

# Roald Hoffmann

## List of Publications by Year in descending order

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313  
papers

36,662  
citations

6486

82  
h-index

3782

185  
g-index

365  
all docs

365  
docs citations

365  
times ranked

20972  
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical Studies of Furan and Thiophene Nanthreads: Structures, Cycloaddition Barriers, and Activation Volumes. <i>Journal of the American Chemical Society</i> , 2022, 144, 9044-9056.	6.6	5
2	Synthesis, structure, and magnetic properties of the quaternary oxysulfides $\text{LnV}_5\text{V}_3\text{O}_7\text{S}_6$ ( $\text{Ln} = \text{La, Ce}$ ). <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2021, 76, 677-688.	0.3	0
3	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part C. Toward Consilience. <i>Angewandte Chemie</i> , 2020, 132, 13798-13814.	1.6	7
4	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part B. The March of Simulation, for Better or Worse. <i>Angewandte Chemie</i> , 2020, 132, 13256-13278.	1.6	2
5	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part A. Stage Setting. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12590-12610.	7.2	18
6	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part B. The March of Simulation, for Better or Worse. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 13156-13178.	7.2	16
7	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part C. Toward Consilience. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 13694-13710.	7.2	12
8	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part A. Stage Setting. <i>Angewandte Chemie</i> , 2020, 132, 12690-12710.	1.6	3
9	Fermi surface studies of the low-temperature structure of sodium. <i>Physical Review B</i> , 2020, 101, .	1.1	5
10	Varying Electronic Configurations in Compressed Atoms: From the Role of the Spatial Extension of Atomic Orbitals to the Change of Electronic Configuration as an Isobaric Transformation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5047-5056.	2.3	14
11	Do Diradicals Behave Like Radicals?. <i>Chemical Reviews</i> , 2019, 119, 11291-11351.	23.0	228
12	Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischer-Tropsch Synthesis. <i>Catalysis Letters</i> , 2019, 149, 645-664.	1.4	19
13	Squeezing All Elements in the Periodic Table: Electron Configuration and Electronegativity of the Atoms under Compression. <i>Journal of the American Chemical Society</i> , 2019, 141, 10253-10271.	6.6	138
14	Cross Conjugation in Polyenes and Related Hydrocarbons: What Can Be Learned from Valence Bond Theory about Single-Molecule Conductance?. <i>Journal of the American Chemical Society</i> , 2019, 141, 6030-6047.	6.6	26
15	Expanding the Frontiers of Higher-Order Cycloadditions. <i>Accounts of Chemical Research</i> , 2019, 52, 3488-3501.	7.6	83
16	Electronegativity Seen as the Ground-State Average Valence Electron Binding Energy. <i>Journal of the American Chemical Society</i> , 2019, 141, 342-351.	6.6	139
17	High-pressure lithium as an elemental topological semimetal. <i>Physical Review Materials</i> , 2019, 3, .	0.9	7
18	Surface Activation of Transition Metal Nanoparticles for Heterogeneous Catalysis: What We Can Learn from Molecular Dynamics. <i>ACS Catalysis</i> , 2018, 8, 3365-3375.	5.5	58

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19	Coarctate and Möbius: The Helical Orbitals of Allene and Other Cumulenes. ACS Central Science, 2018, 4, 688-700.	5.3	46
20	Quantum Interference, Graphs, Walks, and Polynomials. Chemical Reviews, 2018, 118, 4887-4911.	23.0	50
21	High Hydrides of Scandium under Pressure: Potential Superconductors. Journal of Physical Chemistry C, 2018, 122, 6298-6309.	1.5	83
22	All the Ways To Have Substituted Nanothreads. Journal of Chemical Theory and Computation, 2018, 14, 1131-1140.	2.3	14
23	Alkali-Metal Trihalides: $M+X_3$ Ion Pair or $MX_2$ Complex?. Journal of Physical Chemistry B, 2018, 122, 3339-3353.	1.2	8
24	Carbon Nitride Nanowire Crystals Derived from Pyridine. Journal of the American Chemical Society, 2018, 140, 4969-4972.	6.6	81
25	Potential Semiconducting and Superconducting Metastable $Si_3C$ Structures under Pressure. Chemistry of Materials, 2018, 30, 421-427.	3.2	5
26	Alkyl Isosteres. Journal of the American Chemical Society, 2018, 140, 12844-12852.	6.6	4
27	Mirrors of Bonding in Metal Halide Perovskites. Journal of the American Chemical Society, 2018, 140, 12996-13010.	6.6	75
28	Eight-coordinate fluoride in a silicate double-four-ring. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 828-833.	3.3	17
29	Evidence from Fermi surface analysis for the low-temperature structure of lithium. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 5389-5394.	3.3	22
30	An Iodobenzene Story. Journal of the American Chemical Society, 2017, 139, 7124-7129.	6.6	10
31	Ternary Gold Hydrides: Routes to Stable and Potentially Superconducting Compounds. Journal of the American Chemical Society, 2017, 139, 8740-8751.	6.6	47
32	Potential high- $T_c$ superconducting lanthanum and yttrium hydrides at high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6990-6995.	3.3	651
33	Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. Journal of the American Chemical Society, 2017, 139, 9302-9316.	6.6	33
34	Dioxygen: What Makes This Triplet Diradical Kinetically Persistent?. Journal of the American Chemical Society, 2017, 139, 9010-9018.	6.6	147
35	The Green's function for the Hückel (tight binding) model. Journal of Mathematical Physics, 2017, 58, 033505.	0.5	15
36	Quasimolecules in Compressed Lithium. Angewandte Chemie, 2017, 129, 992-995.	1.6	16

