.	2.9	167
6	Inorganic Solid-State Chemistry with Main Group Element Carbodiimides. <i>Chemistry of Materials</i> , 1998, 10, 2964-2979.	3.2	134
7	Vacuum Ultraviolet Detector for Gas Chromatography. <i>Analytical Chemistry</i> , 2014, 86, 8329-8335.	3.2	125
8	Corrugated layered heptazine-based carbon nitride: the lowest energy modifications of C ₃ N ₄ ground state. <i>Journal of Materials Chemistry</i> , 2009, 19, 3013.	6.7	122
9	Monomeric Copper(I), Silver(I), and Gold(I) Alkyne Complexes and the Coinage Metal Family Group Trends. <i>Journal of the American Chemical Society</i> , 2009, 131, 11249-11255.	6.6	117
10	Nitrogen-rich transition metal nitrides. <i>Coordination Chemistry Reviews</i> , 2013, 257, 2063-2072.	9.5	114
11	Magnetism in graphene due to single-atom defects: dependence on the concentration and packing geometry of defects. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 196002.	0.7	96
12	Prediction of Novel Phases of Tantalum(V) Nitride and Tungsten(VI) Nitride That Can Be Synthesized under High Pressure and High Temperature. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 4249-4254.	7.2	83
13	High-Pressure Synthesis of Crystalline Carbon Nitride Imide, C ₂ N ₂ (NH). <i>Angewandte Chemie - International Edition</i> , 2007, 46, 1476-1480.	7.2	82
14	Polymer-Derived Ultra-High Temperature Ceramics (UHTCs) and Related Materials. <i>Advanced Engineering Materials</i> , 2019, 21, 1900269.	1.6	80
15	Metastability of Corundum-Type In ₂ O ₃ . <i>Chemistry - A European Journal</i> , 2008, 14, 3306-3310.	1.7	77
16	First-Principles Nuclear Magnetic Resonance Structural Analysis of Vitreous Silica. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7917-7929.	1.5	76
17	Structural, electronic, and magnetic properties of 13-, 55-, and 147-atom clusters of Fe, Co, and Ni: A spin-polarized density functional study. <i>Physical Review B</i> , 2008, 78, .	1.1	70
18	Resolution of isomeric new designer stimulants using gas chromatography – Vacuum ultraviolet spectroscopy and theoretical computations. <i>Analytica Chimica Acta</i> , 2017, 971, 55-67.	2.6	67

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19	Pathways to metastable nitride structures. <i>Journal of Solid State Chemistry</i> , 2003, 176, 530-537.	1.4	65
20	Synthesis, Structure Determination, and Quantum-Chemical Characterization of an Alternate HgNCN Polymorph. <i>Inorganic Chemistry</i> , 2002, 41, 4259-4265.	1.9	62
21	Self-Assembled Peptide Nanofibers Display Natural Antimicrobial Peptides to Selectively Kill Bacteria without Compromising Cytocompatibility. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 28681-28689.	4.0	59
22	Influence of SiO ₂ matrix on electronic and optical properties of Si nanocrystals. <i>Nanotechnology</i> , 2009, 20, 135702.	1.3	58
23	Gold(I) Chloride Coordinated 3-Hexyne. <i>Inorganic Chemistry</i> , 2009, 48, 423-425.	1.9	57
24	First principles study of C ₃ N ₄ carbon nitride nanotubes. <i>Journal of Materials Chemistry</i> , 2009, 19, 3020.	6.7	57
25	Formation of spinel-type gallium oxynitrides: a density-functional study of binary and ternary phases in the system Ga–O–N. <i>Journal of Materials Chemistry</i> , 2005, 15, 3296.	6.7	56
