

Roald Hoffmann

List of Publications by Citations

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337
papers

30,974
citations

79
h-index

170
g-index

365
ext. papers

33,150
ext. citations

9.2
avg, IF

7.39
L-index

#	Paper	IF	Citations
337	An Extended Hückel Theory. I. Hydrocarbons. <i>Journal of Chemical Physics</i> , 1963 , 39, 1397-1412	3.9	4099
336	The Conservation of Orbital Symmetry. <i>Angewandte Chemie International Edition in English</i> , 1969 , 8, 781-853	2132	
335	Interaction of orbitals through space and through bonds. <i>Accounts of Chemical Research</i> , 1971 , 4, 1-9	24.3	1244
334	Orbital interactions in metal dimer complexes. <i>Journal of the American Chemical Society</i> , 1975 , 97, 4884-4899	1197	
333	Stereochemistry of Electrocyclic Reactions. <i>Journal of the American Chemical Society</i> , 1965 , 87, 395-397	16.4	1062
332	Building Bridges Between Inorganic and Organic Chemistry (Nobel Lecture). <i>Angewandte Chemie International Edition in English</i> , 1982 , 21, 711-724	936	
331	Theory of Polyhedral Molecules. I. Physical Factorizations of the Secular Equation. <i>Journal of Chemical Physics</i> , 1962 , 36, 2179-2189	3.9	812
330	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	16.4	600
329	Conservation of orbital symmetry. <i>Accounts of Chemical Research</i> , 1968 , 1, 17-22	24.3	546
328	Selection Rules for Concerted Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 1965 , 87, 2046-2048	16.4	470
327	Planar tetracoordinate carbon. <i>Journal of the American Chemical Society</i> , 1970 , 92, 4992-4993	16.4	446
326	How Chemistry and Physics Meet in the Solid State. <i>Angewandte Chemie International Edition in English</i> , 1987 , 26, 846-878	437	
325	Boron Hydrides: LCAO-MO and Resonance Studies. <i>Journal of Chemical Physics</i> , 1962 , 37, 2872-2883	3.9	407
324	Potential high- superconducting lanthanum and yttrium hydrides at high pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 6990-6995	11.5	387
323	Trimethylene and the addition of methylene to ethylene. <i>Journal of the American Chemical Society</i> , 1968 , 90, 1475-1485	16.4	386
322	Selection Rules for Sigmatropic Reactions. <i>Journal of the American Chemical Society</i> , 1965 , 87, 2511-2513	16.4	364
321	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	16.4	363

320	Brücken zwischen Anorganischer und Organischer Chemie (Nobel-Vortrag). <i>Angewandte Chemie</i> , 2006 , 94, 725-739	3.6	341
319	The chemical imagination at work in very tight places. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 3620-42	16.4	327
318	Orbital Symmetries and endo-exo Relationships in Concerted Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 1965 , 87, 4388-4389	16.4	292
317	Large-scale soft colloidal template synthesis of 1.4 nm thick CdSe nanosheets. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 6861-4	16.4	281
316	How carbon monoxide bonds to metal surfaces. <i>Journal of the American Chemical Society</i> , 1985 , 107, 578-584	16.4	272
315	Predicting molecules--more realism, please!. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7164-7164	16.4	257
314	Extended Hückel Theory. III. Compounds of Boron and Nitrogen. <i>Journal of Chemical Physics</i> , 1964 , 40, 2474-2480	3.9	257
313	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	16.4	253
312	The electronic structure of methylenes. <i>Journal of the American Chemical Society</i> , 1968 , 90, 1485-1499	16.4	248
311	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	16.4	221
310	Stabilizing a singlet methylene. <i>Journal of the American Chemical Society</i> , 1968 , 90, 5457-5460	16.4	219
309	Extended Hückel Theory. IV. Carbonium Ions. <i>Journal of Chemical Physics</i> , 1964 , 40, 2480-2488	3.9	213
308	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, 17640-3	11.5	205
307	Hydrogen Migration in Transition Metal Alkyne and Related Complexes. <i>Helvetica Chimica Acta</i> , 1985 , 68, 1461-1506	2	197
306	Extended Hückel Theory. II. Orbitals in the Azines. <i>Journal of Chemical Physics</i> , 1964 , 40, 2745-2745	3.9	192
305	Bonding in the trihalides (X_3Y), mixed trihalides (X_2Y_2) and hydrogen bihalides (X_2HY). 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	175	
304	Structures and potential superconductivity in at high pressure: en route to "metallic hydrogen". <i>Physical Review Letters</i> , 2006 , 96, 017006	7.4	174
303	Homo Citans and Carbon Allotropes: For an Ethics of Citation. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 10962-76	16.4	172