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37	Enhancing the conductivity of molecular electronic devices. <i>Journal of Chemical Physics</i> , 2017, 146, .	1.2	39
38	Quasimolecules in Compressed Lithium. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 972-975.	7.2	32
39	Reply to Martinez-Canales et al.: The structure(s) of lithium at low temperatures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8810-E8811.	3.3	1
40	Mechanochemical Synthesis of Carbon Nanothread Single Crystals. <i>Journal of the American Chemical Society</i> , 2017, 139, 16343-16349.	6.6	88
41	Stabilizing a different cyclooctatetraene stereoisomer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 9803-9808.	3.3	26
42	Druckeffekte auf organische Reaktionen in Fluiden – eine neue theoretische Perspektive. <i>Angewandte Chemie</i> , 2017, 129, 11278-11295.	1.6	10
43	The Effect of Pressure on Organic Reactions in Fluids – a New Theoretical Perspective. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11126-11142.	7.2	89
44	Donor–Acceptor Strategies for Stabilizing Planar Diphlobenes. <i>Organometallics</i> , 2017, 36, 4825-4833.	1.1	3
45	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. <i>Chemical Reviews</i> , 2016, 116, 8173-8192.	23.0	155
46	Structural Diversity and Electron Confinement in $\text{Li}_4\text{N}$ : Potential for 0-D, 2-D, and 3-D Electrides. <i>Journal of the American Chemical Society</i> , 2016, 138, 14108-14120.	6.6	59
47	Atomic and Ionic Radii of Elements 1–96. <i>Chemistry - A European Journal</i> , 2016, 22, 14625-14632.	1.7	239
48	Semiconductive $\text{K}_2\text{MSb}_3(\text{SH})$ ( $\text{M} = \text{Zn}, \text{Cd}$ ) Featuring One-Dimensional $\text{[M}_2\text{Sb}_2\text{S}_6(\text{SH})_2]$ Chains. <i>Inorganic Chemistry</i> , 2016, 55, 9742-9747.		18
49	<i>Homo Citans</i> und Kohlenstoffallotrope: Für eine Ethik des Zitierens. <i>Angewandte Chemie</i> , 2016, 128, 11122-11139.	1.6	17
50	<i>Homo Citans</i> and Carbon Allotropes: For an Ethics of Citation. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10962-10976.	7.2	251
51	Helical Oligoenes: Conformations, Bond Alternation, and Competing Through-Bond and Through-Space Transmission. <i>Chemistry - A European Journal</i> , 2016, 22, 4878-4888.	1.7	21
52	$\text{AuO}$ : Evolving from Dis- to Comproportionation and Back Again. <i>Inorganic Chemistry</i> , 2016, 55, 1278-1286.	1.9	24
53	The Dimerization of $\text{H}_2\text{NO}$ . <i>Journal of Physical Chemistry A</i> , 2016, 120, 1283-1296.	1.1	3
54	Distinguishing Bonds. <i>Journal of the American Chemical Society</i> , 2016, 138, 3731-3744.	6.6	48

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55	Close relation between quantum interference in molecular conductance and diradical existence. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E413-9.	3.3	77
56	Molecular CsF <sub>5</sub> and CsF <sub>2</sub> <sup>+</sup> . Angewandte Chemie - International Edition, 2015, 54, 8275-8278.	7.2	17
57	Molecular CsF <sub>5</sub> and CsF <sub>2</sub> <sup>+</sup> . Angewandte Chemie, 2015, 127, 8393-8396.	1.6	7
58	Anomalous orbital admixture in ammine complexes. Journal of Organometallic Chemistry, 2015, 792, 6-12.	0.8	5
59	Theoretical Study of Phase Separation of Scandium Hydrides under High Pressure. Journal of Physical Chemistry C, 2015, 119, 5614-5625.	1.5	37
60	High-Pressure Electrides: The Chemical Nature of Interstitial Quasiatoms. Journal of the American Chemical Society, 2015, 137, 3631-3637.	6.6	134
61	Toward an Experimental Quantum Chemistry: Exploring a New Energy Partitioning. Journal of the American Chemical Society, 2015, 137, 10282-10291.	6.6	36
62	Exponential Attenuation of Through-Bond Transmission in a Polyene: Theory and Potential Realizations. ACS Nano, 2015, 9, 11109-11120.	7.3	45
63	Linearly Polymerized Benzene Arrays As Intermediates, Tracing Pathways to Carbon Nanotubes. Journal of the American Chemical Society, 2015, 137, 14373-14386.	6.6	86
64	For the M. Hargittai issue. Structural Chemistry, 2015, 26, 1165-1165.	1.0	1
65	Chemical bonding in hydrogen and lithium under pressure. Journal of Chemical Physics, 2015, 143, 064702.	1.2	24
66	Tension in Chemistry and Its Contents. Accountability in Research, 2015, 22, 330-345.	1.6	2
67	Li-Filled, B-Substituted Carbon Clathrates. Journal of the American Chemical Society, 2015, 137, 12639-12652.	6.6	42
68	Tuning the Ground State Symmetry of Acetylenyl Radicals. ACS Central Science, 2015, 1, 270-278.	5.3	5
69	The Many Guises of Aromaticity. American Scientist, 2015, 103, 18.	0.1	77
70	Quantum interference in polyenes. Journal of Chemical Physics, 2014, 141, 224311.	1.2	55
71	High Pressure Electrides: A Predictive Chemical and Physical Theory. Accounts of Chemical Research, 2014, 47, 1311-1317.	7.6	199
72	Frontier Orbital Control of Molecular Conductance and its Switching. Angewandte Chemie - International Edition, 2014, 53, 4093-4097.	7.2	75

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73	Lithium hydroxide, LiOH, at elevated densities. Journal of Chemical Physics, 2014, 141, 024505.	1.2	20
74	Seeking Small Molecules for Singlet Fission: A Heteroatom Substitution Strategy. Journal of the American Chemical Society, 2014, 136, 12638-12647.	6.6	121
75	The Low-Lying Electronic States of Pentacene and Their Roles in Singlet Fission. Journal of the American Chemical Society, 2014, 136, 5755-5764.	6.6	197
76	The Unusual and the Expected in the Si/C Phase Diagram. Journal of the American Chemical Society, 2013, 135, 11651-11656.	6.6	42
77	Squaroglitter: A 3,4-Connected Carbon Net. Journal of Chemical Theory and Computation, 2013, 9, 3855-3859.	2.3	8
78	Evolving Structural Diversity and Metallicity in Compressed Lithium Azide. Journal of Physical Chemistry C, 2013, 117, 20838-20846.	1.5	51
79	Isotopic differentiation and sublattice melting in dense dynamic ice. Physical Review B, 2013, 88, .	1.1	14
80	Small but Strong Lessons from Chemistry for Nanoscience. Angewandte Chemie - International Edition, 2013, 52, 93-103.	7.2	88
81	Binary Compounds of Boron and Beryllium: A Rich Structural Arena with Space for Predictions. Chemistry - A European Journal, 2013, 19, 4184-4197.	1.7	26
82	One Molecule, Two Atoms, Three Views, Four Bonds?. Angewandte Chemie - International Edition, 2013, 52, 3020-3033.	7.2	129
83	Two-Dimensional CdSe Nanosheets and their Interaction with Stabilizing Ligands. Advanced Materials, 2013, 25, 261-266.	11.1	39
84	A Response to the Critical Comments on "One Molecule, Two Atoms, Three Views, Four Bonds?". Angewandte Chemie - International Edition, 2013, 52, 5926-5928.	7.2	55
85	Hypervalent Compounds as Ligands: I <sub>3</sub> -Anion Adducts with Transition Metal Pentacarbonyls. Inorganic Chemistry, 2013, 52, 7161-7171.	1.9	23
86	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. Physical Review B, 2013, 88, .	1.1	63
87	The Close Relationships between the Crystal Structures of MO and MSO <sub>4</sub> (M = Group 10, 11, or 12) Tj ETQq1 1 0.784314 rgBT /Overlaid 5 2013, 2013, 5094-5102.	1.0	5
88	LiB and its boron-deficient variants under pressure. Physical Review B, 2012, 86, .	1.1	23
89	High pressure ices. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 745-750.	3.3	92
90	Molecular Orbitals of the Oxocarbons (CO) <sub>2</sub> , (CO) <sub>3</sub> , (CO) <sub>4</sub> . Why Does (CO) <sub>4</sub> Have a Triplet Ground State?. Journal of the American Chemical Society, 2012, 134, 10259-10270.	6.6	43

