Eva Zurek

List of Publications by Citations

160 papers	8,068 citations	38 h-index	87 g-index
175 ext. papers	9,858 ext. citations	6.7 avg, IF	6.41 L-index

#	Paper	IF	Citations
160	Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. *Journal of Cheminformatics*, **2012**, 4, 17	8.6	3841
159	XtalOpt: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, **2011**, 182, 372-387	4.2	211
158	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, 17640-3	11.5	205
157	Theoretical studies of the structure and function of MAO (methylaluminoxane). *Progress in Polymer Science*, **2004**, 29, 107-148	29.6	163
156	Density functional calculations of the 13C NMR chemical shifts in (9,0) single-walled carbon nanotubes. *Journal of the American Chemical Society*, **2004**, 126, 13079-88	16.4	148
155	A molecular perspective on lithium-ammonia solutions. *Angewandte Chemie - International Edition*, **2009**, 48, 8198-232	16.4	133
154	Graphene-like Boron-Carbon-Nitrogen Monolayers. *ACS Nano*, **2017**, 11, 2486-2493	16.7	110
153	Decomposition Products of Phosphine Under Pressure: PH2 Stable and Superconducting?. *Journal of the American Chemical Society*, **2016**, 138, 1884-92	16.4	85
152	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, 361-70	5.1	85
151	Predicting crystal structures and properties of matter under extreme conditions via quantum mechanics: the pressure is on. *Physical Chemistry Chemical Physics*, **2015**, 17, 2917-34	3.6	81
150	Pressure-stabilized sodium polyhydrides: NaH(n) (n>1). *Physical Review Letters*, **2011**, 106, 237002	7.4	80
149	High-temperature superconductivity in alkaline and rare earth polyhydrides at high pressure: A theoretical perspective. *Journal of Chemical Physics*, **2019**, 150, 050901	3.9	77
148	Metallization of magnesium polyhydrides under pressure. *Physical Review B*, **2013**, 87,	3.3	76
147	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	3.8	75
146	Enantioselective copper-catalyzed carboetherification of unactivated alkenes. *Angewandte Chemie - International Edition*, **2014**, 53, 6383-7	16.4	71
145	Polyhydrides of the Alkaline Earth Metals: A Look at the Extremes under Pressure. *Journal of Physical Chemistry C*, **2013**, 117, 2982-2992	3.8	71
144	Toward the Identification of Dormant and Active Species in MAO (Methylaluminoxane)-Activated, Dimethylzirconocene-Catalyzed Olefin Polymerization. *Organometallics*, **2002**, 21, 83-92	3.8	64

