Richard Dronskowski

List of Publications by Year
in descending order

477 papers	21,500 citations	23879 60 h-index	15698 129 g-index
489 all docs	489 docs citations	489 times ranked	16334 citing authors

#	Article	IF	Citations
1	The Orbital Origins of Chemical Bonding in Geâ^'Sbâ^'Te Phaseâ€Change Materials**. Angewandte Chemie - International Edition, 2022, 61, .	7.2	19
2	First-Principles Plane-Wave-Based Exploration of Cathode and Anode Materials for Li- and Na-Ion Batteries Involving Complex Nitrogen-Based Anions. Chemistry of Materials, 2022, 34, 652-668.	3.2	9
3	Temperature-Resolved Anisotropic Displacement Parameters from Theory and Experiment: A Case Study. Crystals, 2022, 12, 283.	1.0	0
4	Existence of BeCN₂ and Its First-Principles Phase Diagram: Be and C Introducing Structural Diversity. Journal of the American Chemical Society, 2022, 144, 5155-5162.	6.6	12
5	InnenrÃ¼cktitelbild: Orbitale als Ausgangspunkt der Chemischen Bindung in Geâ^'Sbâ^'Teâ€Phasenwechselmaterialien (Angew. Chem. 17/2022). Angewandte Chemie, 2022, 134, .	1.6	0
6	Reaction pathways on N-substituted carbon catalysts during the electrochemical reduction of nitrate to ammonia. Catalysis Science and Technology, 2022, 12, 3582-3593.	2.1	6
7	Chemical Reactions and Phase Stabilities in the Siâ€"Te System at High Pressures and High Temperatures. Inorganic Chemistry, 2022, 61, 7349-7357.	1.9	0
8	Predicting Nitrogenâ€Based Families of Compounds: Transitionâ€Metal Guanidinates TCN₃ (T=V, Nb, Ta) and Orthoâ€Nitrido Carbonates Tâ€²₂CN₄ (Tâ€²=Ti, Zr, Hf). Angewandte Chemie - International Edition, 2021, 60, 486-492.	7.2	18
9	Vorhersage stickstoffbasierter Verbindungsklassen: Guanidinate TCN₃ (T=V,) Tj ETQq1 1 0.784314 rgBT /O Ãœbergangsmetallen. Angewandte Chemie, 2021, 133, 490-497.	1.6	2
10	Nonlinear optical effects in two mercury cyanamide/guanidinium chlorides Hg3(NCN)2Cl2 and Hg2(C(NH2)3)Cl5. Journal of Materials Chemistry C, 2021, 9, 967-974.	2.7	3
11	Sensibilization of p-NiO with ZnSe/CdS and CdS/ZnSe quantum dots for photoelectrochemical water reduction. Nanoscale, 2021, 13, 869-877.	2.8	8
12	Displacement parameters from density-functional theory and their validation in the experimental charge density of tartaric acid. CrystEngComm, 2021, 23, 1052-1058.	1.3	1
13	Graphitic nitrogen in carbon catalysts is important for the reduction of nitrite as revealed by naturally abundant¹⁵N NMR spectroscopy. Dalton Transactions, 2021, 50, 6857-6866.	1.6	8
14	Metathesis and Redetermination of the Crystal Structure of Cadmium Carbodiimide, CdNCN. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 496-499.	0.6	3
15	Combining Electrocatalysts and Biobased Adsorbents for Sustainable Denitrification. ACS Sustainable Chemistry and Engineering, 2021, 9, 3658-3667.	3.2	9
16	Crystal Orbital Bond Index: Covalent Bond Orders in Solids. Journal of Physical Chemistry C, 2021, 125, 7959-7970.	1.5	96
17	Exploring the Possible Anionic Redox Mechanism in Li-Rich Transition-Metal Carbodiimides. Journal of Physical Chemistry C, 2021, 125, 8479-8487.	1.5	2
18	CeTiO₂N oxynitride perovskite: paramagnetic ¹⁴N MAS NMR without paramagnetic shifts. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2021, 76, 275-280.	0.3	4