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91	Graphane Nanotubes. ACS Nano, 2012, 6, 7142-7150.	7.3	32
92	A fresh look at dense hydrogen under pressure. I. An introduction to the problem, and an index probing equalization of H-H distances. Journal of Chemical Physics, 2012, 136, 074501.	1.2	61
93	A fresh look at dense hydrogen under pressure. II. Chemical and physical models aiding our understanding of evolving H-H separations. Journal of Chemical Physics, 2012, 136, 074502.	1.2	42
94	A fresh look at dense hydrogen under pressure. III. Two competing effects and the resulting intra-molecular H-H separation in solid hydrogen under pressure. Journal of Chemical Physics, 2012, 136, 074503.	1.2	35
95	A fresh look at dense hydrogen under pressure. IV. Two structural models on the road from paired to monatomic hydrogen, via a possible non-crystalline phase. Journal of Chemical Physics, 2012, 136, 074504.	1.2	29
96	LiBeB: A predicted phase with structural and electronic peculiarities. Physical Review B, 2012, 86, .	1.1	14
97	Editorial: Was, wieder ein Chemie-Nobelpreis für einen Nichtchemiker?. Angewandte Chemie, 2012, 124, 1768-1769.	1.6	2
98	Stabilizing $H_3^+$ : Or Are We Stabilizing a Proton?. ChemPhysChem, 2012, 13, 2286-2288.	1.0	8
99	WH <sub>6</sub> under pressure. Journal of Physics Condensed Matter, 2012, 24, 155701.	0.7	29
100	Hunting dimers. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	6
101	Editorial: What, Another Nobel Prize in Chemistry to a Nonchemist?. Angewandte Chemie - International Edition, 2012, 51, 1734-1735.	7.2	5
102	Hunting dimers. Highlights in Theoretical Chemistry, 2012, , 3-13.	0.0	0
103	Molecular models for WH <sub>6</sub> under pressure. New Journal of Chemistry, 2011, 35, 2349.	1.4	10
104	Connecting the Chemical and Physical Viewpoints of What Determines Structure: From 1-D Chains to $\beta$ -Brasses. Chemical Reviews, 2011, 111, 4522-4545.	23.0	50
105	BH <sub>3</sub> under Pressure: Leaving the Molecular Diborane Motif. Journal of the American Chemical Society, 2011, 133, 21002-21009.	6.6	31
106	(Barely) Solid Li(NH <sub>3</sub> ) <sub>4</sub> : The Electronics of an Expanded Metal. Journal of the American Chemical Society, 2011, 133, 3535-3547.	6.6	35
107	Benzene under High Pressure: a Story of Molecular Crystals Transforming to Saturated Networks, with a Possible Intermediate Metallic Phase. Journal of the American Chemical Society, 2011, 133, 9023-9035.	6.6	146
108	High Pressure Stabilization and Emergent Forms of $PbH_4$ . Physical Review Letters, 2011, 107, 037002.	2.9	55

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109	International Year of Chemistry 2011: Sustainable Development. <i>Clinical Chemistry</i> , 2011, 57, 144-144.	1.5	1
110	Segregation into Layers: A General Problem for Structural Instability under Pressure, Exemplified by $\text{SnH}_4$ . <i>ChemPhysChem</i> , 2010, 11, 3105-3112.	1.0	14
111	Exploring Group 14 Structures: 1D to 2D to 3D. <i>Chemistry - A European Journal</i> , 2010, 16, 6555-6566.	1.7	29
112	JUST WHEN WE ARE SAFEST. <i>Yale Review</i> , 2010, 98, 126-127.	0.0	0
113	Reconstructing a solid-solid phase transformation pathway in CdSe nanosheets with associated soft ligands. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 17119-17124.	3.3	120
114	Compressing the Most Hydrogen-Rich Inorganic Ion. <i>Journal of the American Chemical Society</i> , 2010, 132, 748-755.	6.6	25
115	Two Lives. <i>American Scientist</i> , 2010, 98, 117.	0.1	6
116	Element Lines: Bonding in the Ternary Gold Polyphosphides, $\text{Au}_2\text{MP}_2$ with M = Pb, Tl, or Hg. <i>Journal of the American Chemical Society</i> , 2009, 131, 2199-2207.	6.6	22
117	A little bit of lithium does a lot for hydrogen. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 17640-17643.	3.3	245
118	Group 12 Dihalides: Structural Predilections from Gases to Solids. <i>Chemistry - A European Journal</i> , 2009, 15, 158-177.	1.7	45
119	A Bonding Quandary – A Demonstration of the Fact That Scientists Are Not Born With Logic. <i>Chemistry - A European Journal</i> , 2009, 15, 8358-8373.	1.7	77
120	A Molecular Perspective on Lithium-Ammonia Solutions. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 8198-8232.	7.2	155
121	Large-Scale Soft Colloidal Template Synthesis of 1.4-...nm Thick CdSe Nanosheets. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 6861-6864.	7.2	298
122	$\frac{1}{2}$ Bonds in an Unusual Coordinated $\text{S}_4^{2-}$ Rectangle. <i>Chemistry - an Asian Journal</i> , 2009, 4, 302-313.	1.7	10
123	Cover Picture: $\frac{1}{2}$ Bonds in an Unusual Coordinated $\text{S}_4^{2-}$ Rectangle (Chem. Asian J. 2/2009). <i>Chemistry - an Asian Journal</i> , 2009, 4, 215-215.	1.7	0
124	Teaching and Learning Strategies That Work. <i>Science</i> , 2009, 325, 1203-1204.	6.0	8
125	$\text{S}_4^{2-}$ Rings, Disulfides, and Sulfides in Transition-Metal Complexes: The Subtle Interplay of Oxidation and Structure. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 2864-2868.	7.2	43
126	Learning from Molecules in Distress. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 4474-4481.	7.2	86



