

# Peter Kroll

## List of Publications by Citations

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139  
papers

5,032  
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157  
ext. papers

5,432  
ext. citations

5.7  
avg. IF

5.69  
L-index

#	Paper	IF	Citations
139	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> , <b>2003</b> , 125, 10288-300	16.4	805
138	Synthesis of cubic silicon nitride. <i>Nature</i> , <b>1999</b> , 400, 340-342	50.4	549
137	Tri-s-triazine derivatives. Part I. From trichloro-tri-s-triazine to graphitic C <sub>3</sub> N <sub>4</sub> structures. <i>New Journal of Chemistry</i> , <b>2002</b> , 26, 508-512	3.6	500
136	High-pressure chemistry of nitride-based materials. <i>Chemical Society Reviews</i> , <b>2006</b> , 35, 987-1014	58.5	185
135	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> , <b>2003</b> , 90, 125501	7.4	149
134	Inorganic Solid-State Chemistry with Main Group Element Carbodiimides. <i>Chemistry of Materials</i> , <b>1998</b> , 10, 2964-2979	9.6	120
133	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> , <b>2009</b> , 131, 11249-55	16.4	103
132	Vacuum ultraviolet detector for gas chromatography. <i>Analytical Chemistry</i> , <b>2014</b> , 86, 8329-35	7.8	102
131	Corrugated layered heptazine-based carbon nitride: the lowest energy modifications of C <sub>3</sub> N <sub>4</sub> ground state. <i>Journal of Materials Chemistry</i> , <b>2009</b> , 19, 3013		101
130	Nitrogen-rich transition metal nitrides. <i>Coordination Chemistry Reviews</i> , <b>2013</b> , 257, 2063-2072	23.2	87
129	Magnetism in graphene due to single-atom defects: dependence on the concentration and packing geometry of defects. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 196002	1.8	84
128	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> , <b>2005</b> , 44, 4249-54	16.4	79
127	High-pressure synthesis of crystalline carbon nitride imide, C <sub>2</sub> N <sub>2</sub> (NH). <i>Angewandte Chemie - International Edition</i> , <b>2007</b> , 46, 1476-80	16.4	74
126	Metastability of corundum-type In <sub>2</sub> O <sub>3</sub> . <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 3306-10	4.8	70
125	First-Principles Nuclear Magnetic Resonance Structural Analysis of Vitreous Silica. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 7917-7929	3.8	68
124	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> , <b>2008</b> , 78,	3.3	64
123	Pathways to metastable nitride structures. <i>Journal of Solid State Chemistry</i> , <b>2003</b> , 176, 530-537	3.3	62

122	Influence of SiO <sub>2</sub> matrix on electronic and optical properties of Si nanocrystals. <i>Nanotechnology</i> , <b>2009</b> , 20, 135702	3.4	57
121	Gold(I) chloride coordinated 3-hexyne. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 423-5	5.1	54
120	Resolution of isomeric new designer stimulants using gas chromatography - Vacuum ultraviolet spectroscopy and theoretical computations. <i>Analytica Chimica Acta</i> , <b>2017</b> , 971, 55-67	6.6	53
119	Synthesis, structure determination, and quantum-chemical characterization of an alternate HgNCN polymorph. <i>Inorganic Chemistry</i> , <b>2002</b> , 41, 4259-65	5.1	53
118	Formation of spinel-type gallium oxynitrides: a density-functional study of binary and ternary phases in the system Ga <sub>2</sub> O <sub>3</sub> -N <sub>2</sub> . <i>Journal of Materials Chemistry</i> , <b>2005</b> , 15, 3296		51
117	Analysis and deconvolution of dimethylnaphthalene isomers using gas chromatography vacuum ultraviolet spectroscopy and theoretical computations. <i>Analytica Chimica Acta</i> , <b>2016</b> , 945, 1-8	6.6	49
116	Theoretical Tracing of a Novel Route from Molecular Precursors through Polymers to Dense, Hard C <sub>3</sub> N <sub>4</sub> Solids. <i>Journal of the American Chemical Society</i> , <b>1999</b> , 121, 4696-4703	16.4	48
115	Polymer-Derived Ultra-High Temperature Ceramics (UHTCs) and Related Materials. <i>Advanced Engineering Materials</i> , <b>2019</b> , 21, 1900269	3.5	47
114	Isolable, gold carbonyl complexes supported by N-heterocyclic carbenes. <i>Chemical Communications</i> , <b>2011</b> , 47, 4478-80	5.8	46
113	Searching insight into the atomistic structure of SiCO ceramics. <i>Journal of Materials Chemistry</i> , <b>2010</b> , 20, 10528		46
112	First principles study of C <sub>3</sub> N <sub>4</sub> carbon nitride nanotubes. <i>Journal of Materials Chemistry</i> , <b>2009</b> , 19, 3020		46
111	Modelling and simulation of amorphous silicon oxycarbide. <i>Journal of Materials Chemistry</i> , <b>2003</b> , 13, 1657		44
110	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> , <b>2006</b> , 26, 1325-1335	6	43
109	Orthorhombic In <sub>2</sub> O <sub>3</sub> : a metastable polymorph of indium sesquioxide. <i>Angewandte Chemie - International Edition</i> , <b>2013</b> , 52, 6531-5	16.4	40
108	A density functional study of phosphorus nitride P <sub>3</sub> N <sub>5</sub> : refined geometries, properties, and relative stability of alpha-P <sub>3</sub> N <sub>5</sub> and gamma-P <sub>3</sub> N <sub>5</sub> and a further possible high-pressure phase delta-P <sub>3</sub> N <sub>5</sub> with kyanite-type structure. <i>Chemistry - A European Journal</i> , <b>2002</b> , 8, 3530-7	4.8	40
107	Theoretical Investigation of the Solid State Reaction of Silicon Nitride and Silicon Dioxide forming Silicon Oxynitride (Si <sub>2</sub> N <sub>2</sub> O) under Pressure. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2003</b> , 629, 1737-1750	1.3	40
106	Modelling polymer-derived ceramics. <i>Journal of the European Ceramic Society</i> , <b>2005</b> , 25, 163-174	6	39
105	Self-Assembled Peptide Nanofibers Display Natural Antimicrobial Peptides to Selectively Kill Bacteria without Compromising Cytocompatibility. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 28681-28689	9.5	38