143	Rubidium polyhydrides under pressure: emergence of the linear H3(-) species. *Chemistry - A European Journal*, **2012**, 18, 5013-21	4.8	62
142	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, 11995-2004	2.8	62
141	Relativistic Density-Functional Computations of the Chemical Shift of 129Xe in 60. *Journal of Physical Chemistry A*, **2003**, 107, 4967-4972	2.8	59
140	High Hydrides of Scandium under Pressure: Potential Superconductors. *Journal of Physical Chemistry C*, **2018**, 122, 6298-6309	3.8	57
139	A combined quantum mechanical and statistical mechanical study of the equilibrium of trimethylaluminum (TMA) and oligomers of (AlOCH(3))(n) found in methylaluminoxane (MAO) solution. *Inorganic Chemistry*, **2001**, 40, 3279-92	5.1	57
138	Identifying duplicate crystal structures: XtalComp, an open-source solution. *Computer Physics Communications*, **2012**, 183, 690-697	4.2	55
137	High Pressure Potassium Polyhydrides: A Chemical Perspective. *Journal of Physical Chemistry C*, **2012**, 116, 13322-13328	3.8	55
136	Surface state engineering of molecule-molecule interactions. *Physical Chemistry Chemical Physics*, **2012**, 14, 4971-6	3.6	52
135	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. *Computational Materials Science*, **2018**, 152, 134-145	3.2	51
134	Composition and Constitution of Compressed Strontium Polyhydrides. *Journal of Physical Chemistry C*, **2014**, 118, 6433-6447	3.8	50
133	Synthesis of Yttrium Superhydride Superconductor with a Transition Temperature up to 262 K by Catalytic Hydrogenation at High Pressures. *Physical Review Letters*, **2021**, 126, 117003	7.4	49
132	Compressed cesium polyhydrides: Cs+ sublattices and H3(-) three-connected nets. *Inorganic Chemistry*, **2012**, 51, 9333-42	5.1	46
131	Route to high-Tc superconductivity via CH4-intercalated H3S hydride perovskites. *Physical Review B* , **2020**, 101,	3.3	45
130	A density functional study of the 13C NMR chemical shifts in functionalized single-walled carbon nanotubes. *Journal of the American Chemical Society*, **2007**, 129, 4430-9	16.4	45
129	Density Functional Study of the 13C NMR Chemical Shifts in Single-Walled Carbon Nanotubes with Stone Wales Defects. *Journal of Physical Chemistry C*, **2008**, 112, 11744-11750	3.8	44
128	Predicting superhard materials via a machine learning informed evolutionary structure search. *Npj Computational Materials*, **2019**, 5,	10.9	43
127	Muffin-tin orbital Wannier-like functions for insulators and metals. *ChemPhysChem*, **2005**, 6, 1934-42	3.2	43
126	Chemistry under high pressure. *Nature Reviews Chemistry*, **2020**, 4, 508-527	34.6	43

125	Reactivity of He with ionic compounds under high pressure. *Nature Communications*, **2018**, 9, 951	17.4	42
124	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, 93-109; discussion 145-53, 453-5	3.6	42
123	Self-assembly of strongly dipolar molecules on metal surfaces. *Journal of Chemical Physics*, **2015**, 142, 101921	3.9	38
122	Effects of Nonhydrostatic Stress on Structural and Optoelectronic Properties of Methylammonium Lead Bromide Perovskite. *Journal of Physical Chemistry Letters*, **2017**, 8, 3457-3465	6.4	37
121	XtalOpt version r7: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, **2011**, 182, 2305-2306	4.2	37
120	Superconducting High-Pressure Phases Composed of Hydrogen and Iodine. *Journal of Physical Chemistry Letters*, **2015**, 6, 4067-72	6.4	36
119	Locking and Unlocking the Molecular Spin Crossover Transition. *Advanced Materials*, **2017**, 29, 1702257	24	36
118	Electron Counting and a Large Family of Two-Dimensional Semiconductors. *Chemistry of Materials*, **2016**, 28, 1994-1999	9.6	35
117	The Dynamic Equilibrium Between (AlOMe)n Cages and (AlOMe)n(AlMe3)m Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation. *Macromolecules*, **2014**, 47, 8556-8569	5.5	35
116	A Review of Equation-of-State Models for Inertial Confinement Fusion Materials. *High Energy Density Physics*, **2018**, 28, 7-24	1.2	33
115	Hydrides of the Alkali Metals and Alkaline Earth Metals Under Pressure. *Comments on Inorganic Chemistry*, **2017**, 37, 78-98	3.9	28
114	Epitaxial growth of aligned atomically precise chevron graphene nanoribbons on Cu(111). *Chemical Communications*, **2017**, 53, 8463-8466	5.8	28
113	Dipole driven bonding schemes of quinonoid zwitterions on surfaces. *Chemical Communications*, **2012**, 48, 7143-5	5.8	28
112	A density functional study of the 13C NMR chemical shifts in fluorinated single-walled carbon nanotubes. *Journal of Physical Chemistry A*, **2009**, 113, 4117-24	2.8	28
111	Determining the Diameter of Functionalized Single-Walled Carbon Nanotubes with 13C NMR: A Theoretical Study. *Journal of Physical Chemistry C*, **2008**, 112, 9267-9271	3.8	28
110	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. *Journal of Physical Chemistry C*, **2018**, 122, 19370-19378	3.8	27
109	Lithium Subhydrides under Pressure and Their Superatom-like Building Blocks. *ChemPlusChem*, **2012**, 77, 969-972	2.8	27
108	Substituted Benzene Derivatives on the Cu(111) Surface. *Journal of Physical Chemistry C*, **2012**, 116, 12636-12643	3.6	27

