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	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
2	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
3	Halogen and structure sensitivity of halobenzene adsorption on copper surfaces. Physical Chemistry Chemical Physics, 2022, 24, 4485-4492.	2.8	2
4	Insight into the Adsorption Structure of TIPS-Pentacene on Noble Metal Surfaces. Journal of Physical Chemistry C, 2022, 126, 2689-2698.	3.1	0
5	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
6	Nature of the bonded-to-atomic transition in liquid silica to TPa pressures. Journal of Applied Physics, 2022, 131, .	2.5	4
7	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
8	Structural Diversity and Superconductivity in Sâ€“Pâ€“H Ternary Hydrides under Pressure. Journal of Physical Chemistry C, 2022, 126, 7208-7220.	3.1	8
9	Dilute carbon in H3S under pressure. Npj Computational Materials, 2022, 8, .	8.7	9
10	Materials under high pressure: a chemical perspective. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	2.3	15
11	Computational materials discovery. Journal of Chemical Physics, 2022, 156, .	3.0	2
12	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie - International Edition, 2022, 61, .	13.8	5
13	The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure. Angewandte Chemie, 2022, 134, .	2.0	3
14	The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction. Journal of Physical Chemistry C, 2021, 125, 1601-1620.	3.1	42
15	An electrochemically controlled release of NHCs using iron bis(dithiolene) N-heterocyclic carbene complexes. Inorganic Chemistry Frontiers, 2021, 8, 59-71.	6.0	4
16	Copper-catalyzed enantioselective alkene carboetherification for the synthesis of saturated six-membered cyclic ethers. Chemical Communications, 2021, 57, 10099-10102.	4.1	8
17	Fluorides of Silver Under Large Compression**. Chemistry - A European Journal, 2021, 27, 5536-5545.	3.3	14
18	Superalkaliâ€“Alkalide Interactions and Ion Pairing in Low-Polarity Solvents. Journal of the American Chemical Society, 2021, 143, 3934-3943.	13.7	17

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19	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
20	The Liâ€“Fâ€“H ternary system at high pressures. Journal of Chemical Physics, 2021, 154, 124709.	3.0	2
21	Pressure-induced yttrium oxides with unconventional stoichiometries and novel properties. Physical Review Materials, 2021, 5, .	2.4	8
22	Structural motifs and bonding in two families of boron structures predicted at megabar pressures. Physical Review Materials, 2021, 5, .	2.4	8
23	Reliable folding of hybrid tetrapeptides into short Î²-hairpins. Chinese Chemical Letters, 2021, , .	9.0	0
24	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
25	Laserâ€induced Cooperative Transition in Molecular Electronic Crystal. Advanced Materials, 2021, 33, e2103000.	21.0	6
26	Electronic Structure and Superconductivity of Compressed Metal Tetrahydrides. Chemistry - A European Journal, 2021, 27, 14858-14870.	3.3	11
27	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
28	Laserâ€induced Cooperative Transition in Molecular Electronic Crystal (Adv. Mater. 39/2021). Advanced Materials, 2021, 33, .	21.0	0
29	Nano-makisu: highly anisotropic two-dimensional carbon allotropes made by weaving together nanotubes. Nanoscale, 2020, 12, 347-355.	5.6	3
30	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
31	Compression of curium pyrrolidine-dithiocarbamate enhances covalency. Nature, 2020, 583, 396-399.	27.8	34
32	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
33	Chemistry under high pressure. Nature Reviews Chemistry, 2020, 4, 508-527.	30.2	117
34	Major Factors for the Persistent Folding of Hybrid Î±, Î², Î³-Hybrid Peptides Into Hairpins. Frontiers in Chemistry, 2020, 8, 530083.	3.6	2
35	Predicted CsSi compound: a promising material for photovoltaic applications. Physical Chemistry Chemical Physics, 2020, 22, 11578-11582.	2.8	7
36	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