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19	Solidâ€state quantum chemistry with ÎĨ¦ (ThetaPhi): Spinâ€liquids , superconductors, and magnetic superstructures made computationally available. Journal of Computational Chemistry, 2021, 42, 1498-1513.	1.5	1
20	Synthesis and characterisation of the quaternary cyanamide Li₂MgSn₂(NCN)₆. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 2162-2166.	0.6	4
21	Longâ€Range Forces in Rockâ€Saltâ€Type Tellurides and How they Mirror the Underlying Chemical Bonding. Advanced Materials, 2021, 33, e2100163.	11.1	26
22	Synthesis, Crystal Structure, Symmetry Relationships, and Electronic Structure of Bismuth Carbodiimide Bi₂(NCN)₃ and Its Ammonia Adduct Bi₂(NCN)₃Â·NH₃. Inorganic Chemistry, 2021, 60, 12664-12670.	1.9	4
23	Conduction Band Control of Oxyhalides with a Triple-Fluorite Layer for Visible Light Photocatalysis. Journal of the American Chemical Society, 2021, 143, 2491-2499.	6.6	52
24	Bonding diversity in rock salt-type tellurides: examining the interdependence between chemical bonding and materials properties. RSC Advances, 2021, 11, 20679-20686.	1.7	14
25	Structural Properties of NdTiO2+xN1â€“x and Its Application as Photoanode. Inorganic Chemistry, 2021, 60, 919-929.	1.9	7
26	Deprotonating Melamine to Gain Highly Interconnected Materials: Melaminate Salts of Potassium and Rubidium. Inorganic Chemistry, 2021, 60, 15069-15077.	1.9	3
27	Elemental electrical switch enabling phase segregationâ€“free operation. Science, 2021, 374, 1390-1394.	6.0	73
28	Preferred selenium incorporation and unexpected interlayer bonding in the layered structure of Sb₂Te_{3â^'} _x Se _x . Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2020, 75, 41-50.	0.3	2
29	Reversible High Capacity and Reaction Mechanism of Cr₂(NCN)₃ Negative Electrodes for Liâ€ion Batteries. Energy Technology, 2020, 8, 1901260.	1.8	9
30	Nanostructured coreâ€“shell metal boridesâ€“oxides as highly efficient electrocatalysts for photoelectrochemical water oxidation. Nanoscale, 2020, 12, 3121-3128.	2.8	29
31	ÎĨ¦: Solid state package allowing Bardeenâ€“Cooperâ€“Schrieffer and magnetic superstructure electronic states. Computer Physics Communications, 2020, 251, 107079.	3.0	4
32	Arndt Simon zum 80. Geburtstag gewidmet. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2020, 75, 1-2.	0.3	0
33	Quantumâ€Chemical Study of the FeNCN Conversionâ€Reaction Mechanism in Lithiumâ€and Sodiumâ€Ion Batteries. Angewandte Chemie - International Edition, 2020, 59, 3718-3723.	7.2	24
34	Exploring the Origins of Improved Photocurrent by Acidic Treatment for Quaternary Tantalum-Based Oxynitride Photoanodes on the Example of CaTaO₂N. Journal of Physical Chemistry C, 2020, 124, 152-160.	1.5	28
35	Semi-transparent quaternary oxynitride photoanodes on GaN underlayers. Chemical Communications, 2020, 56, 13193-13196.	2.2	16
36	Metathetic synthesis of lead cyanamide as a p-type semiconductor. Dalton Transactions, 2020, 49, 14061-14067.	1.6	16

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37	Deductive molecular mechanics of carbon allotropes (Review article). Low Temperature Physics, 2020, 46, 655-670.	0.2	3
38	Structural evolution of CrN nanocube electrocatalysts during nitrogen reduction reaction. Nanoscale, 2020, 12, 19276-19283.	2.8	24
39	Tailoring the Surface Properties of Bi₂O₂NCN by in Situ Activation for Augmented Photoelectrochemical Water Oxidation on WO₃ and CuWO₄ Heterojunction Photoanodes. Inorganic Chemistry, 2020, 59, 13589-13597.	1.9	7
