

Roald Hoffmann

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Fermi surface studies of the low-temperature structure of sodium. <i>Physical Review B</i> , 2020 , 101,	3.3	1
336	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	6.4	5
335	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part C. Toward Consilience. <i>Angewandte Chemie</i> , 2020 , 132, 13798-13814	3.6	1
334	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	3.6	1
333	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part A. Stage Setting. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 12590-12610	16.4	9
332	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	16.4	9
331	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part C. Toward Consilience. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 13694-13710	16.4	8
330	Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part A. Stage Setting. <i>Angewandte Chemie</i> , 2020 , 132, 12690-12710	3.6	1
329	Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischer-Tropsch Synthesis. <i>Catalysis Letters</i> , 2019 , 149, 645-664	2.8	13
328	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
327	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	16.4	14
326	Do Diradicals Behave Like Radicals?. <i>Chemical Reviews</i> , 2019 , 119, 11291-11351	68.1	116
325	High-pressure lithium as an elemental topological semimetal. <i>Physical Review Materials</i> , 2019 , 3,	3.2	3
324	Expanding the Frontiers of Higher-Order Cycloadditions. <i>Accounts of Chemical Research</i> , 2019 , 52, 3488-3501	39	39
323	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
322	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
321	Coarctate and Möbius: The Helical Orbitals of Allene and Other Cumulenes. <i>ACS Central Science</i> , 2018 , 4, 688-700	16.8	34

320	Quantum Interference, Graphs, Walks, and Polynomials. <i>Chemical Reviews</i> , 2018 , 118, 4887-4911	68.1	37
319	High Hydrides of Scandium under Pressure: Potential Superconductors. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 6298-6309	3.8	57
318	All the Ways To Have Substituted Nанothreads. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1131-1140	6.4	11
317	Alkali-Metal Trihalides: MX Ion Pair or MX-X Complex?. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 3339-3353	3.4	5
316	Carbon Nitride Nanothread Crystals Derived from Pyridine. <i>Journal of the American Chemical Society</i> , 2018 , 140, 4969-4972	16.4	56
315	Potential Semiconducting and Superconducting Metastable Si ₃ C Structures under Pressure. <i>Chemistry of Materials</i> , 2018 , 30, 421-427	9.6	4
314	Alkyl Isosteres. <i>Journal of the American Chemical Society</i> , 2018 , 140, 12844-12852	16.4	3
313	Mirrors of Bonding in Metal Halide Perovskites. <i>Journal of the American Chemical Society</i> , 2018 , 140, 12996-13040	16.4	10
312	Eight-coordinate fluoride in a silicate double-four-ring. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 828-833	11.5	11
311	Evidence from Fermi surface analysis for the low-temperature structure of lithium. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 5389-5394	11.5	12
310	An Iodobenzene Story. <i>Journal of the American Chemical Society</i> , 2017 , 139, 7124-7129	16.4	9
309	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
308	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
307	Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9302-9316	16.4	23
306	Dioxygen: What Makes This Triplet Diradical Kinetically Persistent?. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9010-9018	16.4	94
305	The Green's Function for the Hückel (tight binding) model. <i>Journal of Mathematical Physics</i> , 2017 , 58, 033505	1.2	11
304	Quasimolecules in Compressed Lithium. <i>Angewandte Chemie</i> , 2017 , 129, 992-995	3.6	15
303	Enhancing the conductivity of molecular electronic devices. <i>Journal of Chemical Physics</i> , 2017 , 146, 092310	3.7	37