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37	Pressure-Induced Superconductivity in the Wide-Band-Gap Semiconductor Cu2Br2Se6 with a Robust Framework. Chemistry of Materials, 2020, 32, 6237-6246.	6.7	6
38	M-graphene: a metastable two-dimensional carbon allotrope. 2D Materials, 2020, 7, 025047.	4.4	30
39	Reverse Turn Foldamers: An Expanded Î²-Turn Motif Reinforced by Double Hydrogen Bonds. Organic Letters, 2020, 22, 1003-1007.	4.6	9
40	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 mathvariant="n	3.2	98
41	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
42	The Computational Design of Two-Dimensional Materials. Journal of Chemical Education, 2019, 96, 2308-2314.	2.3	8
43	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
44	Building egg-tray-shaped graphenes that have superior mechanical strength and band gap. Npj Computational Materials, 2019, 5, .	8.7	19
45	Predicting superhard materials via a machine learning informed evolutionary structure search. Npj Computational Materials, 2019, 5, .	8.7	74
46	A First-Principles Exploration of NaxSy Binary Phases at 1 atm and Under Pressure. Crystals, 2019, 9, 441.	2.2	8
47	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0
48	The Search for Superconductivity in High Pressure Hydrides. , 2019, , .		27
49	Silanization of superficially porous silica particles with p-aminophenyltrimethoxysilane. Microchemical Journal, 2019, 147, 263-268.	4.5	8
50	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
51	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
52	XtalOptÂVersion r12: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2019, 237, 274-275.	7.5	37
53	Anchoring effect of distorted octahedra on the stability and strength of platinum metal pernitrides. Physical Review Materials, 2019, 3, .	2.4	1
54	Reactivity ofÂHe withÂionic compounds under high pressure. Nature Communications, 2018, 9, 951.	12.8	59

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55	High Hydrides of Scandium under Pressure: Potential Superconductors. Journal of Physical Chemistry C, 2018, 122, 6298-6309.	3.1	83
56	Crystal Structures and Electronic Properties of Xeâ€“Cl Compounds at High Pressure. Journal of Physical Chemistry C, 2018, 122, 2941-2950.	3.1	7
57	XtalOptÂversion r11: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2018, 222, 418-419.	7.5	11
58	Extended HÃ¼ckel Calculations on Solids Using the Avogadro Molecular Editor and Visualizer. Journal of Chemical Education, 2018, 95, 331-337.	2.3	22
59	Materials genome approach to organic ferroelectrics and piezoelectrics. International Journal of Nanotechnology, 2018, 15, 784.	0.2	1
60	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
61	Crystal Structures and Properties of Iron Hydrides at High Pressure. Journal of Physical Chemistry C, 2018, 122, 24262-24269.	3.1	24
62	Electrochemical Atomic Force Microscopy and First-Principles Calculations of Ferriprotoporphyrin Adsorption and Polymerization. Langmuir, 2018, 34, 11335-11346.	3.5	0
63	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	3.0	72
64	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
65	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. Journal of Physical Chemistry C, 2018, 122, 19370-19378.	3.1	38
66	A Review of Equation-of-State Models for Inertial Confinement Fusion Materials. High Energy Density Physics, 2018, 28, 7-24.	1.5	54
67	Hydrides of the Alkali Metals and Alkaline Earth Metals Under Pressure. Comments on Inorganic Chemistry, 2017, 37, 78-98.	5.2	35
68	Superconductivity in Hydrides Doped with Main Group Elements Under Pressure. Novel Superconducting Materials, 2017, 3, .	0.8	15
69	Graphene-like Boronâ€“Carbonâ€“Nitrogen Monolayers. ACS Nano, 2017, 11, 2486-2493.	14.6	154
70	XtalOptÂVersion r10: An openâ€“source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2017, 217, 210-211.	7.5	11
71	Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen. Angewandte Chemie, 2017, 129, 10326-10329.	2.0	13
72	Helical Folding of Meta-Connected Aromatic Oligoureas. Organic Letters, 2017, 19, 2666-2669.	4.6	11

