Eva Zurek

List of Publications by Year
in descending order

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162	11,781	66336	29154
papers	citations	42 h-index	104 g-index

175	175	175	15471
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. Journal of Cheminformatics, 2012, 4, 17.	6.1	6,063
2	XtalOpt: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2011, 182, 372-387.	7.5	263
3	A little bit of lithium does a lot for hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 17640-17643.	7.1	245
4	Theoretical studies of the structure and function of MAO (methylaluminoxane). Progress in Polymer Science, 2004, 29, 107-148.	24.7	177
5	Synthesis of Yttrium Superhydride Superconductor with a Transition Temperature up to 262ÂK by Catalytic Hydrogenation at High Pressures. Physical Review Letters, 2021, 126, 117003.	7.8	165
6	A Molecular Perspective on Lithiumâ€“Ammonia Solutions. Angewandte Chemie - International Edition, 2009, 48, 8198-8232.	13.8	155
7	Graphene-like Boronâ€“Carbonâ€“Nitrogen Monolayers. ACS Nano, 2017, 11, 2486-2493.	14.6	154
8	Density Functional Calculations of the13C NMR Chemical Shifts in (9,0) Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2004, 126, 13079-13088.	13.7	152
9	High-temperature superconductivity in alkaline and rare earth polyhydrides at high pressure: A theoretical perspective. Journal of Chemical Physics, 2019, 150, 050901.	3.0	126
10	Chemistry under high pressure. Nature Reviews Chemistry, 2020, 4, 508-527.	30.2	117
11	Metallization of magnesium polyhydrides under pressure. Physical Review B, 2013, 87, .	3.2	102
12	Decomposition Products of Phosphine Under Pressure: PH₂ Stable and Superconducting?. Journal of the American Chemical Society, 2016, 138, 1884-1892.	13.7	102
13	Predicting crystal structures and properties of matter under extreme conditions via quantum mechanics: the pressure is on. Physical Chemistry Chemical Physics, 2015, 17, 2917-2934.	2.8	99
14	Route to high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:ma superconductivity via <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml -intercalated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi	3.2	98
15	Modeling the Dynamic Equilibrium between Oligomers of (AlOCH3)n in Methylaluminoxane (MAO). A Theoretical Study Based on a Combined Quantum Mechanical and Statistical Mechanical Approach. Inorganic Chemistry, 2001, 40, 361-370.	4.0	93
16	Pressure-Stabilized Sodium Polyhydrides:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>NaH</mml:mi><mml:mi>n</mml:mi></mml:msub></mml:math>(<mml:math) Tj ETQq0 0 0 rgBT	7.8	93
17	Physical Review Letters, 2011, 106, 237002. Enantioselective Copperâ€Catalyzed Carboetherification of Unactivated Alkenes. Angewandte Chemie - International Edition, 2014, 53, 6383-6387.	13.8	88
18	Polyhydrides of the Alkaline Earth Metals: A Look at the Extremes under Pressure. Journal of Physical Chemistry C, 2013, 117, 2982-2992.	3.1	84