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127	Predicting Moleculesâ€”More Realism, Please!. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7164-7167.	7.2	311
128	Parallel disulfido bridges in bi- and poly-nuclear transition metal compounds: Bonding flexibility induced by redox chemistry. <i>Inorganica Chimica Acta</i> , 2008, 361, 3631-3637.	1.2	7
129	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. <i>Nature</i> , 2008, 451, 445-448.	13.7	111
130	Why Think Up New Molecules?. <i>American Scientist</i> , 2008, 96, 372.	0.1	17
131	Electronic Effects in CO Chemisorption on Ptâˆ”Pb Intermetallic Surfaces:â€” A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17357-17369.	1.5	19
132	Structure and bonding in boron carbide: The invincibility of imperfections. <i>New Journal of Chemistry</i> , 2007, 31, 473.	1.4	118
133	A Quantum Mechanically Guided View of Mg <sub>44</sub> Rh <sub>7</sub> . <i>Chemistry - A European Journal</i> , 2007, 13, 7852-7863.	1.7	20
134	Interpenetrating Polar and Nonpolar Sublattices in Intermetallics: The NaCd <sub>2</sub> Structure. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 1958-1976.	7.2	70
135	The Chemical Imagination at Work in Very Tight Places. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 3620-3642.	7.2	393
136	Cover Picture: Interpenetrating Polar and Nonpolar Sublattices in Intermetallics: The NaCd <sub>2</sub> Structure ( <i>Angew. Chem. Int. Ed.</i> 12/2007). <i>Angewandte Chemie - International Edition</i> , 2007, 46, 1927-1927.	7.2	2
137	Blow-Up: Making Sense of the Image in the Nanoworld. <i>Small</i> , 2007, 3, 368-371.	5.2	0
138	What might philosophy of science look like if chemists built it?. <i>Synthese</i> , 2007, 155, 321-336.	0.6	38
139	Prediction of thermodynamic stability and electronic structure of novel ternary lanthanide hydrides. <i>Journal of Materials Chemistry</i> , 2006, 16, 1154.	6.7	10
140	Theoretical studies on doubly and triply linked polymers of Ge <sub>9</sub> clusters. <i>Inorganica Chimica Acta</i> , 2006, 359, 3776-3784.	1.2	9
141	Structures and Potential Superconductivity in SiH <sub>4</sub> at High Pressure: En Route to “Metallic Hydrogen”. <i>Physical Review Letters</i> , 2006, 96, 017006.	2.9	187
142	Solid Memory: Structural Preferences in Group 2 Dihalide Monomers, Dimers, and Solids. <i>Journal of the American Chemical Society</i> , 2006, 128, 11236-11249.	6.6	33
143	Richard Kuhn, das Dritte Reich und die GDCh. <i>Nachrichten Aus Der Chemie</i> , 2006, 54, 1019-1024.	0.0	0
144	Adsorption of CO on PtBi <sub>2</sub> and PtBi surfaces. <i>Surface Science</i> , 2005, 574, 1-16.	0.8	59

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145	Squeezing C≡C Bonds. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 7549-7553.	7.2	50
146	How do electrons travel in unusual metallic fluorides of Ag <sub>2</sub> ?. <i>Physica Status Solidi (B): Basic Research</i> , 2005, 242, R1-R3.	0.7	14
147	Transition Metal Complexes of Cyclic and Open Ozone and Thiozone. <i>Journal of the American Chemical Society</i> , 2005, 127, 1278-1285.	6.6	41
148	Theoretical Chemistry. <i>Foundations of Chemistry</i> , 2004, 6, 11.	0.4	0
149	A Claim on the Development of the Frontier Orbital Explanation of Electrocyclic Reactions. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 6586-6590.	7.2	27
150	Hydrogen Migration Over Organic Tapes: [1,5] Sigmatropic Shiftamers. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 273-280.	1.2	6
151	Thinking about metal-metal quadruple bonding in extended structures: a hypothetical A <sub>2</sub> M <sub>6</sub> E <sub>8</sub> network. <i>New Journal of Chemistry</i> , 2004, 28, 185.	1.4	5
152	Dicyclobuta[de,ij]naphthalene and Dicyclopenta[cd,gh]pentalene: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 8093-8100.	1.7	8
153	Main Group Element Nets to a T. <i>Inorganic Chemistry</i> , 2004, 43, 2526-2540.	1.9	14
154	Planar Tetracoordinate Carbon in Extended Systems. <i>Journal of the American Chemical Society</i> , 2004, 126, 15309-15315.	6.6	126
155	The Nowotny Chimney Ladder Phases: Following the pseudo Clue toward an Explanation of the 14 Electron Rule. <i>Inorganic Chemistry</i> , 2004, 43, 6151-6158.	1.9	79
156	The Nowotny Chimney Ladder Phases: Whence the 14 Electron Rule?. <i>Inorganic Chemistry</i> , 2004, 43, 6159-6167.	1.9	98
157	Extended Barbaralanes: Sigmatropic Shiftamers or <i>f</i> -Polyacenes?. <i>Journal of the American Chemical Society</i> , 2004, 126, 4256-4263.	6.6	26
158	Meissen Chymistry. <i>American Scientist</i> , 2004, 92, 312.	0.1	2
159	A Conversation on VB vs MO Theory: A Never-Ending Rivalry?. <i>Accounts of Chemical Research</i> , 2003, 36, 750-756.	7.6	144
160	The RE <sub>2</sub> ME Phases. <i>Helvetica Chimica Acta</i> , 2003, 86, 1653-1682.	1.0	61
161	The RE <sub>2</sub> ME Phases. <i>Helvetica Chimica Acta</i> , 2003, 86, 1683-1708.	1.0	39
162	Helicoid Shiftamers for the Transport of $\pi$ -Clumps and Charges. <i>Helvetica Chimica Acta</i> , 2003, 86, 3525-3532.	1.0	9