104	Assessment of the HfN <sub>x</sub> , ZrN <sub>x</sub> and TiN <sub>x</sub> phase diagrams at high pressures and temperatures: balancing between MN and M <sub>3</sub> N <sub>4</sub> (M = Hf, Zr, Ti). <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, S1235-S1244	18	38
103	SrSi <sub>6</sub> N <sub>8</sub> —a reduced nitridosilicate with a Si-Si bond. <i>Angewandte Chemie - International Edition</i> , <b>2005</b> , 44, 567-70	16.4	35
102	Modeling the free carbon phase in amorphous silicon oxycarbide. <i>Journal of Non-Crystalline Solids</i> , <b>2005</b> , 351, 1121-1126	3.9	34
101	High-pressure high-temperature synthesis of Rh <sub>2</sub> O <sub>3</sub> -II-type In <sub>2</sub> O <sub>3</sub> polymorph. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2008</b> , 2, 269-271	2.5	32
100	HP-Ca <sub>2</sub> Si <sub>5</sub> N <sub>8</sub> —a new high-pressure nitridosilicate: synthesis, structure, luminescence, and DFT calculations. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 7892-902	4.8	31
99	Structure and reactivity of amorphous silicon nitride investigated with density-functional methods. <i>Journal of Non-Crystalline Solids</i> , <b>2001</b> , 293-295, 238-243	3.9	30
98	Silylated carbodiimides in molecular and extended structures. <i>Physical Review B</i> , <b>1999</b> , 60, 3126-3139	3.3	30
97	Band alignment at a nonplanar Si/SiO <sub>2</sub> interface. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	28
96	Post-Spinel Phases of Silicon Nitride. <i>Physica Status Solidi (B): Basic Research</i> , <b>2001</b> , 226, R6-R7	1.3	28
95	First-principles lattice dynamics calculations of the phase boundary between beta-Si <sub>3</sub> N <sub>4</sub> and gamma-Si <sub>3</sub> N <sub>4</sub> at elevated temperatures and pressures. <i>Journal of Computational Chemistry</i> , <b>2008</b> , 29, 2255-9	3.5	27
94	Shell-like structure of valence band orbitals of silicon nanocrystals in silica glass. <i>Physica Status Solidi (B): Basic Research</i> , <b>2006</b> , 243, R47-R49	1.3	27
93	Tunneling of electrons between Si nanocrystals embedded in a SiO <sub>2</sub> matrix. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	26
92	Silicon Boron Nitrides: Hypothetical Polymorphs of Si B N. <i>Angewandte Chemie - International Edition</i> , <b>1998</b> , 37, 2527-2530	16.4	26
91	Spinel-type gallium oxynitrides attainable at high pressure and high temperature. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	23
90	Compressing the most hydrogen-rich inorganic ion. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 748-55	16.4	22
89	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> , <b>2010</b> , 291, 118-124	1.9	22
88	High-Pressure Synthesis of Crystalline Carbon Nitride Imide, C <sub>2</sub> N <sub>2</sub> (NH). <i>Angewandte Chemie</i> , <b>2007</b> , 119, 1498-1502	3.6	21
87	Silicon monoxide at 1 atm and elevated pressures: crystalline or amorphous?. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 3410-23	16.4	20