302	The low-lying electronic states of pentacene and their roles in singlet fission. <i>Journal of the American Chemical Society</i> , 2014 , 136, 5755-64	16.4	161
301	Interaction of nonconjugated double bonds. <i>Journal of the American Chemical Society</i> , 1970 , 92, 706-707	16.4	158
300	Bent cis d0 MoO ₂₂ ⁺ vs. linear trans d0f0 UO ₂₂ ⁺ : a significant role for nonvalence 6p orbitals in uranyl. <i>Inorganic Chemistry</i> , 1980 , 19, 2656-2658	5.1	153
299	Description of diatomic molecules using one electron configuration energies with two-body interactions. <i>Journal of Chemical Physics</i> , 1974 , 60, 4271-4273	3.9	151
298	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	5.1	149
297	Representation in Chemistry. <i>Angewandte Chemie International Edition in English</i> , 1991 , 30, 1-16		149
296	Atomic and Ionic Radii of Elements 1-96. <i>Chemistry - A European Journal</i> , 2016 , 22, 14625-32	4.8	143
295	Hypothetical metallic allotrope of carbon. <i>Journal of the American Chemical Society</i> , 1983 , 105, 4831-4832	16.4	143
294	High pressure electrides: a predictive chemical and physical theory. <i>Accounts of Chemical Research</i> , 2014 , 47, 1311-7	24.3	139
293	A molecular perspective on lithium-ammonia solutions. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 8198-232	16.4	133
292	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	3.9	128
291	Bridged and unbridged M ₂ L ₁₀ complexes. <i>Journal of the American Chemical Society</i> , 1980 , 102, 4555-4572	16.4	126
290	Benzene under high pressure: a story of molecular crystals transforming to saturated networks, with a possible intermediate metallic phase. <i>Journal of the American Chemical Society</i> , 2011 , 133, 9023-35	16.4	125
289	A conversation on VB vs MO theory: a never-ending rivalry?. <i>Accounts of Chemical Research</i> , 2003 , 36, 750-6	24.3	124
288	The TiNiSi Family of Compounds: Structure and Bonding. <i>Inorganic Chemistry</i> , 1998 , 37, 5754-5763	5.1	124
287	Real and Hypothetical Intermediate-Valence Ag /Ag and Ag /Ag Fluoride Systems as Potential Superconductors. <i>Angewandte Chemie - International Edition</i> , 2001 , 40, 2742-2781	16.4	119
286	Potential surface for a nonconcerted reaction. Tetramethylene. <i>Journal of the American Chemical Society</i> , 1970 , 92, 7091-7097	16.4	119
285	Do Diradicals Behave Like Radicals?. <i>Chemical Reviews</i> , 2019 , 119, 11291-11351	68.1	116