#	ARTICLE	IF	CITATIONS
163	Polyhedral Boranes with Exo Multiple Bonds: Three-Dimensional Inorganic Analogues of Quinones. <i>ChemInform</i> , 2003, 34, no.	0.1	0
164	Vibronic Coupling in Molecules and in Solids. <i>Chemistry - A European Journal</i> , 2003, 9, 575-587.	1.7	18
165	Polyhedral Boranes with Exo Multiple Bonds: Three-Dimensional Inorganic Analogues of Quinones. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3777-3781.	7.2	12
166	Breaking Down Barriers: The Liaison Between Sigmatropic Shifts, Electrocyclic Reactions, and Three-Center Cations. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 5877-5882.	7.2	20
167	Cover Picture: Breaking Down Barriers: The Liaison Between Sigmatropic Shifts, Electrocyclic Reactions, and Three-Center Cations ( <i>Angew. Chem. Int. Ed.</i> 47/2003). <i>Angewandte Chemie - International Edition</i> , 2003, 42, 5777-5777.	7.2	0
168	Propensity of Different AgBr Surfaces for Photoinduced Silver Cluster Formation: A Molecular Orbital Analysis. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8184-8190.	1.1	13
169	Why Buy That Theory?. <i>American Scientist</i> , 2003, 91, 9.	0.1	28
170	Electron-Rich Three-Center Bonding: Role of s,p Interactions across the p-Block. <i>Journal of the American Chemical Society</i> , 2002, 124, 4787-4795.	6.6	69
171	Bcc and Fcc Transition Metals and Alloys: A Central Role for the Jahn-Teller Effect in Explaining Their Ideal and Distorted Structures. <i>Journal of the American Chemical Society</i> , 2002, 124, 4811-4823.	6.6	33
172	Electronic Properties of the Silver-Silver Chloride Cluster Interface. <i>Chemistry - A European Journal</i> , 2002, 8, 1785.	1.7	88
173	Sigmatropic Shiftamers: Fluxionality in Broken Ladderane Polymers. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1033-1036.	7.2	35
174	Band structure representations of the electronic structure of one-dimensional materials with helical symmetry. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 272-281.	0.5	10
175	Structure and physical properties of CeSbTe. <i>Journal of Alloys and Compounds</i> , 2001, 314, 132-139.	2.8	21
176	Chemistry of vibronic coupling. Part 2. How to maximize the dynamic diagonal vibronic coupling constant for T1 states in AB systems (A, B=H, Li, Na, K, Rb, Cs, F, Cl, Br or I)?. <i>New Journal of Chemistry</i> , 2001, 25, 108-115.	1.4	12
177	Electron-Rich Bonding and the Importance of s,p Mixing as One Moves Across a Period: A Lesson from the LiSn System. <i>Journal of the American Chemical Society</i> , 2001, 123, 2317-2325.	6.6	20
178	Electron-Rich Rods as Building Blocks for Sb Strips and Te Sheets. <i>Journal of the American Chemical Society</i> , 2001, 123, 6600-6608.	6.6	41
179	A Comparative Study of the p(2 Å <sup>2</sup> -2)-CO/M(111), M=Pt,Cu,Al Chemisorption Systems. <i>Journal of Physical Chemistry B</i> , 2001, 105, 3245-3260.	1.2	22
180	Origin of the Broken Conjugation in m-Phenylene Linked Conjugated Polymers. <i>Macromolecules</i> , 2001, 34, 6474-6481.	2.2	92

#	ARTICLE	IF	CITATIONS
181	Complicated Goings-On in the Metal-Manipulated Ring-Opening of Cyclobutene. <i>Journal of the American Chemical Society</i> , 2001, 123, 9855-9859.	6.6	25
182	Chemistry of vibronic coupling. Part 1: How to maximize vibronic coupling constants in a diabatic harmonic potential model?. <i>Chemical Physics</i> , 2001, 265, 153-163.	0.9	6
183	Demonic Intervention in the Thermal Electrocyclic Ring Opening of Cyclobutenes: Fe(CO) <sub>3</sub> Complexation of Pericyclic Transition Structures. <i>Helvetica Chimica Acta</i> , 2001, 84, 1396-1404.	1.0	19
184	Protean. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1033-1036.	7.2	6
185	Real and Hypothetical Intermediate-Valence AgII/AgIII and AgII/AgI Fluoride Systems as Potential Superconductors. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2742-2781.	7.2	139
186	Not a Library. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 3337-3340.	7.2	36
187	Coping with Fritz Haber's Somber Literary Shadow. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 4599-4604.	7.2	8
188	Disrotatory and Conrotatory Transition Structures for the Fe(CO) <sub>3</sub> -Templated Rearrangement of Methylene cyclopropane to Trimethylenemethane. <i>Organometallics</i> , 2001, 20, 4562-4564.	1.1	20
189	Demonic Intervention in the Thermal Electrocyclic Ring Opening of Cyclobutenes: Fe(CO) <sub>3</sub> Complexation of Pericyclic Transition Structures. , 2001, 84, 1396.		1
190	Demonic Intervention in the Thermal Electrocyclic Ring Opening of Cyclobutenes: Fe(CO) <sub>3</sub> Complexation of Pericyclic Transition Structures. , 2001, 84, 1396.		1
191	Benjamin Lee Whorf: once a chemist .... <i>Interdisciplinary Science Reviews</i> , 2001, 26, 15-19.	1.0	3
192	Ferrocene: Ironclad History or Rashomon Tale?. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 123-124.	7.2	65
193	Generalized perturbational molecular orbital (PMO) theory. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 408-420.	1.0	14
194	Hypervalent Bonding in One, Two, and Three Dimensions: Extending the Zintl-Klemm Concept to Nonclassical Electron-Rich Networks. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 2408-2448.	7.2	261
195	Chemistry of Vibronic Coupling. 3. How One Might Maximize Off-Diagonal Dynamic Vibronic Coupling Constants for Intervalence Charge-Transfer (IVCT) States in an ABA System (A, B = Alkali Metal, H, ) <a href="#">TJ ETQq1 1 0.784314 8gBT /Over</a>		
196	A comparative study of Hamilton and overlap population methods for the analysis of chemical bonding. <i>Journal of Chemical Physics</i> , 2000, 113, 1698-1704.	1.2	39
197	Exquisite Control. <i>American Scientist</i> , 2000, 88, 14.	0.1	5
198	Total energy partitioning within a one-electron formalism: A Hamilton population study of surface CO interaction in the c(2Å-2)-CO/ Ni(100) chemisorption system. <i>Journal of Chemical Physics</i> , 1999, 111, 893-910.	1.2	49