302	Quasimolecules in Compressed Lithium. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 972-975	16.4	25
301	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	11.5	1
300	Mechanochemical Synthesis of Carbon Nanothread Single Crystals. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16343-16349	16.4	61
299	Stabilizing a different cyclooctatetraene stereoisomer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 9803-9808	11.5	17
298	Druckeffekte auf organische Reaktionen in Fluiden – Eine neue theoretische Perspektive. <i>Angewandte Chemie</i> , 2017 , 129, 11278-11295	3.6	5
297	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
296	Donor-Acceptor Strategies for Stabilizing Planar Diplumbenes. <i>Organometallics</i> , 2017 , 36, 4825-4833	3.8	2
295	Atomic and Ionic Radii of Elements 1-96. <i>Chemistry - A European Journal</i> , 2016 , 22, 14625-32	4.8	143
294	Semiconductive KMSb(SH) (M = Zn, Cd) Featuring One-Dimensional [MSb(SH)] Chains. <i>Inorganic Chemistry</i> , 2016 , 55, 9742-9747	5.1	14
293	Homo Citans und Kohlenstoffallotrope: Für eine Ethik des Zitierens. <i>Angewandte Chemie</i> , 2016 , 128, 11122-11139	3.6	14
292	Homo Citans and Carbon Allotropes: For an Ethics of Citation. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 10962-76	16.4	172
291	Helical Oligoenes: Conformations, Bond Alternation, and Competing Through-Bond and Through-Space Transmission. <i>Chemistry - A European Journal</i> , 2016 , 22, 4878-88	4.8	15
290	AuO: Evolving from Dis- to Comproportionation and Back Again. <i>Inorganic Chemistry</i> , 2016 , 55, 1278-86	5.1	23
289	The Dimerization of H ₂ NO. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 1283-96	2.8	3
288	Distinguishing Bonds. <i>Journal of the American Chemical Society</i> , 2016 , 138, 3731-44	16.4	32
287	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
286	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. <i>Chemical Reviews</i> , 2016 , 116, 8173-92	68.1	94
285	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

284	High-pressure electrides: the chemical nature of interstitial quasiatoms. <i>Journal of the American Chemical Society</i> , 2015 , 137, 3631-7	16.4	94
283	Toward an Experimental Quantum Chemistry: Exploring a New Energy Partitioning. <i>Journal of the American Chemical Society</i> , 2015 , 137, 10282-91	16.4	24
282	Exponential Attenuation of Through-Bond Transmission in a Polyene: Theory and Potential Realizations. <i>ACS Nano</i> , 2015 , 9, 11109-20	16.7	33
281	Linearly Polymerized Benzene Arrays As Intermediates, Tracing Pathways to Carbon Nanothreads. <i>Journal of the American Chemical Society</i> , 2015 , 137, 14373-86	16.4	69
280	For the M. Hargittai issue. <i>Structural Chemistry</i> , 2015 , 26, 1165-1165	1.8	1
279	Chemical bonding in hydrogen and lithium under pressure. <i>Journal of Chemical Physics</i> , 2015 , 143, 064703	3.9	21
278	Tension in Chemistry and Its Contents. <i>Accountability in Research</i> , 2015 , 22, 330-45	1.9	2
277	Li-Filled, B-Substituted Carbon Clathrates. <i>Journal of the American Chemical Society</i> , 2015 , 137, 12639-52	16.4	26
276	Tuning the Ground State Symmetry of Acetylenyl Radicals. <i>ACS Central Science</i> , 2015 , 1, 270-8	16.8	5
275	Molecular CsF5 and CsF2+. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 8275-8	16.4	12
274	Molecular CsF5 and CsF2+. <i>Angewandte Chemie</i> , 2015 , 127, 8393-8396	3.6	6
273	Anomalous orbital admixture in ammine complexes. <i>Journal of Organometallic Chemistry</i> , 2015 , 792, 6-12	2.3	5
272	Theoretical Study of Phase Separation of Scandium Hydrides under High Pressure. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 5614-5625	3.8	26
271	The Many Guises of Aromaticity. <i>American Scientist</i> , 2015 , 103, 18	2.7	54
270	Frontier orbital control of molecular conductance and its switching. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 4093-7	16.4	68
269	Lithium hydroxide, LiOH, at elevated densities. <i>Journal of Chemical Physics</i> , 2014 , 141, 024505	3.9	14
268	Frontier Orbital Control of Molecular Conductance and its Switching. <i>Angewandte Chemie</i> , 2014 , 126, 4177-4181	3.6	19
267	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