26	Analysis and deconvolution of dimethylnaphthalene isomers using gas chromatography vacuum ultraviolet spectroscopy and theoretical computations. <i>Analytica Chimica Acta</i> , 2016, 945, 1-8.	2.6	56
27	Isolable, gold carbonyl complexes supported by N-heterocyclic carbenes. <i>Chemical Communications</i> , 2011, 47, 4478.	2.2	53
28	Searching insight into the atomistic structure of SiCO ceramics. <i>Journal of Materials Chemistry</i> , 2010, 20, 10528.	6.7	52
29	Modelling and simulation of amorphous silicon oxycarbide. <i>Journal of Materials Chemistry</i> , 2003, 13, 1657.	6.7	50
30	Theoretical Tracing of a Novel Route from Molecular Precursors through Polymers to Dense, Hard C ₃ N ₄ Solids. <i>Journal of the American Chemical Society</i> , 1999, 121, 4696-4703.	6.6	49
31	A Density Functional Study of Phosphorus Nitride P ₃ N ₅ : Refined Geometries, Properties, and Relative Stability of \bar{I} -P ₃ N ₅ and \bar{I}^3 -P ₃ N ₅ and a Further Possible High-Pressure Phase \bar{I} -P ₃ N ₅ with Kyanite-Type Structure. <i>Chemistry - A European Journal</i> , 2002, 8, 3530.	1.7	48
32	Theoretical Investigation of the Solid State Reaction of Silicon Nitride and Silicon Dioxide forming Silicon Oxynitride (Si ₂ N ₂ O) under Pressure. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2003, 629, 1737-1750.	0.6	48
33	Hard silicon carbonitride films obtained by RF-plasma-enhanced chemical vapour deposition using the single-source precursor bis(trimethylsilyl)carbodiimide. <i>Journal of the European Ceramic Society</i> , 2006, 26, 1325-1335.	2.8	48
34	Modelling polymer-derived ceramics. <i>Journal of the European Ceramic Society</i> , 2005, 25, 163-174.	2.8	43
35	Assessment of the Hf–N, Zr–N and Ti–N phase diagrams at high pressures and temperatures: balancing between MN and M ₃ N ₄ (M = Hf, Zr, Ti). <i>Journal of Physics Condensed Matter</i> , 2004, 16, S1235-S1244.	0.7	42
36	SrSi ₆ N ₈ -A Reduced Nitridosilicate with a Si–Si Bond. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 567-570.	7.2	42

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37	Orthorhombic In_2O_3 : A Metastable Polymorph of Indium Sesquioxide. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6531-6535.	7.2	42
38	Silylated carbodiimides in molecular and extended structures. <i>Physical Review B</i> , 1999, 60, 3126-3139.	1.1	38
39	Modeling the sp^2 -free carbon phase in amorphous silicon oxycarbide. <i>Journal of Non-Crystalline Solids</i> , 2005, 351, 1121-1126.	1.5	35
40	$\text{HPaCa}_2\text{Si}_5\text{N}_8$ "A New High-Pressure Nitridosilicate: Synthesis, Structure, Luminescence, and DFT Calculations. <i>Chemistry - A European Journal</i> , 2008, 14, 7892-7902.	1.7	35
41	Structure and reactivity of amorphous silicon nitride investigated with density-functional methods. <i>Journal of Non-Crystalline Solids</i> , 2001, 293-295, 238-243.	1.5	33
42	High-pressure high-temperature synthesis of Rh_2O_3 type In_2O_3 polymorph. <i>Physica Status Solidi - Rapid Research Letters</i> , 2008, 2, 269-271.	1.2	32