#	ARTICLE	IF	CITATIONS
199	Direct and indirect band gap types in one-dimensional conjugated or stacked organic materials. <i>Theoretical Chemistry Accounts</i> , 1999, 102, 23-32.	0.5	48
200	Chemical Bonding in the Ternary Transition Metal Bismuthides $Ti_4Tb_2$ with $T = Cr, Mn, Fe, Co,$ and $Ni$ . <i>Inorganic Chemistry</i> , 1999, 38, 1609-1617.	1.9	19
201	Pulse, Pump & Probe. <i>American Scientist</i> , 1999, 87, 308.	0.1	3
202	Kenichi Fukui (1918-98). <i>Nature</i> , 1998, 391, 750-750.	13.7	3
203	Building up Complexity from Strips and Sheets: The Electronic Structure of the $La_{12}Mn_2Sb_3$ Alloy. <i>Journal of Solid State Chemistry</i> , 1998, 139, 8-21.	1.4	34
204	Might $BF$ and $BNR_2$ be alternatives to $CO$ ? A theoretical quest for new ligands in organometallic chemistry. <i>New Journal of Chemistry</i> , 1998, 22, 1-3.	1.4	61
205	Magic Electron Counts for Networks of Condensed Clusters: A Vertex-Sharing Aluminum Octahedra. <i>Journal of the American Chemical Society</i> , 1998, 120, 4200-4208.	6.6	27
206	The $TiNiSi$ Family of Compounds: A Structure and Bonding. <i>Inorganic Chemistry</i> , 1998, 37, 5754-5763.	1.9	152
207	Is $CO$ a Special Ligand in Organometallic Chemistry? Theoretical Investigation of $AB$ , $Fe(CO)_4AB$ , and $Fe(AB)_5$ ( $AB = N_2, CO, BF, SiO$ ). <i>Inorganic Chemistry</i> , 1998, 37, 1080-1090.	1.9	162
208	Bonding in an Unusual Nickel Carbide. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 1998, 53, 322-332.	0.3	23
209	Orbital Interaction Analysis of McConnell's Model for Through-Space Magnetic Coupling. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 305, 157-166.	0.3	7
210	Sulfur Multicenter Bonding and Distortions in a Hypothetical Polydithioquinone. <i>Chemistry of Materials</i> , 1997, 9, 573-579.	3.2	6
211	Forbidden Four-Center Reactions: A Molecular Orbital Considerations for $N_2^+ + N_2$ and $N_2 + N_2^+$ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 8255-8263.	1.1	16
212	Bonding in the trihalides ( $X_3$ ), mixed trihalides ( $X_2Y$ ) and hydrogen bihalides ( $X_2H$ ). The connection between hypervalent, electron-rich three-center, donor-acceptor and strong hydrogen bonding. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 3605-3613.	1.1	187
213	The Electronic Structure of $[Te_5Br_4][MoOBr_4]_2$ and Some General Aspects of Bonding in Classical and Hypervalent Tellurium Halides. <i>Chemische Berichte</i> , 1997, 130, 463-472.	0.2	2
214	Teach to Search: ACS 1996 Pimentel Award. <i>Journal of Chemical Education</i> , 1996, 73, A202.	1.1	4
215	Electronic Structure, Bonding, and Electrical Properties of $MoNiP_8$ . <i>Inorganic Chemistry</i> , 1996, 35, 4683-4689.	1.9	8
216	The Four-Connected Net in the $CeCu_2$ Structure and Its Ternary Derivatives. Its Electronic and Structural Properties. <i>Inorganic Chemistry</i> , 1996, 35, 6922-6932.	1.9	121

#	ARTICLE	IF	CITATIONS
217	The d <sup>2</sup> â€M(NR) <sub>2</sub> Fragment, High Valent and Low Valent Organometallic Equivalents, and an Unusual Mode of Ethylene Complexation. <i>Chemische Berichte</i> , 1996, 129, 1345-1353.	0.2	4
218	Polyamidoimidonitride Clusters of Zirconium - a molecular orbital study. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 1996, 622, 392-400.	0.6	11
219	Chemical Said Song. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 284, 1-2.	0.3	0
220	Potential Linearâ€Chain Organic Ferromagnets. <i>Chemistry - A European Journal</i> , 1995, 1, 403-413.	1.7	53
221	The role of orbital interactions in determining ferromagnetic coupling in organic molecular assemblies. <i>Journal of the American Chemical Society</i> , 1995, 117, 6921-6926.	6.6	107
222	Polythiene, a Novel Hypothetical Carbon-Sulfur Polymer. <i>Journal of the American Chemical Society</i> , 1995, 117, 12328-12335.	6.6	22
223	Adhesion of Rh, Pd, and Pt to Alumina and NO Reactions on Resulting Surfaces. <i>ACS Symposium Series</i> , 1994, , 140-156.	0.5	0
224	Bondâ€Stretch Isomers and Spinâ€State Isomers: A Comment on the Article â€œBondâ€Stretch Isomers: Fact not Fictionâ€ <sup>[1]</sup> . <i>Angewandte Chemie</i> , 1994, 106, 1530-1530.	1.6	11
225	A Hypothetical Dense 3,4-Connected Carbon Net and Related B <sub>2</sub> C and CN <sub>2</sub> Nets Built from 1,4-Cyclohexadienoid Units. <i>Journal of the American Chemical Society</i> , 1994, 116, 11456-11464.	6.6	101
226	[Ni(PtBu) <sub>6</sub> ] and [Ni(SiH <sub>2</sub> ) <sub>6</sub> ] Are Isolobal, Related to [In{Mn(CO) <sub>4</sub> } <sub>5</sub> ] <sup>2+</sup> , and Have 16-Electron Counts. <i>Angewandte Chemie International Edition in English</i> , 1993, 32, 1616-1618.	4.4	22
227	How Should Chemists Think?. <i>Scientific American</i> , 1993, 268, 66-73.	1.0	59
228	Rhenium-carbon bonding in erbium rhenium carbide (Er <sub>2</sub> ReC <sub>2</sub> ), an organometallic polymer in the solid state. <i>Inorganic Chemistry</i> , 1993, 32, 1991-1996.	1.9	15
229	A theoretical study of the initial stages of Si(111)â€7Ã—7 oxidation. I. The molecular precursor. <i>Journal of Chemical Physics</i> , 1993, 98, 7593-7605.	1.2	81
230	A theoretical study of the initial stages of Si(111)â€7Ã—7 oxidation. II. The dissociated state and formation of SiO <sub>4</sub> . <i>Journal of Chemical Physics</i> , 1993, 98, 7606-7612.	1.2	33
231	[Ni(P<i>t</i>Bu) <sub>6</sub> ] und [Ni(SiH <sub>2</sub> ) <sub>6</sub> ] sind isolobal, verwandt mit [In{Mn(CO) <sub>4</sub> } <sub>5</sub> ] <sup>2+</sup> und haben jeweils 16 Valenzelektronen. <i>Angewandte Chemie</i> , 1993, 105, 1682-1684.	1.6	5
232	Bonding in halocuprates. <i>Inorganic Chemistry</i> , 1992, 31, 1021-1029.	1.9	96
233	The electronic structure of two novel carbides, Ca <sub>3</sub> Cl <sub>2</sub> C <sub>3</sub> and Sc <sub>3</sub> C <sub>4</sub> , containing C <sub>3</sub> units. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 1992, 607, 57-71.	0.6	30
234	Structure-Bonding Relationships in the Laves Phases. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 1992, 616, 105-120.	0.6	127