284	Orbital Symmetries and Orientational Effects in a Sigmatropic Reaction. <i>Journal of the American Chemical Society</i> , 1965 , 87, 4389-4390	16.4	116
283	Planar tetracoordinate carbon in extended systems. <i>Journal of the American Chemical Society</i> , 2004 , 126, 15309-15	16.4	113
282	Site preferences and bond length differences in CaAl ₂ Si ₂ -type Zintl compounds. <i>Journal of the American Chemical Society</i> , 1986 , 108, 1876-1884	16.4	113
281	One molecule, two atoms, three views, four bonds?. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 3020-33	16.4	110
280	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	5.1	110
279	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		110
278	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, 17119-24	11.5	106
277	Structure and bonding in boron carbide: The invincibility of imperfections. <i>New Journal of Chemistry</i> , 2007 , 31, 473	3.6	103
276	Structure-Bonding Relationships in the Laves Phases. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 1992 , 616, 105-120	1.3	103
275	Square nets of main-group elements in solid-state materials. <i>Journal of the American Chemical Society</i> , 1987 , 109, 124-140	16.4	102
274	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	16.4	101
273	Seeking small molecules for singlet fission: a heteroatom substitution strategy. <i>Journal of the American Chemical Society</i> , 2014 , 136, 12638-47	16.4	100
272	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	16.4	97
271	Dioxygen: What Makes This Triplet Diradical Kinetically Persistent?. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9010-9018	16.4	94
270	High-pressure electrides: the chemical nature of interstitial quasiatoms. <i>Journal of the American Chemical Society</i> , 2015 , 137, 3631-7	16.4	94
269	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. <i>Chemical Reviews</i> , 2016 , 116, 8173-92	68.1	94
268	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. <i>Nature</i> , 2008 , 451, 445-8	50.4	93
267	Bonding in halocuprates. <i>Inorganic Chemistry</i> , 1992 , 31, 1021-1029	5.1	90

266	Electronegativity Seen as the Ground-State Average Valence Electron Binding Energy. <i>Journal of the American Chemical Society</i> , 2019 , 141, 342-351	16.4	90
265	High pressure ices. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 745-50	11.5	86
264	Origin of the Broken Conjugation in m-Phenylene Linked Conjugated Polymers. <i>Macromolecules</i> , 2001 , 34, 6474-6481	5.5	84
263	The Nowotny chimney ladder phases: whence the 14 electron rule?. <i>Inorganic Chemistry</i> , 2004 , 43, 6159-671	83	
262	The Interaction of Nonbonding Orbitals in Carbonyls. <i>Helvetica Chimica Acta</i> , 1970 , 53, 2331-2338	2	83
261	Electronic properties of the silver-silver chloride cluster interface. <i>Chemistry - A European Journal</i> , 2002 , 8, 1785-94	4.8	81
260	A Hypothetical Dense 3,4-Connected Carbon Net and Related B2C and CN2 Nets Built from 1,4-Cyclohexadienoid Units. <i>Journal of the American Chemical Society</i> , 1994 , 116, 11456-11464	16.4	81
259	Small but strong lessons from chemistry for nanoscience. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 93-103	16.4	80
258	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	16.4	76
257	A theoretical study of the initial stages of Si(111) oxidation. I. The molecular precursor. <i>Journal of Chemical Physics</i> , 1993 , 98, 7593-7605	3.9	76
256	Complementary local and extended views of bonding in the ThCr ₂ Si ₂ and CaAl ₂ Si ₂ structures. <i>Journal of Solid State Chemistry</i> , 1988 , 72, 58-71	3.3	76
255	Learning from molecules in distress. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 4474-81	16.4	71
254	The Nowotny chimney ladder phases: following the c(pseudo) clue toward an explanation of the 14 electron rule. <i>Inorganic Chemistry</i> , 2004 , 43, 6151-8	5.1	70
253	Linearly Polymerized Benzene Arrays As Intermediates, Tracing Pathways to Carbon Nanowires. <i>Journal of the American Chemical Society</i> , 2015 , 137, 14373-86	16.4	69
252	Frontier orbital control of molecular conductance and its switching. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 4093-7	16.4	68
251	A bonding quandary--or--a demonstration of the fact that scientists are not born with logic. <i>Chemistry - A European Journal</i> , 2009 , 15, 8358-73	4.8	68
250	Close relation between quantum interference in molecular conductance and diradical existence. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, E413-9	11.5	66
249	Interpenetrating polar and nonpolar sublattices in intermetallics: the NaCd(2) structure. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 1958-76	16.4	62