40	Phonon Spectroscopy in Antimony and Tellurium Oxides. Journal of Physical Chemistry A, 2020, 124, 7869-7880.	1.1	6
41	Silver Cyanoguanidine Nitrate Hydrate: Ag(C2N4H4)NO3Â·Â½ H2O, a Cyanoguanidine Compound Coordinating by an Inner Nitrogen Atom. Inorganics, 2020, 8, 64.	1.2	3
42	NiO/Poly(4-alkylthiazole) Hybrid Interface for Promoting Spatial Charge Separation in Photoelectrochemical Water Reduction. ACS Applied Materials & Interfaces, 2020, 12, 29173-29180.	4.0	7
43	Elucidation of the Active Sites for Monodisperse FePt and Pt Nanocrystal Catalysts for p-WSe₂ Photocathodes. Journal of Physical Chemistry C, 2020, 124, 11877-11885.	1.5	10
44	It's All in the (Cyanamide) Tilt: Synthesis and Structure of NaSc(NCN)₂. European Journal of Inorganic Chemistry, 2020, 2020, 2596-2602.	1.0	9
45	<scp>LOBSTER</scp>: Local orbital projections, atomic charges, and chemicalâ€bonding analysis from <scp>projectorâ€augmentedâ€waveâ€based</scp> densityâ€functional theory. Journal of Computational Chemistry, 2020, 41, 1931-1940.	1.5	523
46	Syntheses, Crystal Structures, and Vibrational Properties of Two Lead Azide Halides PbN 3 X (X = Cl,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.6	3
47	Quantumâ€Chemical Study of the FeNCN Conversionâ€Reaction Mechanism in Lithiumâ€and Sodiumâ€Ion Batteries. Angewandte Chemie, 2020, 132, 3747-3752.	1.6	2
48	Increased photocurrent of CuWO₄ photoanodes by modification with the oxide carbodiimide Sn₂O(NCN). Dalton Transactions, 2020, 49, 3450-3456.	1.6	14
49	Revisiting the Zintlâ€'Klemm Concept for ALn2Ag3Te5-Type Alkaline-Metal (A) Lanthanide (Ln) Silver Tellurides. Crystals, 2020, 10, 184.	1.0	12
50	Time-dependent density-functional theory molecular-dynamics study on amorphization of Sc-Sb-Te alloy under optical excitation. Npj Computational Materials, 2020, 6, .	3.5	32
51	Lattice Dynamics of Sb₂Se₃ from Inelastic Neutron and Xâ€Ray Scattering. Physica Status Solidi (B): Basic Research, 2020, 257, 2000063.	0.7	6
52	Ammonothermal Synthesis, Crystal Structure, and Vibrational Properties of the Doubly Deprotonated Calcium Guanidinate, CaC(NH)₃. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 180-183.	0.6	5
53	Can we trust the experiment? Anisotropic displacement parameters in 1-(halomethyl)-3-nitrobenzene (halogen = Cl or Br). Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 591-597.	0.2	2
54	Deductive molecular mechanics of four-coordinated carbon allotropes. Physical Chemistry Chemical Physics, 2019, 21, 18138-18148.	1.3	4

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55	Direct atomic insight into the role of dopants in phase-change materials. Nature Communications, 2019, 10, 3525.	5.8	56
56	Local magnetic cluster size identified by neutron total scattering in the site-diluted spin glass SnxFe4â^'xN (x=0.88). Physical Review B, 2019, 100, .	1.1	10
57	Impact of Bonding on the Stacking Defects in Layered Chalcogenides. Advanced Functional Materials, 2019, 29, 1902332.	7.8	21
58	Melting Behavior of Alkaline-Earth Metal Carbodiimides and Their Thermochemistry from First-Principles. Inorganic Chemistry, 2019, 58, 8938-8942.	1.9	13
59	Understanding the Structure and Properties of Sesquiâ€Chalcogenides (i.e.,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 587 Td (V	11.1	98