#	ARTICLE	IF	CITATIONS
235	Representation in Chemistry. <i>Angewandte Chemie International Edition in English</i> , 1991, 30, 1-16.	4.4	191
236	Darstellungen in der Chemie â€” die Sprache der Chemiker. <i>Angewandte Chemie</i> , 1991, 103, 1-16.	1.6	32
237	From chemisorption to mechanism on surfaces: An exploration of the pyrolysis of triisobutylaluminum in the chemical vapor deposition of aluminum thin films. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1991, 9, 1569-1580.	0.9	12
238	Chemisorption of carbon monoxide on three metal surfaces: nickel(111), palladium(111), and platinum(111): a comparative study. <i>The Journal of Physical Chemistry</i> , 1991, 95, 859-867.	2.9	116
239	A one-electron perturbation theory of chemisorption. <i>Journal of Chemical Physics</i> , 1990, 93, 3635-3644.	1.2	3
240	PF <sub>3</sub> , PF <sub>2</sub> , and PF on Ni(111): Theoretical aspects of their chemisorption. <i>Journal of Chemical Physics</i> , 1990, 92, 699-708.	1.2	28
241	A SIMPLE WAY TO UNDERSTAND THE ELECTRONIC STRUCTURES OF THE Tiâ€”Baâ€”Caâ€”Cuâ€”O HIGH T <sub>c</sub> SUPERCONDUCTORS. <i>International Journal of Modern Physics B</i> , 1990, 04, 677-699.	1.0	2
242	Molecular Beauty. <i>Journal of Aesthetics and Art Criticism</i> , 1990, 48, 191.	0.1	20
243	Polyisocyanides: electronic or steric reasons for their presumed helical structure?. <i>Journal of the American Chemical Society</i> , 1990, 112, 8230-8238.	6.6	56
244	TiI-TiI Interactions in the Molecular State?an MO Analysis. <i>Angewandte Chemie International Edition in English</i> , 1989, 28, 1688-1690.	4.4	45
245	How carbon-carbon bonds are formed and how they influence structural choices in some binary and ternary metal carbides. <i>Chemistry of Materials</i> , 1989, 1, 83-101.	3.2	42
246	Under the Surface of the Chemical Article. <i>Angewandte Chemie International Edition in English</i> , 1988, 27, 1593-1602.	4.4	24
247	Complementary local and extended views of bonding in the ThCr <sub>2</sub> Si <sub>2</sub> and CaAl <sub>2</sub> Si <sub>2</sub> structures. <i>Journal of Solid State Chemistry</i> , 1988, 72, 58-71.	1.4	84
248	Summary Abstract: The adsorption of benzotriazole on copper and cuprous oxide. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1988, 6, 885-886.	0.9	10
249	FLUORITE. <i>The Sciences</i> , 1988, 28, 31-31.	0.1	5
250	Summary Abstract: Electronic factors in thiophene adsorption and hydrodesulfurization on MoS <sub>2</sub> surfaces. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1987, 5, 635-637.	0.9	5
251	3,4-Connected carbon nets: through-space and through-bond interactions in the solid state. <i>Journal of the American Chemical Society</i> , 1987, 109, 6742-6751.	6.6	113
252	Square nets of main-group elements in solid-state materials. <i>Journal of the American Chemical Society</i> , 1987, 109, 124-140.	6.6	134

#	ARTICLE	IF	CITATIONS
253	How Chemistry and Physics Meet in the Solid State. <i>Angewandte Chemie International Edition in English</i> , 1987, 26, 846-878.	4.4	531
254	Site preferences and bond length differences in CaAl <sub>2</sub> Si <sub>2</sub> -type Zintl compounds. <i>Journal of the American Chemical Society</i> , 1986, 108, 1876-1884.	6.6	135
255	Bonding in the BaPdSn <sub>3</sub> Structure. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 1986, 41, 1399-1415.	0.3	12
256	A Novel Electron Count and Metal-Metal Multiple Bonding in Trigonal Prismatic Clusters. <i>Angewandte Chemie International Edition in English</i> , 1986, 25, 822-823.	4.4	17
257	A theoretical and chemical view of surface chemistry: Chemisorption and reactions of acetylene. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1986, 4, 1336-1341.	0.9	6
258	Hydrogen Migration in Transition Metal Alkyne and Related Complexes. <i>Helvetica Chimica Acta</i> , 1985, 68, 1461-1506.	1.0	217
259	How carbon monoxide bonds to metal surfaces. <i>Journal of the American Chemical Society</i> , 1985, 107, 578-584.	6.6	302
260	Hydride bridges between LnCp <sub>2</sub> centers. <i>Inorganic Chemistry</i> , 1985, 24, 2095-2104.	1.9	65
261	Alkyl Shifts between Transition Metals and Coordinated Main Group Atoms. <i>Helvetica Chimica Acta</i> , 1984, 67, 1-17.	1.0	67
262	Reactivity of transition metal cluster carbides which have an exposed carbon atom. <i>Organometallics</i> , 1984, 3, 962-970.	1.1	36
263	Chains of trans-edge-sharing molybdenum octahedra: metal-metal bonding in extended systems. <i>Journal of the American Chemical Society</i> , 1983, 105, 3528-3537.	6.6	423
264	Hypothetical metallic allotrope of carbon. <i>Journal of the American Chemical Society</i> , 1983, 105, 4831-4832.	6.6	165
265	Building Bridges Between Inorganic and Organic Chemistry (Nobel Lecture). <i>Angewandte Chemie International Edition in English</i> , 1982, 21, 711-724.	4.4	1,090
266	Brücken zwischen Anorganischer und Organischer Chemie (Nobelvortrag). <i>Angewandte Chemie</i> , 1982, 94, 725-739.	1.6	426
267	Bent cis d <sup>0</sup> MoO <sub>2</sub> <sup>2+</sup> vs. linear trans d <sup>0</sup> UO <sub>2</sub> <sup>2+</sup> : a significant role for nonvalence 6p orbitals in uranyl. <i>Inorganic Chemistry</i> , 1980, 19, 2656-2658.	1.9	171
268	Why some binuclear complexes bridge, while others, even though they might have a quadruple bond available to them, do not. <i>Journal of the American Chemical Society</i> , 1980, 102, 1194-1196.	6.6	16
269	Bridged and unbridged M <sub>2</sub> L <sub>10</sub> complexes. <i>Journal of the American Chemical Society</i> , 1980, 102, 4555-4572.	6.6	141
270	Tempered orbital energies in SCF MO calculations and their relation to the ordinate in Mulliken-Walsh correlation diagrams and extended Hückel orbital energies. <i>Theoretica Chimica Acta</i> , 1978, 48, 301-321.	0.9	25