266	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
265	Quantum interference in polyenes. <i>Journal of Chemical Physics</i> , 2014 , 141, 224311	3.9	46
264	High pressure electrides: a predictive chemical and physical theory. <i>Accounts of Chemical Research</i> , 2014 , 47, 1311-7	24.3	139
263	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
262	Squareglitter: A 3,4-Connected Carbon Net. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3855-96.4	7	
261	Evolving Structural Diversity and Metallicity in Compressed Lithium Azide. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 20838-20846	3.8	41
260	Isotopic differentiation and sublattice melting in dense dynamic ice. <i>Physical Review B</i> , 2013 , 88,	3.3	14
259	Small but strong lessons from chemistry for nanoscience. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 93-103	16.4	80
258	Klein, aber oho: was die Nanowissenschaft von der Chemie lernen kann. <i>Angewandte Chemie</i> , 2013 , 125, 99-111	3.6	15
257	Binary compounds of boron and beryllium: a rich structural arena with space for predictions. <i>Chemistry - A European Journal</i> , 2013 , 19, 4184-97	4.8	21
256	One molecule, two atoms, three views, four bonds?. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 3020-33	16.4	110
255	Two-dimensional CdSe nanosheets and their interaction with stabilizing ligands. <i>Advanced Materials</i> , 2013 , 25, 261-6	24	34
254	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
253	A Response to the Critical Comments on One Molecule, Two Atoms, Three Views, Four Bonds? <i>Angewandte Chemie</i> , 2013 , 125, 6040-6042	3.6	14
252	Hypervalent compounds as ligands: I3-anion adducts with transition metal pentacarbonyls. <i>Inorganic Chemistry</i> , 2013 , 52, 7161-71	5.1	20
251	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. <i>Physical Review B</i> , 2013 , 88,	3.3	52
250	The Close Relationships between the Crystal Structures of MO and MSO ₄ (M = Group 10, 11, or 12 Metal), and the Predicted Structures of AuO and PtSO ₄ . <i>European Journal of Inorganic Chemistry</i> , 2013 , 2013, 5094-5102	2.3	5
249	Ein Molek \ddot{u} zwei Atome, drei Ansichten, vier Bindungen?. <i>Angewandte Chemie</i> , 2013 , 125, 3094-3109	3.6	30

248	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
247	Molecular orbitals of the oxocarbons (CO) _n , n = 2-6. Why does (CO) ₄ have a triplet ground state?. <i>Journal of the American Chemical Society</i> , 2012 , 134, 10259-70	16.4	39
246	Graphane nanotubes. <i>ACS Nano</i> , 2012 , 6, 7142-50	16.7	30
245	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
244	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
243	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. <i>Journal of Chemical Physics</i> , 2012 , 136, 074503	3.9	28
242	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. <i>Journal of Chemical Physics</i> , 2012 , 136, 074504	3.9	25
241	LiBeB: A predicted phase with structural and electronic peculiarities. <i>Physical Review B</i> , 2012 , 86,	3.3	13
240	Stabilizing H ₃ -: or are we stabilizing a proton?. <i>ChemPhysChem</i> , 2012 , 13, 2286-8	3.2	7
239	WH(n) under pressure. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 155701	1.8	24
238	Hunting dimers. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	5
237	LiB and its boron-deficient variants under pressure. <i>Physical Review B</i> , 2012 , 86,	3.3	20
236	Hunting dimers. <i>Highlights in Theoretical Chemistry</i> , 2012 , 3-13		
235	(Barely) solid Li(NH ₃) ₄ : the electronics of an expanded metal. <i>Journal of the American Chemical Society</i> , 2011 , 133, 3535-47	16.4	24
234	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
233	Molecular models for WH ₆ under pressure. <i>New Journal of Chemistry</i> , 2011 , 35, 2349	3.6	9
232	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
231	BH ₃ under pressure: leaving the molecular diborane motif. <i>Journal of the American Chemical Society</i> , 2011 , 133, 21002-9	16.4	26