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19	High Hydrides of Scandium under Pressure: Potential Superconductors. Journal of Physical Chemistry C, 2018, 122, 6298-6309.	3.1	83
20	Theoretical Study of the Interactions between Cations and Anions in Group IV Transition-Metal Catalysts for Single-Site Homogeneous Olefin Polymerization. Organometallics, 2002, 21, 2444-2453.	2.3	79
21	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
22	Predicting superhard materials via a machine learning informed evolutionary structure search. Npj Computational Materials, 2019, 5, .	8.7	74
23	Toward the Identification of Dormant and Active Species in MAO (Methylaluminoxane)-Activated, Dimethylzirconocene-Catalyzed Olefin Polymerization. Organometallics, 2002, 21, 83-92.	2.3	73
24	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	3.0	72
25	Identifying duplicate crystal structures: XtalComp, an open-source solution. Computer Physics Communications, 2012, 183, 690-697.	7.5	71
26	Relativistic Density-Functional Computations of the Chemical Shift of129Xe in Xe@C60. Journal of Physical Chemistry A, 2003, 107, 4967-4972.	2.5	70
27	Rubidium Polyhydrides Under Pressure: Emergence of the Linear H₃^{â^'} Species. Chemistry - A European Journal, 2012, 18, 5013-5021.	3.3	68
28	High Pressure Potassium Polyhydrides: A Chemical Perspective. Journal of Physical Chemistry C, 2012, 116, 13322-13328.	3.1	63
29	A Combined Quantum Mechanical and Statistical Mechanical Study of the Equilibrium of Trimethylaluminum (TMA) and Oligomers of (AlOCH3)nFound in Methylaluminoxane (MAO) Solution. Inorganic Chemistry, 2001, 40, 3279-3292.	4.0	62
30	Density Functional Study of the 13C NMR Chemical Shifts in Small-to-Medium-Diameter Infinite Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2006, 110, 11995-12004.	2.5	62
31	Composition and Constitution of Compressed Strontium Polyhydrides. Journal of Physical Chemistry C, 2014, 118, 6433-6447.	3.1	59
32	Reactivity ofÂHe withÂionic compounds under high pressure. Nature Communications, 2018, 9, 951.	12.8	59
33	Density Functional Study of the ¹³C NMR Chemical Shifts in Single-Walled Carbon Nanotubes with Stoneâ^'Wales Defects. Journal of Physical Chemistry C, 2008, 112, 11744-11750.	3.1	56
34	Surface state engineering of moleculeâ€“molecule interactions. Physical Chemistry Chemical Physics, 2012, 14, 4971.	2.8	56
35	Locking and Unlocking the Molecular Spin Crossover Transition. Advanced Materials, 2017, 29, 1702257.	21.0	55
36	Compressed Cesium Polyhydrides: Cs⁺ Sublattices and H₃^{â€“} Three-Connected Nets. Inorganic Chemistry, 2012, 51, 9333-9342.	4.0	54

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37	A Review of Equation-of-State Models for Inertial Confinement Fusion Materials. High Energy Density Physics, 2018, 28, 7-24.	1.5	54
38	Effects of Nonhydrostatic Stress on Structural and Optoelectronic Properties of Methylammonium Lead Bromide Perovskite. Journal of Physical Chemistry Letters, 2017, 8, 3457-3465.	4.6	53
39	Electron Counting and a Large Family of Two-Dimensional Semiconductors. Chemistry of Materials, 2016, 28, 1994-1999.	6.7	52
40	Muffin-Tin Orbital Wannier-Like Functions for Insulators and Metals. ChemPhysChem, 2005, 6, 1934-1942.	2.1	49
41	A Density Functional Study of the13C NMR Chemical Shifts in Functionalized Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2007, 129, 4430-4439.	13.7	47
42	Self-Assembly and Molecular Recognition in Water: Tubular Stacking and Guest-Templated Discrete Assembly of Water-Soluble, Shape-Persistent Macrocycles. Journal of the American Chemical Society, 2020, 142, 2915-2924.	13.7	44
43	A theoretical study of the insertion barrier of MAO (methylaluminoxane)-activated, Cp2ZrMe2-catalyzed ethylene polymerization: further evidence for the structural assignment of active and dormant species. Faraday Discussions, 2003, 124, 93.	3.2	43
44	The Dynamic Equilibrium Between (AlOMe)_n Cages and (AlOMe)_nÂ·(AlMe₃)_m Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation. Macromolecules, 2014, 47, 8556-8569.	4.8	43
45	The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction. Journal of Physical Chemistry C, 2021, 125, 1601-1620.	3.1	42
46	XtalOpt version r7: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2011, 182, 2305-2306.	7.5	41
47	Superconducting High-Pressure Phases Composed of Hydrogen and Iodine. Journal of Physical Chemistry Letters, 2015, 6, 4067-4072.	4.6	41
48	Self-assembly of strongly dipolar molecules on metal surfaces. Journal of Chemical Physics, 2015, 142, 101921.	3.0	38
49	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. Journal of Physical Chemistry C, 2018, 122, 19370-19378.	3.1	38
50	XtalOptÂVersion r12: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2019, 237, 274-275.	7.5	37
51	Epitaxial growth of aligned atomically precise chevron graphene nanoribbons on Cu(111). Chemical Communications, 2017, 53, 8463-8466.	4.1	36
52	(Barely) Solid Li(NH₃)₄: The Electronics of an Expanded Metal. Journal of the American Chemical Society, 2011, 133, 3535-3547.	13.7	35
53	Hydrides of the Alkali Metals and Alkaline Earth Metals Under Pressure. Comments on Inorganic Chemistry, 2017, 37, 78-98.	5.2	35
54	Compression of curium pyrrolidine-dithiocarbamate enhances covalency. Nature, 2020, 583, 396-399.	27.8	34