#	ARTICLE	IF	CITATIONS
271	Counterintuitive orbital mixing. <i>Journal of Chemical Physics</i> , 1978, 68, 5498-5500.	1.2	45
272	Bis[ $\mu$ -methyl-1,3-dimethyl-h <sup>3</sup> -allyl-nickel] Struktur und Bindungsverhältnisse eines Alkyl-verbrückten Ni-Ni-Systems / Bis [ $\mu$ -methyl-1,3-dimethyl-h <sup>3</sup> -allyl-nickel] The Bonding in an Alkyl-Bridged Ni-Ni System. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 1978, 33, 1110-1115.	0.3	33
273	Di- $\mu$ -hydrido-bis[1,3-propanbis(dicyclohexylphosphin)]dinickel(Ni <sub>2</sub> Ni) " Der Bindungszustand in einem Dreizentren-Wasserstoff- $\mu$ -berbrückten Ni <sub>2</sub> Ni-System. <i>Chemische Berichte</i> , 1977, 110, 3900-3909.	0.2	42
274	Orbital interactions in metal dimer complexes. <i>Journal of the American Chemical Society</i> , 1975, 97, 4884-4899.	6.6	1,305
275	Molecular orbital studies of dissociative chemisorption of first period diatomic molecules and ethylene on (100) W and Ni surfaces. <i>Journal of Chemical Physics</i> , 1974, 61, 4545-4559.	1.2	140
276	Description of diatomic molecules using one electron configuration energies with two-body interactions. <i>Journal of Chemical Physics</i> , 1974, 60, 4271-4273.	1.2	166
277	Detailed orbital theory of substituent effects. Charge transfer, polarization, and the methyl group. <i>Journal of the American Chemical Society</i> , 1974, 96, 1370-1383.	6.6	267
278	Zur Stabilisierung des Phenyl-Kations. <i>Chemische Berichte</i> , 1972, 105, 8-23.	0.2	37
279	Effect of Protonation on Aziridine and Oxirane Bond Strengths. <i>Angewandte Chemie International Edition in English</i> , 1972, 11, 825-826.	4.4	11
280	Beeinflussung der Bindungsstärken im Aziridin und Oxiran durch Protonierung. <i>Angewandte Chemie</i> , 1972, 84, 820-821.	1.6	9
281	The Stabilization of Bridged Structures of Ethanes. <i>Helvetica Chimica Acta</i> , 1972, 55, 67-75.	1.0	22
282	Orbital Theory of Heterolytic Fragmentation and Remote Effects on Nitrogen Inversion Equilibria. <i>Helvetica Chimica Acta</i> , 1972, 55, 893-906.	1.0	53
283	Interaction of orbitals through space and through bonds. <i>Accounts of Chemical Research</i> , 1971, 4, 1-9.	7.6	1,402
284	The Interaction of Nonbonding Orbitals in Carbonyls. <i>Helvetica Chimica Acta</i> , 1970, 53, 2331-2338.	1.0	92
285	The interaction of sulphur atoms with ethylene. <i>Molecular Physics</i> , 1970, 19, 113-120.	0.8	17
286	Potential surface for a nonconcerted reaction. Tetramethylene. <i>Journal of the American Chemical Society</i> , 1970, 92, 7091-7097.	6.6	131
287	Planar tetracoordinate carbon. <i>Journal of the American Chemical Society</i> , 1970, 92, 4992-4993.	6.6	541
288	Interaction of nonconjugated double bonds. <i>Journal of the American Chemical Society</i> , 1970, 92, 706-707.	6.6	181

#	ARTICLE	IF	CITATIONS
289	Quantum mechanical approach to the conformational analysis of macromolecules in ground and excited states. <i>Biopolymers</i> , 1969, 7, 207-213.	1.2	54
290	Formal Diradicals Which Should Have Singlet Ground States. <i>Angewandte Chemie International Edition in English</i> , 1969, 8, 214-215.	4.4	8
291	The Conservation of Orbital Symmetry. <i>Angewandte Chemie International Edition in English</i> , 1969, 8, 781-853.	4.4	2,636
292	The electronic structure of methylenes. <i>Journal of the American Chemical Society</i> , 1968, 90, 1485-1499.	6.6	274
293	Conservation of orbital symmetry. <i>Accounts of Chemical Research</i> , 1968, 1, 17-22.	7.6	626
294	Stabilizing a singlet methylene. <i>Journal of the American Chemical Society</i> , 1968, 90, 5457-5460.	6.6	241
295	Trimethylene and the addition of methylene to ethylene. <i>Journal of the American Chemical Society</i> , 1968, 90, 1475-1485.	6.6	430
296	Benzynes, dehydroconjugated molecules, and the interaction of orbitals separated by a number of intervening sigma bonds. <i>Journal of the American Chemical Society</i> , 1968, 90, 1499-1509.	6.6	662
297	Transition State for the Hydrogen-Iodine and the Hydrogen Exchange Reactions. <i>Journal of Chemical Physics</i> , 1968, 49, 3739-3740.	1.2	60
298	THE ELECTRONIC STRUCTURE OF SOME INTERMEDIATES AND TRANSITION STATES IN ORGANIC REACTIONS*. <i>Transactions of the New York Academy of Sciences</i> , 1966, 28, 475-479.	0.2	19
299	Stereochemistry of Electrocyclic Reactions. <i>Journal of the American Chemical Society</i> , 1965, 87, 395-397.	6.6	1,267
300	Selection Rules for Sigmatropic Reactions. <i>Journal of the American Chemical Society</i> , 1965, 87, 2511-2513.	6.6	421
301	Orbital Symmetries and endo-exo Relationships in Concerted Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 1965, 87, 4388-4389.	6.6	353
302	Selection Rules for Concerted Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 1965, 87, 2046-2048.	6.6	562
303	Orbital Symmetries and Orientational Effects in a Sigmatropic Reaction. <i>Journal of the American Chemical Society</i> , 1965, 87, 4389-4390.	6.6	150
304	Theoretical Investigations on Boron-Nitrogen Molecules. <i>Advances in Chemistry Series</i> , 1964, , 78-86.	0.6	24
305	Extended Hückel Theory. IV. Carbonium Ions. <i>Journal of Chemical Physics</i> , 1964, 40, 2480-2488.	1.2	233
306	Distribution of Electronic Levels in Alkanes. <i>Journal of Chemical Physics</i> , 1964, 40, 2047-2048.	1.2	32

#	ARTICLE	IF	CITATIONS
307	Extended Hückel Theory. II. $\pi$ Orbitals in the Azines. Journal of Chemical Physics, 1964, 40, 2745-2745.	1.2	209
308	Extended Hückel Theory. III. Compounds of Boron and Nitrogen. Journal of Chemical Physics, 1964, 40, 2474-2480.	1.2	290
309	An Extended Hückel Theory. I. Hydrocarbons. Journal of Chemical Physics, 1963, 39, 1397-1412.	1.2	4,583
310	Theory of Polyhedral Molecules. II. A Crystal Field Model. Journal of Chemical Physics, 1962, 36, 2189-2195.	1.2	62
311	Sequential Substitution Reactions on $B_{10}H_{10}^{2-}$ and $B_{12}H_{12}^{2-}$ . Journal of Chemical Physics, 1962, 37, 520-523.	1.2	33
312	Theory of Polyhedral Molecules. I. Physical Factorizations of the Secular Equation. Journal of Chemical Physics, 1962, 36, 2179-2189.	1.2	937
313	Boron Hydrides: LCAO-MO and Resonance Studies. Journal of Chemical Physics, 1962, 37, 2872-2883.	1.2	464