107	NMR computations for carbon nanotubes from first principles: Present status and future directions. *International Journal of Quantum Chemistry*, **2009**, 109, 3343-3367	2.1	25
106	(Barely) solid Li(NH3)4: the electronics of an expanded metal. *Journal of the American Chemical Society*, **2011**, 133, 3535-47	16.4	24
105	Charge-Transfer-Induced Magic Cluster Formation of Azaborine Heterocycles on Noble Metal Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 6020-6030	3.8	23
104	Enantioselective Copper-Catalyzed Carboetherification of Unactivated Alkenes. *Angewandte Chemie*, **2014**, 126, 6501-6505	3.6	21
103	Proton transfer in surface-stabilized chiral motifs of croconic acid. *Physical Review B*, **2013**, 87,	3.3	21
102	XtalOpt Version r12: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, **2019**, 237, 274-275	4.2	21
101	Coverage-Dependent Interactions at the Organics Metal Interface: Quinonoid Zwitterions on Au(111). *Journal of Physical Chemistry C*, **2013**, 117, 16406-16415	3.8	20
100	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,	3.3	20
99	Magic Electret Clusters of 4-Fluorostyrene on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2012**, 3, 2069-2075	6.4	20
98	Alkali metals in ethylenediamine: a computational study of the optical absorption spectra and NMR parameters of [M(en)3( )M( )] ion pairs. *Journal of the American Chemical Society*, **2011**, 133, 4829-39	16.4	20
97	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	16.4	20
96	Equation of state, adiabatic sound speed, and Gr eisen coefficient of boron carbide along the principal Hugoniot to 700 GPa. *Physical Review B*, **2016**, 94,	3.3	20
95	Benzene derivatives adsorbed to the Ag(111) surface: Binding sites and electronic structure. *Journal of Chemical Physics*, **2015**, 142, 101924	3.9	19
94	Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen. *Angewandte Chemie - International Edition*, **2017**, 56, 10192-10195	16.4	19
93	2D Cocrystallization from H-Bonded Organic Ferroelectrics. *Journal of Physical Chemistry Letters*, **2016**, 7, 435-40	6.4	18
92	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	13.1	18
91	Pressure induced structural transitions in KH, RbH, and CsH. *Journal of Applied Physics*, **2012**, 111, 112611	2.5	18
90	RandSpg: An open-source program for generating atomistic crystal structures with specific spacegroups. *Computer Physics Communications*, **2017**, 213, 208-216	4.2	17