60	The gapless energy spectrum and spin-Peierls instability of 1D Heisenberg spin systems in polymeric complexes of transition metals and hypothetical carbon allotropes. Journal of Physics Condensed Matter, 2019, 31, 305601.	0.7	8
61	Cobalt Carbodiimide as Negative Electrode for Liâ€Ion Batteries: Electrochemical Mechanism and Performance. ChemElectroChem, 2019, 6, 5101-5108.	1.7	11
62	Exploring Chemical Bonding in Phaseâ€Change Materials with Orbitalâ€Based Indicators. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800579.	1.2	22
63	A new tilt and an old twist on the nickel arsenide structure-type: synthesis and characterisation of the quaternary transition-metal cyanamides A₂MnSn₂(NCN)₆ (A =) Tj ETQq1 1 0.784314 rgBT	1.1	3
64	K₂Ge₃As₃: Fiberlike Crystals of a Narrow-Band-Gap Zintl Phase with a One-Dimensional Substructure _{âˆž}¹{(Ge₃As₃)^{2â€“}}. Chemistry of Materials, 2019, 31, 8839-8849.	3.2	4
65	First-Principles Study of Divalent 3d Transition-Metal Carbodiimides. Journal of Physical Chemistry A, 2019, 123, 9328-9335.	1.1	16
66	Magnetic Properties of Quasi-One-Dimensional Crystals Formed by Graphene Nanoclusters and Embedded Atoms of the Transition Metals. Crystals, 2019, 9, 251.	1.0	9
67	Revealing the Nature of Chemical Bonding in an ALn2Ag3Te5-Type Alkaline-Metal (A) Lanthanide (Ln) Silver Telluride. Inorganics, 2019, 7, 70.	1.2	12
68	Syntheses and Characterization of Diammineâ€“Nickel/Cobalt(II)â€“Bisdicyanamide M(NH₃)₂[N(CN)₂]₂ with M = Ni and Co. Inorganic Chemistry, 2019, 58, 7803-7811.	1.9	3
69	Quaternary Coreâ€“Shell Oxynitride Nanowire Photoanode Containing a Hole-Extraction Gradient for Photoelectrochemical Water Oxidation. ACS Applied Materials & Interfaces, 2019, 11, 19077-19086.	4.0	35
70	Relative stability of diamond and graphite as seen through bonds and hybridizations. Physical Chemistry Chemical Physics, 2019, 21, 10961-10969.	1.3	20
71	Covalent bonding versus total energy: On the attainability of certain predicted low-energy carbon allotropes. Carbon, 2019, 148, 151-158.	5.4	14
72	Band Gap Tuning in Bismuth Oxide Carbodiimide Bi₂O₂NCN. Inorganic Chemistry, 2019, 58, 6467-6473.	1.9	28

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73	Achieving band convergence by tuning the bonding ionicity in nâ€type Mg₃Sb₂. Journal of Computational Chemistry, 2019, 40, 1693-1700.	1.5	68
74	Ammonothermal Synthesis, Xâ€Ray and Timeâ€ofâ€Flight Neutron Crystalâ€Structure Determination, and Vibrational Properties of Barium Guanidinate, Ba(CN₃H₄)₂. ChemistryOpen, 2019, 8, 327-332.	0.9	8
75	New insights on the GeSe _x Te_{1â^'x} phase diagram from theory and experiment. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 246-256.	0.5	6
76	Electrochemical Evaluation of Pb, Ag, and Zn Cyanamides/Carbodiimides. ACS Omega, 2019, 4, 4339-4347.	1.6	16
77	Synthesis and characterisation of a quaternary nitride series with spin-glass behaviour: Sn_xGe_{1â^'x}Fe₃N. Journal of Materials Chemistry C, 2019, 7, 3822-3828.	2.7	4
78	Construction of a hybrid clamped cell for high-pressure neutron-diffraction experiments with a large diamond window. Review of Scientific Instruments, 2019, 90, 026103.	0.6	1
79	A new tool for validating theoretically derived anisotropic displacement parameters with experiment: directionality of prolate displacement ellipsoids. CrystEngComm, 2019, 21, 6396-6404.	1.3	4