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73	Epitaxial growth of aligned atomically precise chevron graphene nanoribbons on Cu(111). Chemical Communications, 2017, 53, 8463-8466.	4.1	36
74	RandSpg: An open-source program for generating atomistic crystal structures with specific spacegroups. Computer Physics Communications, 2017, 213, 208-216.	7.5	30
75	Locking and Unlocking the Molecular Spin Crossover Transition. Advanced Materials, 2017, 29, 1702257.	21.0	55
76	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
77	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
78	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
79	Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen. Angewandte Chemie - International Edition, 2017, 56, 10192-10195.	13.8	27
80	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
81	Crystal Field Splitting is Limiting the Stability and Strength of Ultra-incompressible Orthorhombic Transition Metal Tetraborides. Scientific Reports, 2016, 6, 23088.	3.3	18
82	Electronic Structure of Iron Porphyrin Adsorbed to the Pt(111) Surface. Journal of Physical Chemistry C, 2016, 120, 29173-29181.	3.1	13
83	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
84	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me)₄N]₂PuCl₆. Inorganic Chemistry, 2016, 55, 8371-8380.	4.0	20
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	Decomposition Products of Phosphine Under Pressure: PH₂ Stable and Superconducting?. Journal of the American Chemical Society, 2016, 138, 1884-1892.	13.7	102
87	2D Cocrystallization from H-Bonded Organic Ferroelectrics. Journal of Physical Chemistry Letters, 2016, 7, 435-440.	4.6	19
88	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
89	XtalOpt Âversion r9: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2016, 199, 178-179.	7.5	16
90	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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91	First principles investigation on how site preference and entropy affect the stability of (Eu_xM_{1â€“}_x)₂Ge₂Pb (M = Ca,) Tj ET Q q 1 1 0.784314	1	7
92	Structure and Proton-Transfer Mechanism in One-Dimensional Chains of Benzimidazoles. Journal of Physical Chemistry C, 2016, 120, 5804-5809.	3.1	8
93	Electron Counting and a Large Family of Two-Dimensional Semiconductors. Chemistry of Materials, 2016, 28, 1994-1999.	6.7	52
94	Theoretical Predictions of Novel Superconducting Phases of BaGe3 Stable at Atmospheric and High Pressures. Inorganic Chemistry, 2015, 54, 2875-2884.	4.0	17
95	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
96	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
97	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
98	Theoretical predictions of novel potassium chloride phases under pressure. Physical Chemistry Chemical Physics, 2015, 17, 12265-12272.	2.8	6
99	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
100	Self-assembly of strongly dipolar molecules on metal surfaces. Journal of Chemical Physics, 2015, 142, 101921.	3.0	38
101	Benzene derivatives adsorbed to the Ag(111) surface: Binding sites and electronic structure. Journal of Chemical Physics, 2015, 142, 101924.	3.0	22
102	Superconducting High-Pressure Phases Composed of Hydrogen and Iodine. Journal of Physical Chemistry Letters, 2015, 6, 4067-4072.	4.6	41
103	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
104	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
105	Chiral surface networks of 3-HPLN â€" A molecular analog of rounded triangle assembly. Surface Science, 2014, 629, 65-74.	1.9	7
106	Enantioselective Copperâ€Catalyzed Carboetherification of Unactivated Alkenes. Angewandte Chemie - International Edition, 2014, 53, 6383-6387.	13.8	88
107	Dimerization of cobalt-substituted Keggin phosphotungstate, [PW₁₁O₃₉Co(X)]^{5â^'}, in nonpolar solvents. Journal of Coordination Chemistry, 2014, 67, 2830-2842.	2.2	2
108	Kagome-like lattice of Ï€â€“Ï€ stacked 3-hydroxyphenalenone on Cu(111). Chemical Communications, 2014, 50, 8659-8662.	4.1	19