230	High pressure stabilization and emergent forms of PbH4. <i>Physical Review Letters</i> , 2011 , 107, 037002	7.4	51
229	International Year of Chemistry 2011: Sustainable Development. <i>Clinical Chemistry</i> , 2011 , 57, 144-144	5.5	1
228	JUST WHEN WE ARE SAFEST. <i>Yale Review</i> , 2010 , 98, 126-127	0	
227	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
226	Compressing the most hydrogen-rich inorganic ion. <i>Journal of the American Chemical Society</i> , 2010 , 132, 748-55	16.4	22
225	Segregation into layers: a general problem for structural instability under pressure, exemplified by SnH4. <i>ChemPhysChem</i> , 2010 , 11, 3105-12	3.2	13
224	Exploring group 14 structures: 1D to 2D to 3D. <i>Chemistry - A European Journal</i> , 2010 , 16, 6555-66	4.8	27
223	Two Lives. <i>American Scientist</i> , 2010 , 98, 117	2.7	6
222	Element lines: bonding in the ternary gold polyphosphides, Au(2)MP(2) with M = Pb, Tl, or Hg. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2199-207	16.4	19
221	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
220	Lithium-Ammoniak-Lösungen: eine molekulare Betrachtung. <i>Angewandte Chemie</i> , 2009 , 121, 8344-8381	3.6	8
219	Group 12 dihalides: structural predilections from gases to solids. <i>Chemistry - A European Journal</i> , 2009 , 15, 158-77	4.8	41
218	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
217	Large-Scale Soft Colloidal Template Synthesis of 1.4 nm Thick CdSe Nanosheets. <i>Angewandte Chemie</i> , 2009 , 121, 6993-6996	3.6	53
216	A molecular perspective on lithium-ammonia solutions. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 8198-232	16.4	133
215	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
214	"Half-bonds" in an unusual coordinated S(4) (2-) rectangle. <i>Chemistry - an Asian Journal</i> , 2009 , 4, 302-13	4.5	9
213	Cover picture: "half-bonds" in an unusual coordinated S4(2-) rectangle (Chem. Asian J. 2/2009). <i>Chemistry - an Asian Journal</i> , 2009 , 4, 215	4.5	

212	Teaching and learning strategies that work. <i>Science</i> , 2009 , 325, 1203-4	33.3	6
211	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. <i>Nature</i> , 2008 , 451, 445-8	50.4	93
210	S4(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	Learning from molecules in distress. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 4474-81	16.4	71
208	Predicting molecules--more realism, please!. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7164-7164	16.4	257
207	S42 Rings, Disulfides, and Sulfides in Transition-Metal Complexes: The Subtle Interplay of Oxidation and Structure. <i>Angewandte Chemie</i> , 2008 , 120, 2906-2910	3.6	11
206	Moleküle in Not und was wir von ihnen lernen. <i>Angewandte Chemie</i> , 2008 , 120, 4548-4556	3.6	28
205	Die Vorhersage von Molekülen -mehr Realismus bitte!. <i>Angewandte Chemie</i> , 2008 , 120, 7276-7279	3.6	33
204	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	2.7	7
203	Why Think Up New Molecules?. <i>American Scientist</i> , 2008 , 96, 372	2.7	14
202	A quantum mechanically guided view of Mg ₄₄ Rh ₇ . <i>Chemistry - A European Journal</i> , 2007 , 13, 7852-63	4.8	17
201	Interpenetrating polar and nonpolar sublattices in intermetallics: the NaCd(2) structure. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 1958-76	16.4	62
200	The chemical imagination at work in very tight places. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 3620-42	16.4	327
199	Cover Picture: Interpenetrating Polar and Nonpolar Sublattices in Intermetallics: The NaCd ₂ Structure (Angew. Chem. Int. Ed. 12/2007). <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 1927-1927	16.4	2
198	Sich durchdringende polare und unpolare Untergitter in intermetallischen Phasen: die Struktur von NaCd ₂ . <i>Angewandte Chemie</i> , 2007 , 119, 2004-2023	3.6	19
197	Chemie unter hähnsten Drücken: eine Herausforderung für die chemische Intuition. <i>Angewandte Chemie</i> , 2007 , 119, 3694-3717	3.6	40
196	Titelbild: Sich durchdringende polare und unpolare Untergitter in intermetallischen Phasen: die Struktur von NaCd ₂ (Angew. Chem. 12/2007). <i>Angewandte Chemie</i> , 2007 , 119, 1971-1971	3.6	
195	Blow-up: making sense of the image in the nanoworld. <i>Small</i> , 2007 , 3, 368-71	11	