80	Transition Metal Doping of Phase Change Materials: Atomic Arrangement of Cr-Doped Ge₂Sb₂Te₅. Journal of Physical Chemistry C, 2019, 123, 30640-30648.	1.5	10
81	Development of a robust tool to extract Mulliken and LÃ¶wdin charges from plane waves and its application to solid-state materials. RSC Advances, 2019, 9, 29821-29830.	1.7	77
82	Cationic Pb₂ Dumbbells Stabilized in the Highly Covalent Lead Nitridosilicate Pb₂Si₅N₈. Angewandte Chemie - International Edition, 2019, 58, 1432-1436.	7.2	12
83	The many flavours of halogen bonds â€“ message from experimental electron density and Raman spectroscopy. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1190-1201.	0.2	14
84	Mapping the band structure of GeSbTe phase change alloys around the Fermi level. Communications Physics, 2018, 1, .	2.0	16
85	Insights into exfoliation possibility of MAX phases to MXenes. Physical Chemistry Chemical Physics, 2018, 20, 8579-8592.	1.3	182
86	Unique Bond Breaking in Crystalline Phase Change Materials and the Quest for Metavalent Bonding. Advanced Materials, 2018, 30, e1706735.	11.1	175
87	A CALPHAD assessment of the Alâ€“Mnâ€“C system supported by ab initio calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 60, 231-239.	0.7	10
88	SrTaO₂N Nanowire Photoanode Modified with a Ferrihydrite Hole-Storage Layer for Photoelectrochemical Water Oxidation. ACS Applied Nano Materials, 2018, 1, 869-876.	2.4	25
89	An MnNCN-Derived Electrocatalyst for CuWO₄ Photoanodes. Langmuir, 2018, 34, 3845-3852.	1.6	36
90	Itinerant nitrides and salt-like guanidinates â€“ The diversity of solid-state nitrogen chemistry. Progress in Solid State Chemistry, 2018, 51, 1-18.	3.9	14

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91	Syntheses and Characterization of Two Dicyanamide Compounds Containing Monovalent Cations: Hg2[N(CN)2]2 and Tl[N(CN)2]. Inorganics, 2018, 6, 135.	1.2	9
92	Synthesis, Crystal Structure, and Chemical-Bonding Analysis of BaZn(NCN)2. Inorganics, 2018, 6, 1.	1.2	27
93	Highâ€Pressure Behavior of Lead Cyanamide PbNCN. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 1881-1885.	0.6	5
94	Cationic Pb2 Dumbbells Stabilized in the Highly Covalent Lead Nitridosilicate Pb2Si5N8. Angewandte Chemie, 2018, 131, 1446.	1.6	2
95	First-Principles Approaches to Metals, Alloys, and Metallic Compounds. Metals, 2018, 8, 705.	1.0	1
96	Chemical Bonding of Crystalline LnB₆ (Ln = Laâ€“Lu) and Its Relationship with Ln₂B₈ Gas-Phase Complexes. Inorganic Chemistry, 2018, 57, 12999-13008.	1.9	57
97	Synthesis and Characterization of the New Dicyanamide LiCs2[N(CN)2]3. Inorganics, 2018, 6, 108.	1.2	8
98	The low-temperature heat capacity of the Sb₂Te_{3â^'x}Se_xsolid solution from experiment and theory. Journal of Physics Condensed Matter, 2018, 30, 405702.	0.7	3
99	Tin(<scp>ii</scp>) oxide carbodiimide and its relationship to SnO. Dalton Transactions, 2018, 47, 13378-13383.	1.6	17
100	Magnetic inhomogeneity in the copper pseudochalcogenide CuNCN. Physical Review B, 2018, 97, .	1.1	4
101	Discovery of High-Performance Thermoelectric Chalcogenides through Reliable High-Throughput Material Screening. Journal of the American Chemical Society, 2018, 140, 10785-10793.	6.6	134
102	The Crystal Orbital Hamilton Population (COHP) Method as a Tool to Visualize and Analyze Chemical Bonding in Intermetallic Compounds. Crystals, 2018, 8, 225.	1.0	199