89	The Search for Superconductivity in High Pressure Hydrides **2019**,		17
88	Kagome-like lattice of stacked 3-hydroxyphenalenone on Cu(111). *Chemical Communications*, **2014**, 50, 8659-62	5.8	17
87	Crystal Field Splitting is Limiting the Stability and Strength of Ultra-incompressible Orthorhombic Transition Metal Tetraborides. *Scientific Reports*, **2016**, 6, 23088	4.9	17
86	Crystal Structures and Electronic Properties of Single-Layer, Few-Layer, and Multilayer GeH. *Journal of Physical Chemistry C*, **2016**, 120, 793-800	3.8	16
85	Theoretical predictions of novel superconducting phases of BaGe3 stable at atmospheric and high pressures. *Inorganic Chemistry*, **2015**, 54, 2875-84	5.1	16
84	Computational prediction and analysis of the (27)Al solid-state NMR spectrum of methylaluminoxane (MAO) at variable temperatures and field strengths. *Physical Chemistry Chemical Physics*, **2016**, 18, 24106-18	3.6	15
83	XtalOpt version r9: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, **2016**, 199, 178-179	4.2	15
82	A Computational Experiment on Single-Walled Carbon Nanotubes. *Journal of Chemical Education*, **2013**, 90, 651-655	2.4	15
81	Crystal Structures and Properties of Iron Hydrides at High Pressure. *Journal of Physical Chemistry C*, **2018**, 122, 24262-24269	3.8	15
80	Rhodizonic Acid on Noble Metals: Surface Reactivity and Coordination Chemistry. *Journal of Physical Chemistry Letters*, **2013**, 4, 3413-3419	6.4	14
79	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me)4N]2PuCl6. *Inorganic Chemistry*, **2016**, 55, 8371-80	5.1	14
78	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, 2299-305	7.8	13
77	Compression of curium pyrrolidine-dithiocarbamate enhances covalency. *Nature*, **2020**, 583, 396-399	50.4	13
76	Superconductivity in Hydrides Doped with Main Group Elements Under Pressure. *Novel Superconducting Materials*, **2017**, 3,		12
75	Computation of Chemical Shifts for Paramagnetic Molecules: A Laboratory Experiment for the Undergraduate Curriculum. *Journal of Chemical Education*, **2014**, 91, 1058-1063	2.4	12
74	Computational Modeling of the Optical Rotation of Amino Acids: An In Silico Experiment for Physical Chemistry. *Journal of Chemical Education*, **2013**, 90, 656-660	2.4	12
73	Searching for the interlayer band and unravelling the bonding in beta-ThSi(2) and alpha-ThSi(2) with NMTO Wannier-like functions. *Inorganic Chemistry*, **2010**, 49, 1384-96	5.1	12
72	XtalOpt Version r10: An open Source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, **2017**, 217, 210-211	4.2	11

71	Helical Folding of Meta-Connected Aromatic Oligoureas. *Organic Letters*, **2017**, 19, 2666-2669	6.2	11
70	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	3.8	11
69	M-graphene: a metastable two-dimensional carbon allotrope. *2D Materials*, **2020**, 7, 025047	5.9	11
68	XtalOpt version r11: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, **2018**, 222, 418-419	4.2	11
67	Building egg-tray-shaped graphenes that have superior mechanical strength and band gap. *Npj Computational Materials*, **2019**, 5,	10.9	11
66	Low energy structural dynamics and constrained libration of Li(NH3)4, the lowest melting point metal. *Chemical Communications*, **2014**, 50, 10778-81	5.8	11
65	Experimental and theoretical investigations of the thermodynamic stability of Ba-c(60) and K-C(60) compound clusters. *ACS Nano*, **2008**, 2, 1000-14	16.7	11
64	Electronic Structure of Iron Porphyrin Adsorbed to the Pt(111) Surface. *Journal of Physical Chemistry C*, **2016**, 120, 29173-29181	3.8	11
63	The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction. *Journal of Physical Chemistry C* , **2021**, 125, 1601-1620	3.8	11
62	Extended H□kel Calculations on Solids Using the Avogadro Molecular Editor and Visualizer. *Journal of Chemical Education*, **2018**, 95, 331-337	2.4	11
61	Folding and Assembly of Short □□□Hybrid Peptides: Minor Variations in Sequence and Drastic Differences in Higher-Level Structures. *Journal of the American Chemical Society*, **2019**, 141, 14239-14248	16.4	10
60	Properties of B4C in the shocked state for pressures up to 1.5 TPa. *Physical Review B*, **2017**, 95,	3.3	10
59	Magic alkali-fullerene compound clusters of extreme thermal stability. *Journal of Chemical Physics*, **2006**, 125, 191102	3.9	10
58	A Metastable CaSH Phase Composed of HS Honeycomb Sheets that is Superconducting Under Pressure. *Journal of Physical Chemistry Letters*, **2020**, 11, 9629-9636	6.4	10
57	Discovering New Materials via A Priori Crystal Structure Prediction. *Reviews in Computational Chemistry*, **2016**, 274-326		10
56	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	3.8	10
55	The AFLOW Fleet for Materials Discovery **2018**, 1-28		9
54	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9