86	Experimental and quantum-chemical studies on the thermochemical stabilities of mercury carbodiimide and mercury cyanamide. <i>ChemPhysChem</i> , <b>2003</b> , 4, 725-31	3.2	20
85	Isotropic Negative Thermal Expansion in $\text{E}^{\text{Si}}(\text{NCN})_2$ and Its Origin. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 526-531	3.8	19
84	Group II element nitrides $\text{M}_3\text{N}_2$ under pressure: a comparative density functional study. <i>Physica Status Solidi (B): Basic Research</i> , <b>2009</b> , 246, 1604-1613	1.3	19
83	A DFT study of amorphous silicon oxynitride. <i>Journal of Non-Crystalline Solids</i> , <b>2005</b> , 351, 1127-1132	3.9	19
82	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> , <b>2019</b> , 123, 7054-7060	3.8	17
81	In situ high pressure high temperature experiments in multi-anvil assemblies with bixbyite-type $\text{In}_2\text{O}_3$ and synthesis of corundum-type and orthorhombic $\text{In}_2\text{O}_3$ polymorphs. <i>High Pressure Research</i> , <b>2013</b> , 33, 697-711	1.6	16
80	High-Pressure Synthesis of Novel Boron Oxynitride $\text{B}_6\text{N}_4\text{O}_3$ with Sphalerite Type Structure. <i>Chemistry of Materials</i> , <b>2015</b> , 27, 5907-5914	9.6	15
79	Tracing Reversible and Irreversible Li Insertion in SiCO Ceramics with Modeling and Ab-Initio Simulations. <i>Materials Research Society Symposia Proceedings</i> , <b>2011</b> , 1313, 70701		14
78	Comparative analysis of electronic structure and optical properties of crystalline and amorphous silicon nitrides. <i>Journal of Applied Physics</i> , <b>2009</b> , 106, 053717	2.5	13
77	Vacuum ultraviolet absorbance of alkanes: an experimental and theoretical investigation. <i>Structural Chemistry</i> , <b>2019</b> , 30, 2217-2224	1.8	12
76	A density functional study of the high-pressure chemistry of $\text{MSiN}_2$ (M = Be, Mg, Ca): prediction of high-pressure phases and examination of pressure-induced decomposition. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 275407	1.8	12
75	First-Principles Calculations and Analysis of $^{29}\text{Si}$ Nuclear Magnetic Resonance Chemical Shifts in Silicon Oxycarbide Ceramics. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 29952-29961	3.8	11
74	Si and N K-XANES spectroscopic study of novel $\text{Si}_3\text{N}_4$ ceramics. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , <b>1998</b> , 96, 253-257	1.7	11
73	Novel binary and ternary phases in the Si-C-N system. <i>Journal of the Ceramic Society of Japan</i> , <b>2008</b> , 116, 674-680	1	11
72	Crystal Structure, Magnetic Properties, and Electronic Structure of $\text{Ni}(\text{NCNH}_2)_4\text{Cl}_2$ and $\text{Co}(\text{NCNH}_2)_4\text{Cl}_2$ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2001</b> , 627, 1682-1686	1.3	11
71	Reactive Force Field for Simulations of the Pyrolysis of Polysiloxanes into Silicon Oxycarbide Ceramics. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 16804-16812	3.8	10
70	Electronic structure and interfacial properties of Ge nanoclusters embedded in amorphous silica. <i>Journal of Non-Crystalline Solids</i> , <b>2010</b> , 356, 2448-2453	3.9	10
69	Density Functional Study of Calcium Nitride: Refined Geometries and Prediction of High-Pressure Phases. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 2943-2949	3.8	10