43	Band alignment at a nonplanar Si_3N_4 surface. <i>Physical Review B</i> , 2010, 82, .		
44	First-Principles Studies of Extended Nitride Materials. <i>Advanced Materials</i> , 2000, 12, 307-310.	11.1	30
45	Post-Spinel Phases of Silicon Nitride. <i>Physica Status Solidi (B): Basic Research</i> , 2001, 226, R6-R7.	0.7	30
46	Silicon Boron Nitrides: Hypothetical Polymorphs of $\text{Si}_3\text{B}_3\text{N}_7$. <i>Angewandte Chemie - International Edition</i> , 1998, 37, 2527-2530.	7.2	29
47	Tunneling of electrons between Si nanocrystals embedded in a SiO_2 matrix. <i>Physical Review B</i> , 2012, 86, .	1.1	29
48	First-principles lattice dynamics calculations of the phase boundary between Si_3N_4 and Si_3N_4 at elevated temperatures and pressures. <i>Journal of Computational Chemistry</i> , 2008, 29, 2255-2259.	1.5	28
49	Shell-like structure of valence band orbitals of silicon nanocrystals in silica glass. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, R47-R49.	0.7	27
50	Silicon Monoxide at 1 atm and Elevated Pressures: Crystalline or Amorphous?. <i>Journal of the American Chemical Society</i> , 2014, 136, 3410-3423.	6.6	26
51	Group II element nitrides M_3N_2 under pressure: a comparative density functional study. <i>Physica Status Solidi (B): Basic Research</i> , 2009, 246, 1604-1613.	0.7	25
52	Compressing the Most Hydrogen-Rich Inorganic Ion. <i>Journal of the American Chemical Society</i> , 2010, 132, 748-755.	6.6	25
53	Spinel-type gallium oxynitrides attainable at high pressure and high temperature. <i>Physical Review B</i> , 2005, 72, .	1.1	24
54	Study of complexation between cyclofructans and alkali metal cations by electrospray ionization mass spectrometry and density functional theory calculations. <i>International Journal of Mass Spectrometry</i> , 2010, 291, 118-124.	0.7	24

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55	Chemical Potential of Nitrogen at High Pressure and High Temperature: Application to Nitrogen and Nitrogen-Rich Phase Diagram Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7054-7060.	1.5	24
56	Experimental and Quantum-Chemical Studies on the Thermochemical Stabilities of Mercury Carbodiimide and Mercury Cyanamide. <i>ChemPhysChem</i> , 2003, 4, 725-731.	1.0	23
57	Isotropic Negative Thermal Expansion in \hat{I}^2 -Si(NCN) ₂ and Its Origin. <i>Journal of Physical Chemistry C</i> , 2012, 116, 526-531.	1.5	22
58	High-Pressure Synthesis of Novel Boron Oxynitride B ₆ N ₄ O ₃ with Sphalerite Type Structure. <i>Chemistry of Materials</i> , 2015, 27, 5907-5914.	3.2	22
59	Reactive Force Field for Simulations of the Pyrolysis of Polysiloxanes into Silicon Oxycarbide Ceramics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16804-16812.	1.5	21
60	A DFT study of amorphous silicon oxynitride. <i>Journal of Non-Crystalline Solids</i> , 2005, 351, 1127-1132.	1.5	20
61	A density functional study of the high-pressure chemistry of MSiN ₂ (M = Be, Mg, Ca): prediction of high-pressure phases and examination of pressure-induced decomposition. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 275407.	0.7	19
62	Tracing Reversible and Irreversible Li Insertion in SiCO Ceramics with Modeling and Ab-Initio Simulations. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1313, 70701.	0.1	19
63	Vacuum ultraviolet absorbance of alkanes: an experimental and theoretical investigation. <i>Structural Chemistry</i> , 2019, 30, 2217-2224.	1.0	17
64	In situ high pressure high temperature experiments in multi-anvil assemblies with bixbyite-type In ₂ O ₃ and synthesis of corundum-type and orthorhombic In ₂ O ₃ polymorphs. <i>High Pressure Research</i> , 2013, 33, 697-711.	0.4	16
65	First-Principles Calculations and Analysis of ²⁹ Si Nuclear Magnetic Resonance Chemical Shifts in Silicon Oxycarbide Ceramics. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29952-29961.	1.5	16
66	Modeling amorphous silicon nitride: A comparative study of empirical potentials. <i>Computational Materials Science</i> , 2018, 148, 165-175.	1.4	15
67	Ab initio and FTIR Studies of HfSiCNO Processed from the Polymer Route. <i>Journal of the American Ceramic Society</i> , 2014, 97, 742-749.	1.9	14