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109	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
110	Composition and Constitution of Compressed Strontium Polyhydrides. Journal of Physical Chemistry C, 2014, 118, 6433-6447.	3.1	59
111	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
112	Determination of the Structures of Molecularly Imprinted Polymers and Xerogels Using an Automated Stochastic Approach. Analytical Chemistry, 2013, 85, 8577-8584.	6.5	11
113	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
114	A Computational Investigation of a Molecular Switch. Journal of Chemical Education, 2013, 90, 1528-1532.	2.3	9
115	Rhodizonic Acid on Noble Metals: Surface Reactivity and Coordination Chemistry. Journal of Physical Chemistry Letters, 2013, 4, 3413-3419.	4.6	14
116	Metallization of magnesium polyhydrides under pressure. Physical Review B, 2013, 87, .	3.2	102
117	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
118	Proton transfer in surface-stabilized chiral motifs of croconic acid. Physical Review B, 2013, 87, .	3.2	22
119	A Computational Experiment on Single-Walled Carbon Nanotubes. Journal of Chemical Education, 2013, 90, 651-655.	2.3	19
120	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
121	Pressure induced structural transitions in KH, RbH, and CsH. Journal of Applied Physics, 2012, 111, 112611.	2.5	23
122	Compressed Cesium Polyhydrides: Cs⁺ Sublattices and H₃^{â€“} Three-Connected Nets. Inorganic Chemistry, 2012, 51, 9333-9342.	4.0	54
123	Surface state engineering of moleculeâ€“molecule interactions. Physical Chemistry Chemical Physics, 2012, 14, 4971.	2.8	56
124	Dipole driven bonding schemes of quinonoid zwitterions on surfaces. Chemical Communications, 2012, 48, 7143.	4.1	31
125	Magic Electret Clusters of 4-Fluorostyrene on Metal Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 2069-2075.	4.6	22
126	High Pressure Potassium Polyhydrides: A Chemical Perspective. Journal of Physical Chemistry C, 2012, 116, 13322-13328.	3.1	63

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127	Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. Journal of Cheminformatics, 2012, 4, 17.	6.1	6,063
128	Lithium Subhydrides under Pressure and Their Superatomâ€like Building Blocks. ChemPlusChem, 2012, 77, 969-972.	2.8	30
129	Substituted Benzene Derivatives on the Cu(111) Surface. Journal of Physical Chemistry C, 2012, 116, 12636-12643.	3.1	28
130	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
131	Rubidium Polyhydrides Under Pressure: Emergence of the Linear H₃^{â^'} Species. Chemistry - A European Journal, 2012, 18, 5013-5021.	3.3	68
132	Identifying duplicate crystal structures: XtalComp, an open-source solution. Computer Physics Communications, 2012, 183, 690-697.	7.5	71
133	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 ETQq1 1 0.784 Physical Review Letters, 2011, 106, 237002.	7.8	93
134	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
135	(Barely) Solid Li(NH₃)₄: The Electronics of an Expanded Metal. Journal of the American Chemical Society, 2011, 133, 3535-3547.	13.7	35
136	XtalOpt version r7: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2011, 182, 2305-2306.	7.5	41
137	XtalOpt: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2011, 182, 372-387.	7.5	263
138	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
139	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
140	A Molecular Perspective on Lithiumâ€“Ammonia Solutions. Angewandte Chemie - International Edition, 2009, 48, 8198-8232.	13.8	155
141	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
142	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
143	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
144	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

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145	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
146	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
147	Density Functional Studies of the [sup 13]C NMR Chemical Shifts in Singleâ€"Walled Carbon Nanotubes. AIP Conference Proceedings, 2007, , .	0.4	1
148	Downfolding and N-ization of Basis Sets of Slater Type Orbitals. AIP Conference Proceedings, 2007, , .	0.4	2
149	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
150	Magic alkali-fullerene compound clusters of extreme thermal stability. Journal of Chemical Physics, 2006, 125, 191102.	3.0	10
151	Muffin-Tin Orbital Wannier-Like Functions for Insulators and Metals. ChemPhysChem, 2005, 6, 1934-1942.	2.1	49
152	Density Functional Calculations of the13C NMR Chemical Shifts in (9,0) Single-Walled Carbon Nanotubes.. ChemInform, 2004, 35, no.	0.0	0
153	Theoretical studies of the structure and function of MAO (methylaluminoxane). Progress in Polymer Science, 2004, 29, 107-148.	24.7	177
154	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
155	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
156	Relativistic Density-Functional Computations of the Chemical Shift of129Xe in Xe@C60. Journal of Physical Chemistry A, 2003, 107, 4967-4972.	2.5	70
157	Toward the Identification of Dormant and Active Species in MAO (Methylaluminoxane)-Activated, Dimethylzirconocene-Catalyzed Olefin Polymerization. Organometallics, 2002, 21, 83-92.	2.3	73
158	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
159	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
160	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
161	Modeling Methylaluminoxane (MAO). , 2001, , 109-123.		1
162	Pushing Towards Room-Temperature Superconductivity. Physics Magazine, 0, 12, .	0.1	5