68	Compositional and Structural Atomistic Study of Amorphous SiBN Networks of Interest for High-Performance Coatings. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 24346-24353	3.8	10
67	Metal-catalyst-free access to multiwalled carbon nanotubes/silica nanocomposites (MWCNT/SiO) from a single-source precursor. <i>Dalton Transactions</i> , <b>2019</b> , 48, 11018-11033	4.3	9
66	Kinetic control in the synthesis of metastable polymorphs: Bixbyite-to-Rh <sub>2</sub> O <sub>3</sub> (II)-to-corundum transition in In <sub>2</sub> O <sub>3</sub> . <i>Journal of Solid State Chemistry</i> , <b>2015</b> , 229, 278-286	3.3	9
65	Fabrication of SiC quantum dots by photo-assisted electrochemical corrosion of bulk powders. <i>Electrochemistry Communications</i> , <b>2013</b> , 37, 1-4	5.1	9
64	Ab initio and FTIR Studies of HfSiCNO Processed from the Polymer Route. <i>Journal of the American Ceramic Society</i> , <b>2014</b> , 97, 742-749	3.8	9
63	High-pressure phases and transitions of the layered alkaline earth nitridosilicates SrSiN(2) and BaSiN(2). <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 275408	1.8	9
62	Magnetism in strained pseudomorphic ultrathin films of fcc 3d-transition metals (Cr, Mn, Fe, Co and Ni) with lateral lattice parameters of bulk fcc-Cu(001). <i>Journal of Magnetism and Magnetic Materials</i> , <b>2009</b> , 321, 2827-2832	2.8	9
61	Modeling amorphous silicon nitride: A comparative study of empirical potentials. <i>Computational Materials Science</i> , <b>2018</b> , 148, 165-175	3.2	8
60	A Novel High-Pressure Tin Oxynitride Sn N O. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 2187-2194	4.8	8
59	Amorphous Ge quantum dots embedded in crystalline Si: ab initio results. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 405302	1.8	7
58	Advances in Computation of Temperature-Pressure Phase Diagrams of High-Pressure Nitrides. <i>Key Engineering Materials</i> , <b>2008</b> , 403, 77-80	0.4	7
57	SnCN <sub>2</sub> : A Carbodiimide with an Innovative Approach for Energy Storage Systems and Phosphors in Modern LED Technology. <i>ChemElectroChem</i> , <b>2020</b> , 7, 4550-4561	4.3	7
56	Simulation of Vacuum Ultraviolet Absorption Spectra: Paraffin, Isoparaffin, Olefin, Naphthene, and Aromatic Hydrocarbon Class Compounds. <i>Applied Spectroscopy</i> , <b>2020</b> , 74, 72-80	3.1	7
55	First principles modeling and simulation of Zr-Si-B-C-N ceramics: Developing hard and oxidation resistant coatings. <i>Acta Materialia</i> , <b>2017</b> , 125, 246-254	8.4	6
54	New structural insight for antimony(III)-tartrate. <i>Inorganic Chemistry Communication</i> , <b>2010</b> , 13, 1504-1508	3.1	6
53	A DFT study of the compressibility of amorphous silicon oxynitride. <i>Journal of Non-Crystalline Solids</i> , <b>2004</b> , 345-346, 720-723	3.9	6
52	Synthesen bei hohem Druck und hoher Temperatur fñhren zu neuen Phasen von Tantal(V)-nitrid und Wolfram(VI)-nitrid. <i>Angewandte Chemie</i> , <b>2005</b> , 117, 4321-4326	3.6	6
51	Discovery of Ternary Silicon Titanium Nitride with Spinel-Type Structure. <i>Scientific Reports</i> , <b>2020</b> , 10, 7372	4.9	5

50	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> , <b>2006</b> , 958, 1		5
49	XANES Studies at N and C K-Edge of Compounds in the Ternary System Si <sub>3</sub> N <sub>4</sub> . <i>Materials Research Society Symposia Proceedings</i> , <b>1996</b> , 437, 231		5
48	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> , <b>2020</b> , 16, e2002780	11	5
47	Towards Porous Silicon Oxycarbide Materials: Effects of Solvents on Microstructural Features of Poly(methylhydrosiloxane)/Divynilbenzene Aerogels. <i>Materials</i> , <b>2018</b> , 11,	3.5	5
46	Influence of separation of Si nanocrystals embedded in a SiO <sub>2</sub> matrix on electronic and optical properties. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , <b>2012</b> , 177, 1098-1102	3.1	4
45	Doping-induced modulation of electrical and optical properties of silicon nitride. <i>Thin Solid Films</i> , <b>2010</b> , 518, 4918-4922	2.2	4
44	Experimental and Quantum-Chemical Studies on the Thermochemical Stabilities of Mercury Carbodiimide and Mercury Cyanamide. <i>ChemPhysChem</i> , <b>2003</b> , 4, 789-789	3.2	4
43	Si NMR Chemical Shifts in Crystalline and Amorphous Silicon Nitrides. <i>Materials</i> , <b>2018</b> , 11,	3.5	4
42	Impact of Transition Metal Cations on the <sup>29</sup> Si NMR Signal in Metal Oxide Glasses: A DFT Case Study of Hafnia Silica Glass. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 24152-24158	3.8	3
41	Structural Insight into Layered Silicon Hydrogen Phosphates Containing [SiO <sub>6</sub> ] Octahedra Prepared by Different Reaction Routes. <i>European Journal of Inorganic Chemistry</i> , <b>2019</b> , 2019, 828-836	2.3	3
40	Superhard Materials <b>2017</b> , 175-200		3
39	Thinking about metal-metal quadruple bonding in extended structures: a hypothetical A <sub>2</sub> M <sub>6</sub> E <sub>8</sub> network. <i>New Journal of Chemistry</i> , <b>2004</b> , 28, 185	3.6	3
38	The Electronic Structure and other Properties of Amorphous Silicon Nitride Investigated with Density Functional Theory. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 715, 1011		3
37	Computing the ironNitrogen phase diagram at high pressure and high temperature. <i>Journal of Alloys and Compounds</i> , <b>2022</b> , 900, 163533	5.7	3
36	National Hypersonic Science Center for Materials and Structures <b>2014</b> ,		3
35	Computing the TantalumNitrogen Phase Diagram at High Pressure and High Temperature. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 22221-22227	3.8	3
34	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> , <b>2017</b> , 1051, 60-67	3.2	2
33	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> , <b>2018</b> , 101, 3489-3497	3.8	2