53	Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen. *Angewandte Chemie*, **2017**, 129, 10326-10329	3.6	8
52	Determination of the structures of molecularly imprinted polymers and xerogels using an automated stochastic approach. *Analytical Chemistry*, **2013**, 85, 8577-84	7.8	8
51	A Computational Investigation of a Molecular Switch. *Journal of Chemical Education*, **2013**, 90, 1528-1532	2.4	8
50	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	3.8	8
49	Lithium-Ammoniak-Lösungen: eine molekulare Betrachtung. *Angewandte Chemie*, **2009**, 121, 8344-8381	3.6	8
48	Superfast Tetrazole-BCN Cycloaddition Reaction for Bioorthogonal Protein Labeling on Live Cells.. *Journal of the American Chemical Society*, **2021**,	16.4	8
47	Chiral surface networks of 3-HPLN □A molecular analog of rounded triangle assembly. *Surface Science*, **2014**, 629, 65-74	1.8	7
46	The Pressing Role of Theory in Studies of Compressed Matter **2017**, 571-605		6
45	Structure and Proton-Transfer Mechanism in One-Dimensional Chains of Benzimidazoles. *Journal of Physical Chemistry C*, **2016**, 120, 5804-5809	3.8	6
44	The Computational Design of Two-Dimensional Materials. *Journal of Chemical Education*, **2019**, 96, 2308-2314	2.4	6
43	On the nature of Ge-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, 12708-16	16.4	6
42	Silanization of superficially porous silica particles with p-aminophenyltrimethoxysilane. *Microchemical Journal*, **2019**, 147, 263-268	4.8	5
41	Theoretical predictions of novel potassium chloride phases under pressure. *Physical Chemistry Chemical Physics*, **2015**, 17, 12265-72	3.6	5
40	Reverse Turn Foldamers: An Expanded □Turn Motif Reinforced by Double Hydrogen Bonds. *Organic Letters*, **2020**, 22, 1003-1007	6.2	5
39	Inducing a Curl with a Stretch. *Physics Magazine*, **2019**, 12,	1.1	5
38	Fluorides of Silver Under Large Compression*. *Chemistry - A European Journal*, **2021**, 27, 5536-5545	4.8	5
37	Superalkali-Alkalide Interactions and Ion Pairing in Low-Polarity Solvents. *Journal of the American Chemical Society*, **2021**, 143, 3934-3943	16.4	5
36	Pressure-Induced Superconductivity in the Wide-Band-Gap Semiconductor Cu2Br2Se6 with a Robust Framework. *Chemistry of Materials*, **2020**, 32, 6237-6246	9.6	4

35	Crystal Structures and Electronic Properties of Xe□l Compounds at High Pressure. *Journal of Physical Chemistry C*, **2018**, 122, 2941-2950	3.8	4
34	Copper-catalyzed enantioselective alkene carboetherification for the synthesis of saturated six-membered cyclic ethers. *Chemical Communications*, **2021**, 57, 10099-10102	5.8	4
33	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, 070901	2.5	4
32	A First-Principles Exploration of NaxSy Binary Phases at 1 atm and Under Pressure. *Crystals*, **2019**, 9, 441	2.3	3
31	Predicted CsSi compound: a promising material for photovoltaic applications. *Physical Chemistry Chemical Physics*, **2020**, 22, 11578-11582	3.6	3
30	The Ideal Crystal Structure of Cristobalite X-I: A Bridge in SiO2 Densification. *Journal of Physical Chemistry C*, **2018**, 122, 17437-17446	3.8	3
29	Structural motifs and bonding in two families of boron structures predicted at megabar pressures. *Physical Review Materials*, **2021**, 5,	3.2	3
28	Electronic Structure and Superconductivity of Compressed Metal Tetrahydrides. *Chemistry - A European Journal*, **2021**, 27, 14858-14870	4.8	3
27	Major Factors for the Persistent Folding of Hybrid □□Hybrid Peptides Into Hairpins. *Frontiers in Chemistry*, **2020**, 8, 530083	5	2
26	Dimerization of cobalt-substituted Keggin phosphotungstate, [PW11O39Co(X)]5□in nonpolar solvents. *Journal of Coordination Chemistry*, **2014**, 67, 2830-2842	1.6	2
25	Nano-makisu: highly anisotropic two-dimensional carbon allotropes made by weaving together nanotubes. *Nanoscale*, **2020**, 12, 347-355	7.7	2
24	The Li-F-H ternary system at high pressures. *Journal of Chemical Physics*, **2021**, 154, 124709	3.9	2
23	Pressure-induced yttrium oxides with unconventional stoichiometries and novel properties. *Physical Review Materials*, **2021**, 5,	3.2	2
22	Crystal structures of silicon-rich lithium silicides at high pressure. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 1047-1051	2.3	2
21	An electrochemically controlled release of NHCs using iron bis(dithiolene) N-heterocyclic carbene complexes. *Inorganic Chemistry Frontiers*, **2021**, 8, 59-71	6.8	2
20	Surface Magnetism in Pristine □Rhombohedral Boron and Intersurface Exchange Coupling Mechanism of Boron Icosahedra. *Journal of Physical Chemistry Letters*, **2021**, 12, 6812-6817	6.4	2
19	Dilute carbon in H3S under pressure. *Npj Computational Materials*, **2022**, 8,	10.9	2
18	Materials under high pressure: a chemical perspective. *Applied Physics A: Materials Science and Processing*, **2022**, 128, 1	2.6	2