248	Electron-rich three-center bonding: role of s,p interactions across the p-block. <i>Journal of the American Chemical Society</i> , 2002 , 124, 4787-95	16.4	62
247	Mechanochemical Synthesis of Carbon Nanothread Single Crystals. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16343-16349	16.4	61
246	Hydride bridges between LnCp ₂ centers. <i>Inorganic Chemistry</i> , 1985 , 24, 2095-2104	5.1	60
245	Conformational preferences of substituted cyclopentadienyl and heterocyclopentadienyl complexes. <i>Chemische Berichte</i> , 1978 , 111, 1578-1590		60
244	Cycloheptatriene and fulvene Cr(CO) ₃ complexes. <i>Chemische Berichte</i> , 1978 , 111, 1591-1602		59
243	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	3.6	58
242	Alkyl Shifts between Transition Metals and Coordinated Main Group Atoms. <i>Helvetica Chimica Acta</i> , 1984 , 67, 1-17	2	58
241	High Hydrides of Scandium under Pressure: Potential Superconductors. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 6298-6309	3.8	57
240	Carbon Nitride Nanothread Crystals Derived from Pyridine. <i>Journal of the American Chemical Society</i> , 2018 , 140, 4969-4972	16.4	56
239	The Effect of Pressure on Organic Reactions in Fluids-a New Theoretical Perspective. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 11126-11142	16.4	55
238	The RE M E Phases. <i>Helvetica Chimica Acta</i> , 2003 , 86, 1653-1682	2	55
237	Theory of Polyhedral Molecules. II. A Crystal Field Model. <i>Journal of Chemical Physics</i> , 1962 , 36, 2189-2195	5.9	55
236	The Many Guises of Aromaticity. <i>American Scientist</i> , 2015 , 103, 18	2.7	54
235	Large-Scale Soft Colloidal Template Synthesis of 1.4 nm Thick CdSe Nanosheets. <i>Angewandte Chemie</i> , 2009 , 121, 6993-6996	3.6	53
234	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. <i>Physical Review B</i> , 2013 , 88,	3.3	52
233	Adsorption of CO on PtBi ₂ and PtBi surfaces. <i>Surface Science</i> , 2005 , 574, 1-16	1.8	52
232	Transition State for the HydrogenBdine and the Hydrogen Exchange Reactions. <i>Journal of Chemical Physics</i> , 1968 , 49, 3739-3740	3.9	52
231	High pressure stabilization and emergent forms of PbH ₄ . <i>Physical Review Letters</i> , 2011 , 107, 037002	7.4	51