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55	Tuning chemical precompression: Theoretical design and crystal chemistry of novel hydrides in the quest for warm and light superconductivity at ambient pressures. Journal of Applied Physics, 2022, 131, .	2.5	33
56	Dipole driven bonding schemes of quinonoid zwitterions on surfaces. Chemical Communications, 2012, 48, 7143.	4.1	31
57	Determining the Diameter of Functionalized Single-Walled Carbon Nanotubes with 13C NMR: A Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 9267-9271.	3.1	30
58	Lithium Subhydrides under Pressure and Their Superatomâ€like Building Blocks. ChemPlusChem, 2012, 77, 969-972.	2.8	30
59	RandSpg: An open-source program for generating atomistic crystal structures with specific spacegroups. Computer Physics Communications, 2017, 213, 208-216.	7.5	30
60	M-graphene: a metastable two-dimensional carbon allotrope. 2D Materials, 2020, 7, 025047.	4.4	30
61	Identification of Polybrominated Diphenyl Ether Metabolites Based on Calculated Boiling Points from COSMO-RS, Experimental Retention Times, and Mass Spectral Fragmentation Patterns. Analytical Chemistry, 2015, 87, 2299-2305.	6.5	29
62	A Density Functional Study of the 13C NMR Chemical Shifts in Fluorinated Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2009, 113, 4117-4124.	2.5	28
63	Substituted Benzene Derivatives on the Cu(111) Surface. Journal of Physical Chemistry C, 2012, 116, 12636-12643.	3.1	28
64	NMR computations for carbon nanotubes from first principles: Present status and future directions. International Journal of Quantum Chemistry, 2009, 109, 3343-3367.	2.0	27
65	The Search for Superconductivity in High Pressure Hydrides. , 2019, , .		27
66	Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen. Angewandte Chemie - International Edition, 2017, 56, 10192-10195.	13.8	27
67	Accurate and precise ab initio anharmonic free-energy calculations for metallic crystals: Application to hcp Fe at high temperature and pressure. Physical Review B, 2017, 96, .	3.2	25
68	Equation of state, adiabatic sound speed, and GrÃ¼neisen coefficient of boron carbide along the principal Hugoniot to 700 GPa. Physical Review B, 2016, 94, .	3.2	24
69	Crystal Structures and Properties of Iron Hydrides at High Pressure. Journal of Physical Chemistry C, 2018, 122, 24262-24269.	3.1	24
70	Alkali Metals in Ethylenediamine: A Computational Study of the Optical Absorption Spectra and NMR Parameters of [M(en)₃^{Î˙+}Â·M^{Î˙â^’}] Ion Pairs. Journal of the American Chemical Society, 2011, 133, 4829-4839.	13.7	23
71	Pressure induced structural transitions in KH, RbH, and CsH. Journal of Applied Physics, 2012, 111, 112611.	2.5	23
72	Charge-Transfer-Induced Magic Cluster Formation of Azaborine Heterocycles on Noble Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 6020-6030.	3.1	23