103	On the Mnâ€“C Short-Range Ordering in a High-Strength High-Ductility Steel: Small Angle Neutron Scattering and Ab Initio Investigation. Metals, 2018, 8, 44.	1.0	20
104	Carbodiimides as energy materials: which directions for a reasonable future?. Dalton Transactions, 2018, 47, 10827-10832.	1.6	51
105	First Full Structural Characterization of Chloro Formamidinium Salts. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 1485-1491.	0.6	1
106	Controlled Crystal Growth of Indium Selenide, In₂Se₃, and the Crystal Structures of Î±-In₂Se₃. Inorganic Chemistry, 2018, 57, 11775-11781.	1.9	97
107	Synthesis, Crystal Structure, Magnetic Properties, and Stability of the Manganese-Rich â€œMn₃AlCâ€•Î² Phase. Inorganic Chemistry, 2017, 56, 1045-1048.	1.9	13
108	Tetrel Bonds in Infinite Molecular Chains by Electronic Structure Theory and Their Role for Crystal Stabilization. Journal of Physical Chemistry A, 2017, 121, 1381-1387.	1.1	15

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109	Automated firstâ€principles mapping for phaseâ€change materials. Journal of Computational Chemistry, 2017, 38, 620-628.	1.5	9
110	A stable compound of helium and sodium at high pressure. Nature Chemistry, 2017, 9, 440-445.	6.6	276
111	Unerwartete Geâ€Geâ€Kontakte in der zweidimensionalen Phase Ge₄Se₃Te und Analyse ihres chemischen Ursprungs mittels Energiedichte(DOE)â€Funktion. Angewandte Chemie, 2017, 129, 10338-10342.	1.6	2
112	Unexpected Geâ€“Ge Contacts in the Twoâ€Dimensional Ge₄Se₃Te Phase and Analysis of Their Chemical Cause with the Density of Energy (DOE) Function. Angewandte Chemie - International Edition, 2017, 56, 10204-10208.	7.2	64
113	HP-MoO₂: A High-Pressure Polymorph of Molybdenum Dioxide. Inorganic Chemistry, 2017, 56, 2321-2327.	1.9	13
114	Atomic motions in the layered copper pseudochalcogenide CuNCN indicative of a quantum spin-liquid scenario. Journal of Physics Condensed Matter, 2017, 29, 235701.	0.7	5
115	Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. Accounts of Chemical Research, 2017, 50, 1231-1239.	7.6	47
116	Dynamic Uptake and Release of Water in the Mixed-Metal EDTA Complex M₃[Yb(EDTA)(CO₃)] (M = K, Rb, Cs). Crystal Growth and Design, 2017, 17, 80-88.	1.4	11
117	Highâ€Pressure NiAsâ€Type Modification of FeN. Angewandte Chemie - International Edition, 2017, 56, 7302-7306.	7.2	43
118	Bonding analyses of unconventional carbon allotropes. Carbon, 2017, 121, 154-162.	5.4	19
119	Instrumental resolution as a function of scattering angle and wavelength as exemplified for the POWGEN instrument. Journal of Applied Crystallography, 2017, 50, 866-875.	1.9	6
120	Advanced anode materials for sodium ion batteries: carbodiimides. MRS Advances, 2017, 2, 1165-1176.	0.5	11
121	Structure and magnetism of the solid solution Ge_xFe_{4â^'x}N_y (0 â‰¤ x) Tj ETQq1 1 0.784314 rg	2.7	8
122	Synthesis and characterization of metastable transition metal oxides and oxide nitrides. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 3-14.	0.4	5
123	Enhanced Photoelectrochemical Water Oxidation Efficiency of CuWO₄ Photoanodes by Surface Modification with Ag₂NCN. Journal of Physical Chemistry C, 2017, 121, 26265-26274.	1.5	36
124	First-Principles Chemical Bonding Study of Manganese Carbodiimide, MnNCN, As Compared to Manganese Oxide, MnO. Journal of Physical Chemistry A, 2017, 121, 7778-7786.	1.1	22