68	Compositional and Structural Atomistic Study of Amorphous Si ³ N Networks of Interest for High-Performance Coatings. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24346-24353.	1.5	14
69	Comparative analysis of electronic structure and optical properties of crystalline and amorphous silicon nitrides. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	13
70	Density Functional Study of Calcium Nitride: Refined Geometries and Prediction of High-Pressure Phases. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2943-2949.	1.5	13
71	Combined Tumor Environment Triggered Self-Assembling Peptide Nanofibers and Inducible Multivalent Ligand Display for Cancer Cell Targeting with Enhanced Sensitivity and Specificity. <i>Small</i> , 2020, 16, e2002780.	5.2	13
72	SnCN ₂ : A Carbodiimide with an Innovative Approach for Energy Storage Systems and Phosphors in Modern LED Technology. <i>ChemElectroChem</i> , 2020, 7, 4550-4561.	1.7	13

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73	Si and N K-XANES spectroscopic study of novel Si ₃ C ₂ N ₂ ceramics. Journal of Electron Spectroscopy and Related Phenomena, 1998, 96, 253-257.	0.8	12
74	Novel binary and ternary phases in the Si-C-N system. Journal of the Ceramic Society of Japan, 2008, 116, 674-680.	0.5	12
75	High-pressure phases and transitions of the layered alkaline earth nitridosilicates SrSiN ₂ and BaSiN ₂ . Journal of Physics Condensed Matter, 2009, 21, 275408.	0.7	12
76	Amorphous Ge quantum dots embedded in crystalline Si: <i>ab initio</i> results. Journal of Physics Condensed Matter, 2015, 27, 405302.	0.7	12
77	First principles modeling and simulation of Zr-Si-B-C-N ceramics: Developing hard and oxidation resistant coatings. Acta Materialia, 2017, 125, 246-254.	3.8	12
78	Simulation of Vacuum Ultraviolet Absorption Spectra: Paraffin, Isoparaffin, Olefin, Naphthene, and Aromatic Hydrocarbon Class Compounds. Applied Spectroscopy, 2020, 74, 72-80.	1.2	12
79	Crystal Structure, Magnetic Properties, and Electronic Structure of Ni(NCNH ₂) ₄ Cl ₂ and Co(NCNH ₂) ₄ Cl ₂ . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2001, 627, 1682-1686.	0.6	11
80	Electronic structure and interfacial properties of Ge nanoclusters embedded in amorphous silica. Journal of Non-Crystalline Solids, 2010, 356, 2448-2453.	1.5	11
81	Metal-catalyst-free access to multiwalled carbon nanotubes/silica nanocomposites (MWCNT/SiO ₂) from a single-source precursor. Dalton Transactions, 2019, 48, 11018-11033.	1.6	11
82	Fabrication of ¹² C-SiC quantum dots by photo-assisted electrochemical corrosion of bulk powders. Electrochemistry Communications, 2013, 37, 1-4.	2.3	10
83	Magnetism in strained pseudomorphic ultrathin films of fcc 3d-transition metals (Cr, Mn, Fe, Co and Tj) ETQq1 1 0.784314 rgBT /Over 321, 2827-2832.	1.0	9
84	Kinetic control in the synthesis of metastable polymorphs: Bixbyite-to-Rh ₂ O ₃ (II)-to-corundum transition in In ₂ O ₃ . Journal of Solid State Chemistry, 2015, 229, 278-286.	1.4	9
85	A Novel High-Pressure Tin Oxynitride Sn ₂ N ₂ O. Chemistry - A European Journal, 2020, 26, 2187-2194.	1.7	9
86	Towards Porous Silicon Oxycarbide Materials: Effects of Solvents on Microstructural Features of Poly(methylhydrosiloxane)/Divynilbenzene Aerogels. Materials, 2018, 11, 2589.	1.3	8
87	Discovery of Ternary Silicon Titanium Nitride with Spinel-Type Structure. Scientific Reports, 2020, 10, 7372.	1.6	8
88	Advances in Computation of Temperature-Pressure Phase Diagrams of High-Pressure Nitrides. Key Engineering Materials, 0, 403, 77-80.	0.4	7
89	New structural insight for antimony(III)-tartrate. Inorganic Chemistry Communication, 2010, 13, 1504-1508.	1.8	7
90	²⁹ Si NMR Chemical Shifts in Crystalline and Amorphous Silicon Nitrides. Materials, 2018, 11, 1646.	1.3	7

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91	A DFT study of the compressibility of amorphous silicon oxynitride. <i>Journal of Non-Crystalline Solids</i> , 2004, 345-346, 720-723.	1.5	6
92	XANES Studies at N and C K-Edge of Compounds in the Ternary System Si-C-N. <i>Materials Research Society Symposia Proceedings</i> , 1996, 437, 231.	0.1	5