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73	A Metastable CaSH₃ Phase Composed of HS Honeycomb Sheets that is Superconducting Under Pressure. Journal of Physical Chemistry Letters, 2020, 11, 9629-9636.	4.6	23
74	Superfast Tetrazoleâ€“BCN Cycloaddition Reaction for Bioorthogonal Protein Labeling on Live Cells. Journal of the American Chemical Society, 2022, 144, 57-62.	13.7	23
75	Magic Electret Clusters of 4-Fluorostyrene on Metal Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 2069-2075.	4.6	22
76	Proton transfer in surface-stabilized chiral motifs of croconic acid. Physical Review B, 2013, 87, .	3.2	22
77	Benzene derivatives adsorbed to the Ag(111) surface: Binding sites and electronic structure. Journal of Chemical Physics, 2015, 142, 101924.	3.0	22
78	Extended HÃ¼ckel Calculations on Solids Using the Avogadro Molecular Editor and Visualizer. Journal of Chemical Education, 2018, 95, 331-337.	2.3	22
79	Coverage-Dependent Interactions at the Organicsâ€“Metal Interface: Quinonoid Zwitterions on Au(111). Journal of Physical Chemistry C, 2013, 117, 16406-16415.	3.1	21
80	Computation of Chemical Shifts for Paramagnetic Molecules: A Laboratory Experiment for the Undergraduate Curriculum. Journal of Chemical Education, 2014, 91, 1058-1063.	2.3	20
81	DFT-D Investigation of Active and Dormant Methylaluminoxane (MAO) Species Grafted onto a Magnesium Dichloride Cluster: A Model Study of Supported MAO. ACS Catalysis, 2015, 5, 6989-6998.	11.2	20
82	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me)₄N]₂PuCl₆. Inorganic Chemistry, 2016, 55, 8371-8380.	4.0	20
83	A Computational Experiment on Single-Walled Carbon Nanotubes. Journal of Chemical Education, 2013, 90, 651-655.	2.3	19
84	Kagome-like lattice of Ï€â€“Ï€ stacked 3-hydroxyphenalenone on Cu(111). Chemical Communications, 2014, 50, 8659-8662.	4.1	19
85	Computational prediction and analysis of the ²⁷Al solid-state NMR spectrum of methylaluminoxane (MAO) at variable temperatures and field strengths. Physical Chemistry Chemical Physics, 2016, 18, 24106-24118.	2.8	19
86	2D Cocrystallization from H-Bonded Organic Ferroelectrics. Journal of Physical Chemistry Letters, 2016, 7, 435-440.	4.6	19
87	Building egg-tray-shaped graphenes that have superior mechanical strength and band gap. Npj Computational Materials, 2019, 5, .	8.7	19
88	Crystal Field Splitting is Limiting the Stability and Strength of Ultra-incompressible Orthorhombic Transition Metal Tetraborides. Scientific Reports, 2016, 6, 23088.	3.3	18
89	Crystal Structures and Electronic Properties of Single-Layer, Few-Layer, and Multilayer GeH. Journal of Physical Chemistry C, 2016, 120, 793-800.	3.1	18
90	Folding and Assembly of Short Î±, Î², Î³-Hybrid Peptides: Minor Variations in Sequence and Drastic Differences in Higher-Level Structures. Journal of the American Chemical Society, 2019, 141, 14239-14248.	13.7	18

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91	Theoretical Predictions of Novel Superconducting Phases of BaGe3 Stable at Atmospheric and High Pressures. Inorganic Chemistry, 2015, 54, 2875-2884.	4.0	17
92	Superalkaliâ€“Alkalide Interactions and Ion Pairing in Low-Polarity Solvents. Journal of the American Chemical Society, 2021, 143, 3934-3943.	13.7	17
93	XtalOpt Âversion r9: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2016, 199, 178-179.	7.5	16
94	Computational Modeling of the Optical Rotation of Amino Acids: An â€˜in Silicoâ€™ Experiment for Physical Chemistry. Journal of Chemical Education, 2013, 90, 656-660.	2.3	15
95	Low energy structural dynamics and constrained libration of Li(NH₃)₄, the lowest melting point metal. Chemical Communications, 2014, 50, 10778-10781.	4.1	15
96	Superconductivity in Hydrides Doped with Main Group Elements Under Pressure. Novel Superconducting Materials, 2017, 3, .	0.8	15
97	Materials under high pressure: a chemical perspective. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	2.3	15
98	Searching for the Interlayer Band and Unravelling the Bonding in Î²-ThSi₂ and Î±-ThSi₂ with NMTO Wannier-like Functions. Inorganic Chemistry, 2010, 49, 1384-1396.	4.0	14
99	Rhodizonic Acid on Noble Metals: Surface Reactivity and Coordination Chemistry. Journal of Physical Chemistry Letters, 2013, 4, 3413-3419.	4.6	14
100	Fluorides of Silver Under Large Compression**. Chemistry - A European Journal, 2021, 27, 5536-5545.	3.3	14
101	Electronic Structure of Iron Porphyrin Adsorbed to the Pt(111) Surface. Journal of Physical Chemistry C, 2016, 120, 29173-29181.	3.1	13
102	Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen. Angewandte Chemie, 2017, 129, 10326-10329.	2.0	13
103	Experimental and Theoretical Investigations of the Thermodynamic Stability of Baâ^'C₆₀ and Kâ^'C₆₀ Compound Clusters. ACS Nano, 2008, 2, 1000-1014.	14.6	11
104	Determination of the Structures of Molecularly Imprinted Polymers and Xerogels Using an Automated Stochastic Approach. Analytical Chemistry, 2013, 85, 8577-8584.	6.5	11
105	Effect of BN/CC Isosterism on the Thermodynamics of Surface and Bulk Binding: 1,2-Dihydro-1,2-azaborine vs Benzene. Journal of Physical Chemistry C, 2015, 119, 14624-14631.	3.1	11
106	Modulating Bond Lengths via Backdonation: A First-Principles Investigation of a Quinonoid Zwitterion Adsorbed to Coinage Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 6633-6641.	3.1	11
107	XtalOptÂVersion r10: An openâ€“source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2017, 217, 210-211.	7.5	11
108	Helical Folding of Meta-Connected Aromatic Oligoureas. Organic Letters, 2017, 19, 2666-2669.	4.6	11