125	Lattice thermal expansion and anisotropic displacements in urea, bromomalonic aldehyde, pentachloropyridine, and naphthalene. Journal of Chemical Physics, 2017, 147, 074112.	1.2	16
126	Revisiting the Siâ€“Te System: SiTe₂ Finally Found by Means of Experimental and Quantum-Chemical Techniques. Inorganic Chemistry, 2017, 56, 11398-11405.	1.9	21

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127	The Ternary Postâ€transition Metal Carbodiimide SrZn(NCN)₂. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 1456-1461.	0.6	15
128	Chemical Tuning of Carrier Type and Concentration in a Homologous Series of Crystalline Chalcogenides. Chemistry of Materials, 2017, 29, 6749-6757.	3.2	18
129	Molybdenum Oxide Nitrides of the Mo2(O,N,â–¡)5 Type: On the Way to Mo2O5. Inorganic Chemistry, 2017, 56, 8782-8792.	1.9	4
130	InnenrÃ¼cktitelbild: Unerwartete Geâ€Geâ€Kontakte in der zweidimensionalen Phase Ge₄Se₃Te und Analyse ihres chemischen Ursprungs mittels Energiedichte(DOE)â€Funktion (Angew. Chem. 34/2017). Angewandte Chemie, 2017, 129, 10381-10381.	1.6	0
131	Ab initio triangle maps for new insights into the crystal wave functions of carbon allotropes. Carbon, 2017, 123, 708-716.	5.4	3
132	Exploring the subsurface atomic structure of the epitaxially grown phase-change material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="bold">Te</mml:mi><mml:mn>5</mml:mn></mml:mrow></mml:math>. Physical Review B, 2017, 96, .	1.1	10
133	Phase transition and proton ordering at 50â€…K in 3-(pyridin-4-yl)pentane-2,4-dione. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 1172-1178.	0.5	5
134	A density-functional theory approach to the existence and stability of molybdenum and tungsten sesquioxide polymorphs. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 69-75.	0.4	1
135	An Ab Initio Study of Carbon-Induced Ordering in Austenitic Fe-Mn-Al-C Alloys. Steel Research International, 2017, 88, 1600292.	1.0	14
136	Synthesis, Crystal Structure, Polymorphism, and Magnetism of Eu(CN3H4)2 and First Evidence of EuC(NH)3. Inorganics, 2017, 5, 10.	1.2	17
137	The Role of Î²-Carbides as Hydrogen Traps in High-Mn Steels. Metals, 2017, 7, 264.	1.0	27
138	Experimental and Theoretical Investigation of the Elastic Moduli of Silicate Glasses and Crystals. Frontiers in Materials, 2017, 4, .	1.2	13
139	Note: Efficient, low-cost cooling system for gloveboxes. Review of Scientific Instruments, 2016, 87, 106102.	0.6	1
140	Synthesis and Structure Determination of the Quaternary Zinc Nitride Halides Zn2NX1â^'yXâ€²y (X, Xâ€² = Cl,) Tj ETQq0 0 0 rgBT /Overl	1.2	1
141	Ab initio lattice dynamics and thermochemistry of layered bismuth telluride (Bi₂Te₃). Journal of Physics Condensed Matter, 2016, 28, 115401.	0.7	17
142	A Firstâ€Principles Study on the Electronic, Vibrational, and Thermodynamic Properties of Jadeite and its Tentative Lowâ€Density Polymorph. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 590-596.	0.6	4
143	Transitionâ€Metal Carbodiimides as Molecular Negative Electrode Materials for Lithiumâ€and Sodiumâ€Ion Batteries with Excellent Cycling Properties. Angewandte Chemie - International Edition, 2016, 55, 5090-5095.	7.2	86
144	Ãœbergangsmetallcarbodiimide als molekulare negative Elektrodenâ€materialien fÃ¼r Liâ€und Naâ€Ionenbatterien mit hervorragendem Zyklisierungsverhalten. Angewandte Chemie, 2016, 128, 5174-5179.	1.6	11

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