230	A fresh look at dense hydrogen under pressure. I. an introduction to the problem, and an index probing equalization of H-H distances. <i>Journal of Chemical Physics</i> , 2012 , 136, 074501	3.9	50
229	A Class of Trinuclear Clusters with Carbonyl Bridging. <i>Helvetica Chimica Acta</i> , 1980 , 63, 29-49	2	50
228	Ferrocene: Ironclad History or Rashomon Tale?. <i>Angewandte Chemie - International Edition</i> , 2000 , 39, 123-124	16.4	49
227	Quantum mechanical approach to the conformational analysis of macromolecules in ground and excited states. <i>Biopolymers</i> , 1969 , 7, 207-213	2.2	49
226	Mirrors of Bonding in Metal Halide Perovskites. <i>Journal of the American Chemical Society</i> , 2018 , 140, 12996-13040		
225	A response to the critical comments on "One molecule, two atoms, three views, four bonds?". <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 5926-8	16.4	48
224	Potential Linear-Chain Organic Ferromagnets. <i>Chemistry - A European Journal</i> , 1995 , 1, 403-413	4.8	48
223	Orbital Theory of Heterolytic Fragmentation and Remote Effects on Nitrogen Inversion Equilibria. <i>Helvetica Chimica Acta</i> , 1972 , 55, 893-906	2	48
222	Polyisocyanides: electronic or steric reasons for their presumed helical structure?. <i>Journal of the American Chemical Society</i> , 1990 , 112, 8230-8238	16.4	47
221	Quantum interference in polyenes. <i>Journal of Chemical Physics</i> , 2014 , 141, 224311	3.9	46
220	Total energy partitioning within a one-electron formalism: A Hamilton population study of surface-CO interaction in the c(20)-CO/ Ni(100) chemisorption system. <i>Journal of Chemical Physics</i> , 1999 , 111, 893-910	3.9	46
219	How Should Chemists Think?. <i>Scientific American</i> , 1993 , 268, 66-73	0.5	45
218	Squeezing C-C bonds. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 7549-53	16.4	44
217	Surface Activation of Transition Metal Nanoparticles for Heterogeneous Catalysis: What We Can Learn from Molecular Dynamics. <i>ACS Catalysis</i> , 2018 , 8, 3365-3375	13.1	42
216	Connecting the chemical and physical viewpoints of what determines structure: from 1-D chains to brasses. <i>Chemical Reviews</i> , 2011 , 111, 4522-45	68.1	42
215	Evolving Structural Diversity and Metallicity in Compressed Lithium Azide. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 20838-20846	3.8	41
214	Group 12 dihalides: structural predilections from gases to solids. <i>Chemistry - A European Journal</i> , 2009 , 15, 158-77	4.8	41
213	Counterintuitive orbital mixing. <i>Journal of Chemical Physics</i> , 1978 , 68, 5498-5500	3.9	41

212	Chemie unter höchsten Drücken: eine Herausforderung für die chemische Intuition. <i>Angewandte Chemie</i> , 2007 , 119, 3694-3717	3.6	40
211	Molecular orbitals of the oxocarbons (CO_n , $n = 2-6$. Why does $(\text{CO})_4$ have a triplet ground state?. <i>Journal of the American Chemical Society</i> , 2012 , 134, 10259-70	16.4	39
210	$S_4(2)$ -rings, disulfides, and sulfides in transition-metal complexes: the subtle interplay of oxidation and structure. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 2864-8	16.4	39
209	Electron-rich rods as building blocks for Sb strips and Te sheets. <i>Journal of the American Chemical Society</i> , 2001 , 123, 6600-8	16.4	39
208	Expanding the Frontiers of Higher-Order Cycloadditions. <i>Accounts of Chemical Research</i> , 2019 , 52, 3488-3501	35	39
207	TII-TII Interactions in the Molecular State in MO Analysis. <i>Angewandte Chemie International Edition in English</i> , 1989 , 28, 1688-1690		38
206	Enhancing the conductivity of molecular electronic devices. <i>Journal of Chemical Physics</i> , 2017 , 146, 092310	30	37
205	Quantum Interference, Graphs, Walks, and Polynomials. <i>Chemical Reviews</i> , 2018 , 118, 4887-4911	68.1	37
204	Transition metal complexes of cyclic and open ozone and thiozone. <i>Journal of the American Chemical Society</i> , 2005 , 127, 1278-85	16.4	37
203	Direct and indirect band gap types in one-dimensional conjugated or stacked organic materials. <i>Theoretical Chemistry Accounts</i> , 1999 , 102, 23-32	1.9	37
202	Structural Diversity and Electron Confinement in LiN: Potential for 0-D, 2-D, and 3-D Electrides. <i>Journal of the American Chemical Society</i> , 2016 , 138, 14108-14120	16.4	37
201	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	9.6	36
200	Di-Ehydrido-bis[1,3-propanbis(dicyclohexylphosphin)]dinickel(Ni_2Ni) Der Bindungszustand in einem Dreizentren-Wasserstoff-Berbrüchten Ni $_2$ Ni-System. <i>Chemische Berichte</i> , 1977 , 110, 3900-3909		36
199	Coarctate and Möbius: The Helical Orbitals of Allene and Other Cumulenes. <i>ACS Central Science</i> , 2018 , 4, 688-700	16.8	34
198	Two-dimensional CdSe nanosheets and their interaction with stabilizing ligands. <i>Advanced Materials</i> , 2013 , 25, 261-6	24	34
197	A fresh look at dense hydrogen under pressure. II. Chemical and physical models aiding our understanding of evolving H-H separations. <i>Journal of Chemical Physics</i> , 2012 , 136, 074502	3.9	34
196	Hypervalenzbindung in einer, zwei und drei Dimensionen: Erweiterung des Zintl-Klemm-Konzepts auf nichtklassische elektronenreiche Netze. <i>Angewandte Chemie</i> , 2000 , 112, 2500-2544	3.6	34
195	Exponential Attenuation of Through-Bond Transmission in a Polyene: Theory and Potential Realizations. <i>ACS Nano</i> , 2015 , 9, 11109-20	16.7	33