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109	XtalOptÂversion r11: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2018, 222, 418-419.	7.5	11
110	Electronic Structure and Superconductivity of Compressed Metal Tetrahydrides. Chemistry - A European Journal, 2021, 27, 14858-14870.	3.3	11
111	Magic alkali-fullerene compound clusters of extreme thermal stability. Journal of Chemical Physics, 2006, 125, 191102.	3.0	10
112	On the Nature of Geâ€“Pb Bonding in the Solid State. Synthesis, Structural Characterization, and Electronic Structures of Two Unprecedented Germanide-Plumbides. Journal of the American Chemical Society, 2012, 134, 12708-12716.	13.7	10
113	Properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:math> in the shocked state for pressures up to 1.5 TPa. Physical Review B, 2017, 95, .	3.2	10
114	A Computational Investigation of a Molecular Switch. Journal of Chemical Education, 2013, 90, 1528-1532.	2.3	9
115	Interplay between Hydrogen Bonding, Epitaxy, and Charge Transfer in the Self-Assembly of Croconic Acid on Au(111) and Ag(111). Journal of Physical Chemistry C, 2015, 119, 26429-26437.	3.1	9
116	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
117	RbB₃Si₃: An Alkali Metal Borosilicide that is Metastable and Superconducting at 1 atm. Journal of Physical Chemistry C, 2020, 124, 14826-14831.	3.1	9
118	Reverse Turn Foldamers: An Expanded Î²-Turn Motif Reinforced by Double Hydrogen Bonds. Organic Letters, 2020, 22, 1003-1007.	4.6	9
119	Dilute carbon in H3S under pressure. Npj Computational Materials, 2022, 8, .	8.7	9
120	Structure and Proton-Transfer Mechanism in One-Dimensional Chains of Benzimidazoles. Journal of Physical Chemistry C, 2016, 120, 5804-5809.	3.1	8
121	The Computational Design of Two-Dimensional Materials. Journal of Chemical Education, 2019, 96, 2308-2314.	2.3	8
122	A First-Principles Exploration of NaxSy Binary Phases at 1 atm and Under Pressure. Crystals, 2019, 9, 441.	2.2	8
123	Silanization of superficially porous silica particles with p-aminophenyltrimethoxysilane. Microchemical Journal, 2019, 147, 263-268.	4.5	8
124	Copper-catalyzed enantioselective alkene carboetherification for the synthesis of saturated six-membered cyclic ethers. Chemical Communications, 2021, 57, 10099-10102.	4.1	8
125	Pressure-induced yttrium oxides with unconventional stoichiometries and novel properties. Physical Review Materials, 2021, 5, .	2.4	8
126	Structural motifs and bonding in two families of boron structures predicted at megabar pressures. Physical Review Materials, 2021, 5, .	2.4	8