17	RbB3Si3: An Alkali Metal Borosilicide that is Metastable and Superconducting at 1 atm. *Journal of Physical Chemistry C*, **2020**, 124, 14826-14831	3.8	1
16	First principles investigation on how site preference and entropy affect the stability of (EuxM1−x)2Ge2Pb (M = Ca, Sr, Ba) polar intermetallics. *Canadian Journal of Chemistry*, **2016**, 94, 312-320	0.9	1
15	Density Functional Studies of the 13C NMR Chemical Shifts in Single‐Walled Carbon Nanotubes. *AIP Conference Proceedings*, **2007**,	0	1
14	Downfolding and N-ization of Basis Sets of Slater Type Orbitals. *AIP Conference Proceedings*, **2007**,	0	1
13	Interplay of Halogen and Weak Hydrogen Bonds in the Formation of Magic Nanoclusters on Surfaces. *Journal of Physical Chemistry C*, **2022**, 126, 588-596	3.8	1
12	Stable pseudo[3]rotaxanes with strong positive binding cooperativity based on shape-persistent aromatic oligoamide macrocycles. *Chemical Communications*, **2021**, 57, 11645-11648	5.8	1
11	Anchoring effect of distorted octahedra on the stability and strength of platinum metal pernitrides. *Physical Review Materials*, **2019**, 3,	3.2	1
10	The AFLOW Fleet for Materials Discovery **2020**, 1785-1812		1
9	Modeling Methylaluminoxane (MAO) **2001**, 109-123		1
8	Materials genome approach to organic ferroelectrics and piezoelectrics. *International Journal of Nanotechnology*, **2018**, 15, 784	1.5	1
7	Laser-Induced Cooperative Transition in Molecular Electronic Crystal. *Advanced Materials*, **2021**, 33, e2103000	24	1
6	Nature of the bonded-to-atomic transition in liquid silica to TPa pressures. *Journal of Applied Physics*, **2022**, 131, 071101	2.5	1
5	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. *Angewandte Chemie - International Edition*,	16.4	1
4	The AFLOW Fleet for Materials Discovery **2019**, 1-28		
3	Insight into the Adsorption Structure of TIPS-Pentacene on Noble Metal Surfaces. *Journal of Physical Chemistry C*, **2022**, 126, 2689-2698	3.8	
2	Laser-Induced Cooperative Transition in Molecular Electronic Crystal (Adv. Mater. 39/2021). *Advanced Materials*, **2021**, 33, 2170309	24	
1	Electrochemical Atomic Force Microscopy and First-Principles Calculations of Ferriprotoporphyrin Adsorption and Polymerization. *Langmuir*, **2018**, 34, 11335-11346	4	