93	Thinking about metal-metal quadruple bonding in extended structures: a hypothetical A ₂ M ₆ E ₈ network. <i>New Journal of Chemistry</i> , 2004, 28, 185.	1.4	5
94	Nano-sized Crystals of Silicon Embedded in Silica Glass: Large Scale Models and Aspects of the Electronic Structure. <i>Materials Research Society Symposia Proceedings</i> , 2006, 958, 1.	0.1	5
95	Doping-induced modulation of electrical and optical properties of silicon nitride. <i>Thin Solid Films</i> , 2010, 518, 4918-4922.	0.8	5
96	Computing the Tantalum–Nitrogen Phase Diagram at High Pressure and High Temperature. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22221-22227.	1.5	5
97	Differential hysteresis scanning of non-templated monomodal amorphous aerogels. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5422-5430.	1.3	5
98	Experimental and Quantum-Chemical Studies on the Thermochemical Stabilities of Mercury Carbodiimide and Mercury Cyanamide. <i>ChemPhysChem</i> , 2003, 4, 789-789.	1.0	4
99	Influence of separation of Si nanocrystals embedded in a SiO ₂ matrix on electronic and optical properties. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2012, 177, 1098-1102.	1.7	4
100	Polymer-Derived Ultra-High Temperature Ceramics (UHTCs) and Related Materials. <i>PoliTO Springer Series</i> , 2021, , 281-323.	0.3	4
101	Cost-effective carbonized waste corrugated boards with surface decorated by SiC@C nanofibers and nanospheres for electromagnetic interference shielding. <i>Applied Surface Science</i> , 2022, 590, 153151.	3.1	4
102	The Electronic Structure and other Properties of Amorphous Silicon Nitride Investigated with Density Functional Theory. <i>Materials Research Society Symposia Proceedings</i> , 2002, 715, 1011.	0.1	3
103	High-pressure high-temperature synthesis of novel binary and ternary nitride phases of group 4 and 14 elements. <i>Journal of Physics: Conference Series</i> , 2008, 121, 062003.	0.3	3
104	Determination of the interconversion energy barrier of three novel pentahelicene derivative enantiomers by dynamic high resolution liquid chromatography. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2017, 1051, 60-67.	1.2	3
105	Impact of Transition Metal Cations on the ²⁹ Si NMR Signal in Metal Oxide Glasses: A DFT Case Study of Hafnia Silica Glass. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24152-24158.	1.5	3
106	Computational study of impact of composition, density, and temperature on thermal conductivity of amorphous silicon boron nitride. <i>Journal of the American Ceramic Society</i> , 2018, 101, 3489-3497.	1.9	3
107	Structural Insight into Layered Silicon Hydrogen Phosphates Containing [SiO ₆] Octahedra Prepared by Different Reaction Routes. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 828-836.	1.0	3
108	Computing the iron–nitrogen phase diagram at high pressure and high temperature. <i>Journal of Alloys and Compounds</i> , 2022, 900, 163533.	2.8	3

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109	X-Ray Absorption at Si K-Edge for Novel Compounds in the Ternary System Si-C-N. Materials Research Society Symposia Proceedings, 1996, 437, 225.	0.1	2
110	Structural, Electronic and Optical Properties of SiC Quantum Dots. Journal of Nano Research, 2012, 18-19, 77-87.	0.8	2
111	Orthorhombisches In_2O_3 – ein metastabiles Indiums sesquioxid – Polymorph. Angewandte Chemie, 2013, 125, 6659-6663.	1.6	2
112	Novel Sulfur-Containing Cross-Linking Agent for Si-Based Pre-ceramic Polymers. Macromolecular Chemistry and Physics, 2020, 221, 1900380.	1.1	2
113	Base-Catalytic Properties of Solid Silicon Imidonitriles. Materials Research Society Symposia Proceedings, 2002, 731, 591.	0.1	2
114	A DFT-Study of Structure and Properties of Amorphous SiCN. Materials Research Society Symposia Proceedings, 2002, 731, 321.	0.1	1
115	First-Principles Simulation of Hydrogen Interaction in Amorphous Silicon Nitride. Materials Research Society Symposia Proceedings, 2002, 719, 8371.	0.1	1
116	Theoretical Investigation of the Solid State Reaction of Silicon Nitride and Silicon Dioxide Forming Silicon Oxynitride ($\text{Si}_2\text{N}_2\text{O}$) under Pressure. ChemInform, 2003, 34, no.	0.1	1