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127	Structural Diversity and Superconductivity in Sâ€“Pâ€“H Ternary Hydrides under Pressure. Journal of Physical Chemistry C, 2022, 126, 7208-7220.	3.1	8
128	Chiral surface networks of 3-HPLN â€” A molecular analog of rounded triangle assembly. Surface Science, 2014, 629, 65-74.	1.9	7
129	Crystal Structures and Electronic Properties of Xeâ€“Cl Compounds at High Pressure. Journal of Physical Chemistry C, 2018, 122, 2941-2950.	3.1	7
130	Predicted CsSi compound: a promising material for photovoltaic applications. Physical Chemistry Chemical Physics, 2020, 22, 11578-11582.	2.8	7
131	Stable pseudo[3]rotaxanes with strong positive binding cooperativity based on shape-persistent aromatic oligoamide macrocycles. Chemical Communications, 2021, 57, 11645-11648.	4.1	7
132	Interplay of Halogen and Weak Hydrogen Bonds in the Formation of Magic Nanoclusters on Surfaces. Journal of Physical Chemistry C, 2022, 126, 588-596.	3.1	7
133	Theoretical predictions of novel potassium chloride phases under pressure. Physical Chemistry Chemical Physics, 2015, 17, 12265-12272.	2.8	6
134	Pressure-Induced Superconductivity in the Wide-Band-Gap Semiconductor Cu2Br2Se6 with a Robust Framework. Chemistry of Materials, 2020, 32, 6237-6246.	6.7	6
135	Laserâ€Induced Cooperative Transition in Molecular Electronic Crystal. Advanced Materials, 2021, 33, e2103000.	21.0	6
136	Pushing Towards Room-Temperature Superconductivity. Physics Magazine, 0, 12, .	0.1	5
137	Surface Magnetism in Pristine Î± Rhombohedral Boron and Intersurface Exchange Coupling Mechanism of Boron Icosahedra. Journal of Physical Chemistry Letters, 2021, 12, 6812-6817.	4.6	5
138	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie - International Edition, 2022, 61, .	13.8	5
139	The Ideal Crystal Structure of Cristobalite X-I: A Bridge in SiO₂ Densification. Journal of Physical Chemistry C, 2018, 122, 17437-17446.	3.1	4
140	Crystal structures of silicon-rich lithium silicides at high pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 1047-1051.	2.1	4
141	An electrochemically controlled release of NHCs using iron bis(dithiolene) N-heterocyclic carbene complexes. Inorganic Chemistry Frontiers, 2021, 8, 59-71.	6.0	4
142	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
143	Nature of the bonded-to-atomic transition in liquid silica to TPa pressures. Journal of Applied Physics, 2022, 131, .	2.5	4
144	Nano-makisu: highly anisotropic two-dimensional carbon allotropes made by weaving together nanotubes. Nanoscale, 2020, 12, 347-355.	5.6	3

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145	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie, 2022, 134, .	2.0	3
146	Downfolding and N-ization of Basis Sets of Slater Type Orbitals. AIP Conference Proceedings, 2007, , .	0.4	2
147	Dimerization of cobalt-substituted Keggin phosphotungstate, [PW₁₁O₃₉Co(X)]^{5â^'}, in nonpolar solvents. Journal of Coordination Chemistry, 2014, 67, 2830-2842.	2.2	2
148	Major Factors for the Persistent Folding of Hybrid Î±, Î², Î³-Hybrid Peptides Into Hairpins. Frontiers in Chemistry, 2020, 8, 530083.	3.6	2
149	The Liâ€“Fâ€“H ternary system at high pressures. Journal of Chemical Physics, 2021, 154, 124709.	3.0	2
150	Halogen and structure sensitivity of halobenzene adsorption on copper surfaces. Physical Chemistry Chemical Physics, 2022, 24, 4485-4492.	2.8	2
151	Computational materials discovery. Journal of Chemical Physics, 2022, 156, .	3.0	2
152	Density Functional Studies of the [sup 13]C NMR Chemical Shifts in Singleâ€“Walled Carbon Nanotubes. AIP Conference Proceedings, 2007, , .	0.4	1
153	First principles investigation on how site preference and entropy affect the stability of (Eu_xM_{1â€“}_x)₂Ge₂Pb (M = Ca,) Tj ET Qq1 1 0.784314 gr	1.0	1
154	Materials genome approach to organic ferroelectrics and piezoelectrics. International Journal of Nanotechnology, 2018, 15, 784.	0.2	1
155	Modeling Methylaluminoxane (MAO). , 2001, , 109-123.		1
156	Anchoring effect of distorted octahedra on the stability and strength of platinum metal pernitrides. Physical Review Materials, 2019, 3, .	2.4	1
157	Density Functional Calculations of the13C NMR Chemical Shifts in (9,0) Single-Walled Carbon Nanotubes.. ChemInform, 2004, 35, no.	0.0	0
158	Electrochemical Atomic Force Microscopy and First-Principles Calculations of Ferriprotoporphyrin Adsorption and Polymerization. Langmuir, 2018, 34, 11335-11346.	3.5	0
159	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0
160	Reliable folding of hybrid tetrapeptides into short Î²-hairpins. Chinese Chemical Letters, 2021, , .	9.0	0
161	Laserâ€Induced Cooperative Transition in Molecular Electronic Crystal (Adv. Mater. 39/2021). Advanced Materials, 2021, 33, .	21.0	0
162	Insight into the Adsorption Structure of TIPS-Pentacene on Noble Metal Surfaces. Journal of Physical Chemistry C, 2022, 126, 2689-2698.	3.1	0