32	Orthorhombisches In <sub>2</sub> O <sub>3</sub> Ein metastabiles Indiums sesquioxid- Polymorph. <i>Angewandte Chemie</i> , <b>2013</b> , 125, 6659-6663	3.6	2
31	Structural, Electronic and Optical Properties of SiC Quantum Dots. <i>Journal of Nano Research</i> , <b>2012</b> , 18-19, 77-87	1	2
30	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> , <b>2008</b> , 121, 062003	0.3	2
29	X-Ray Absorption at Si K-Edge for Novel Compounds in the Ternary System SiCN. <i>Materials Research Society Symposia Proceedings</i> , <b>1996</b> , 437, 225		2
28	Base-Catalytic properties of Solid Silicon Imidonitriles. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 731, 591		2
27	Differential hysteresis scanning of non-templated monomodal amorphous aerogels. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 5422-5430	3.6	2
26	New Ceramic Phases in the Ternary Si-C-N System. <i>Key Engineering Materials</i> , <b>2008</b> , 403, 147-148	0.4	1
25	A DFT-Study of Structure and properties of Amorphous SiCN. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 731, 321		1
24	First-Principles Simulation of Hydrogen Interaction in Amorphous Silicon Nitride. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 719, 8371		1
23	Novel Sulfur-Containing Cross-Linking Agent for Si-Based Pre-ceramic Polymers. <i>Macromolecular Chemistry and Physics</i> , <b>2020</b> , 221, 1900380	2.6	1
22	Gold(I) Complexes [N{(C <sub>3</sub> F <sub>7</sub> )C(Dipp)N} <sub>2</sub> ]AuL (L = Ethylene, tert-Butyl Isocyanide, Tetrahydrothiophene, Triphenylphosphine) and Different Triazapentadienyl Ligand Coordination Modes. <i>European Journal of Inorganic Chemistry</i> , <b>2016</b> , 2016, 5435-5444	2.3	1
21	Post-Spinel Phases of Silicon Nitride <b>2001</b> , 226, R6		1
20	Chemical Reactivity of Tetrasulfur Tetranitride: Synthesis, Physical Properties, and Structural Characterization of the Amorphous Phase Cu <sub>7</sub> S <sub>4</sub> N <sub>4</sub> . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2003</b> , 629, 1751-1759	1.3	0
19	Polymer-Derived Ultra-High Temperature Ceramics (UHTCs) and Related Materials. <i>Polito Springer Series</i> , <b>2021</b> , 281-323	0.4	0
18	Paving the way for cristobalite TiO <sub>2</sub> and GeO <sub>2</sub> attainable under moderate tensile stress: A DFT study of transformation paths and activation barriers in cristobalite-rutile transformations of MO <sub>2</sub> (M = Si, Ge, Ti). <i>Computational Materials Science</i> , <b>2019</b> , 170, 109170	3.2	
17	Structure and thermodynamic properties of hafnia-silica glasses with low hafnia content. <i>Journal of Non-Crystalline Solids</i> , <b>2015</b> , 416, 14-20	3.9	
16	Modeling Amorphous Ceramic Structures <b>2014</b> , 39-69		
15	Modeling Amorphous Ceramic Structures <b>2011</b> , 39-69		



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