117	Chemical Reactivity of Tetrasulfur Tetranitride: Synthesis, Physical Properties, and Structural Characterization of the Amorphous Phase $\text{Cu}_7\text{S}_4\text{N}_4$. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2003, 629, 1751-1759.	0.6	1
118	New Ceramic Phases in the Ternary Si-C-N System. Key Engineering Materials, 0, 403, 147-148.	0.4	1
119	Structure and thermodynamic properties of hafnia-silica glasses with low hafnia content. Journal of Non-Crystalline Solids, 2015, 416, 14-20.	1.5	1
120	Gold(I) Complexes $[\text{N}(\text{C}_3\text{F}_7)\text{C}(\text{Dipp})\text{N}]_2\text{AuL}$ (L = Ethylene, tert-Butyl Isocyanide, etc.). Modes. European Journal of Inorganic Chemistry, 2016, 2016, 5435-5444.	1.0	1
121	Post-Spinel Phases of Silicon Nitride. , 2001, 226, R6.		1
122	Chemical Reactivity of Tetrasulfur Tetranitride: Synthesis, Physical Properties, and Structural Characterization of the Amorphous Phase $\text{Cu}_7\text{S}_4\text{N}_4$. ChemInform, 2003, 34, no.	0.1	0
123	SrSi_6N_8 ? A Reduced Nitridosilicate with a Si-Si Bond.. ChemInform, 2005, 36, no.	0.1	0
124	Prediction of Novel Phases of Tantalum(V) Nitride and Tungsten(VI) Nitride that Can Be Synthesized under High Pressure and High Temperature.. ChemInform, 2005, 36, no.	0.1	0
125	Nano-sized crystals of silicon embedded in silica glass: large models and new aspects of the electronic structure. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2089-2089.	0.6	0
126	Iron Nanoparticles Embedded in Silica Glass: A Computational Study. Materials Research Society Symposia Proceedings, 2006, 959, 1.	0.1	0

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127	Computation of Temperature-Pressure Phase Diagrams of High-Pressure Nitrides. Materials Research Society Symposia Proceedings, 2006, 987, 1.	0.1	0
128	The Phase Boundary Between β -Si ₃ N ₄ and α -Si ₃ N ₄ at Elevated Temperatures and Pressures. Materials Research Society Symposia Proceedings, 2007, 1040, 1.	0.1	0
129	New Metal Nitride Compounds: Can they be Synthesized at High-Pressures?. Materials Research Society Symposia Proceedings, 2007, 1040, 1.	0.1	0
130	Phase Transitions in Silicon-Carbon-Nitride Compounds. Materials Research Society Symposia Proceedings, 2007, 1040, 1.	0.1	0
131	Negative or Zero Thermal Expansion in Silicon Dicarbondiimide, Si(NCN) ₂ . Materials Research Society Symposia Proceedings, 2007, 1040, 1.	0.1	0
132	Non-planar Corrugated Layered Heptazine-based Carbon Nitride: The Lowest Energy Modifications of C ₃ N ₄ . Materials Research Society Symposia Proceedings, 2007, 1040, 1.	0.1	0
133	A Density Functional Study of Alkaline Earth Nitrides M ₃ N ₂ : Refined Geometries and High-Pressure Phases. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2072-2072.	0.6	0
134	HP-Ca ₂ Si ₅ N ₈ - Density Functional Calculations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2073-2073.	0.6	0
135	Festkörperlperchemie 2007. Nachrichten Aus Der Chemie, 2008, 56, 258-268.	0.0	0
136	A Density Functional Study of Phosphorus Nitride P ₃ N ₅ : Refined Geometries, Properties, and Relative Stability of α -P ₃ N ₅ and β -P ₃ N ₅ and a Further Possible High-Pressure Phase γ -P ₃ N ₅ with Kyanite-type Structure.. ChemInform, 2002, 33, 2-2.	0.1	0
137	Paving the way for cristobalite TiO ₂ and GeO ₂ attainable under moderate tensile stress: A DFT study of transformation paths and activation barriers in cristobalite-rutile transformations of MO ₂ (M = Si, Ge.) Tj ETQq141 0.784314 rgB	0.784314	0
138	Frontispiece: A Novel High-Pressure Tin Oxynitride Sn ₂ N ₂ O. Chemistry - A European Journal, 2020, 26, .	1.7	0
139	Single-Crystals of a New Carbon Nitride Phase with all-sp ³ Carbon. Materials Research Society Symposia Proceedings, 2006, 987, 1.	0.1	0
140	Advances in Computation of Temperature-Pressure Phase Diagrams of High-Pressure Nitrides. Key Engineering Materials, 0, , 77-80.	0.4	0
141	Quantifying Thermal Transport of High-Temperature Ceramics From First Principle Calculations. , 2011, , .		0
142	Optimized Design of Composite Materials for Heat Transport Applications. , 2011, , .		0