194	What might philosophy of science look like if chemists built it?. <i>Synthese</i> , 2007 , 155, 321-336	0.8	31
193	Electronic Effects in CO Chemisorption on PtBb Intermetallic Surfaces: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 17357-17369	3.8	17
192	Structure and bonding in boron carbide: The invincibility of imperfections. <i>New Journal of Chemistry</i> , 2007 , 31, 473	3.6	103
191	Brücken zwischen Anorganischer und Organischer Chemie (Nobel-Vortrag). <i>Angewandte Chemie</i> , 2006 , 94, 725-739	3.6	341
190	Prediction of thermodynamic stability and electronic structure of novel ternary lanthanide hydrides. <i>Journal of Materials Chemistry</i> , 2006 , 16, 1154	10	
189	Theoretical studies on doubly and triply linked polymers of Ge9 clusters. <i>Inorganica Chimica Acta</i> , 2006 , 359, 3776-3784	2.7	8
188	Structures and potential superconductivity in at high pressure: en route to "metallic hydrogen". <i>Physical Review Letters</i> , 2006 , 96, 017006	7.4	174
187	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
186	Richard Kuhn, das Dritte Reich und die GDCh. <i>Nachrichten Aus Der Chemie</i> , 2006 , 54, 1019-1024	0.1	
185	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
184	Adsorption of CO on PtBi2 and PtBi surfaces. <i>Surface Science</i> , 2005 , 574, 1-16	1.8	52
183	Squeezing C-C bonds. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 7549-53	16.4	44
182	Squeezing C?C Bonds. <i>Angewandte Chemie</i> , 2005 , 117, 7721-7725	3.6	17
181	How do electrons travel in unusual metallic fluorides of Ag2+?. <i>Physica Status Solidi (B): Basic Research</i> , 2005 , 242, R1-R3	1.3	14
180	Theoretical Chemistry. <i>Foundations of Chemistry</i> , 2004 , 6, 11	0.7	
179	A claim on the development of the frontier orbital explanation of electrocyclic reactions. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 6586-90	16.4	22
178	A Claim on the Development of the Frontier Orbital Explanation of Electrocyclic Reactions. <i>Angewandte Chemie</i> , 2004 , 116, 6748-6752	3.6	6
177	Hydrogen Migration Over Organic Tapes: [1,5] Sigmatropic Shiftamers. <i>European Journal of Organic Chemistry</i> , 2004 , 2004, 273-280	3.2	4

176	Thinking about metal-metal quadruple bonding in extended structures: a hypothetical A2M6E8 network. <i>New Journal of Chemistry</i> , 2004 , 28, 185	3.6	3
175	Dicyclobuta[de,ij]naphthalene and dicyclopenta[cd,gh]pentalene: a theoretical study. <i>Journal of Organic Chemistry</i> , 2004 , 69, 8093-100	4.2	8
174	Main group element nets to a T. <i>Inorganic Chemistry</i> , 2004 , 43, 2526-40	5.1	13
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