194	Building up Complexity from Strips and Sheets: The Electronic Structure of the La ₁₂ Mn ₂ Sb ₃₀ Alloy. <i>Journal of Solid State Chemistry</i> , 1998 , 139, 8-21	3.3	33
193	Die Vorhersage von Molekülen – mehr Realismus bitte!. <i>Angewandte Chemie</i> , 2008 , 120, 7276-7279	3.6	33
192	The RE M E Phases. <i>Helvetica Chimica Acta</i> , 2003 , 86, 1683-1708	2	33
191	Not a Library I am grateful to Albert Eschenmoser, Sylvie Coyaud, and Henning Hopf for their comments.. <i>Angewandte Chemie - International Edition</i> , 2001 , 40, 3337-3340	16.4	33
190	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	3.9	33
189	Reactivity of transition metal cluster carbides which have an exposed carbon atom. <i>Organometallics</i> , 1984 , 3, 962-970	3.8	33
188	Zur Stabilisierung des Phenyl-Kations. <i>Chemische Berichte</i> , 1972 , 105, 8-23		33
187	Ternary Gold Hydrides: Routes to Stable and Potentially Superconducting Compounds. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8740-8751	16.4	32
186	Distinguishing Bonds. <i>Journal of the American Chemical Society</i> , 2016 , 138, 3731-44	16.4	32
185	The unusual and the expected in the Si/C phase diagram. <i>Journal of the American Chemical Society</i> , 2013 , 135, 11651-6	16.4	32
184	What might philosophy of science look like if chemists built it?. <i>Synthese</i> , 2007 , 155, 321-336	0.8	31
183	Solid memory: structural preferences in group 2 dihalide monomers, dimers, and solids. <i>Journal of the American Chemical Society</i> , 2006 , 128, 11236-49	16.4	31
182	A theoretical study of the initial stages of Si(111)–O oxidation. II. The dissociated state and formation of SiO ₄ . <i>Journal of Chemical Physics</i> , 1993 , 98, 7606-7612	3.9	31
181	Graphane nanotubes. <i>ACS Nano</i> , 2012 , 6, 7142-50	16.7	30
180	Ein Moleköl zwei Atome, drei Ansichten, vier Bindungen?. <i>Angewandte Chemie</i> , 2013 , 125, 3094-3109	3.6	30
179	Sequential Substitution Reactions on B ₁₀ H ₁₀ and B ₁₂ H ₁₂ . <i>Journal of Chemical Physics</i> , 1962 , 37, 520-523	3.9	30
178	Distribution of Electronic Levels in Alkanes. <i>Journal of Chemical Physics</i> , 1964 , 40, 2047-2048	3.9	30
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