Bun Chan

List of Publications by Year in Descending Order

152 papers	3,576 citations	34 h-index	52 g-index
165 ext. papers	4,247 ext. citations	5.9 avg, IF	6.03 L-index

#	Paper	IF	Citations
152	Higher-order transition state approximation.. *Journal of Chemical Physics*, **2022**, 156, 114112	3.9	1
151	Accurate Quantum Chemical Prediction of Gas-Phase Anion Binding Affinities and Their Structure-Binding Relationships. *Journal of Physical Chemistry A*, **2021**, 125, 9838-9851	2.8	2
150	Multi-interactive Coordination Network Featuring a Ligand with Topologically Isolated p Orbitals. *Inorganic Chemistry*, **2021**, 60, 17858-17864	5.1	0
149	Fluorescence Enhancement through Confined Oligomerization in Nanochannels: An Anthryl Oligomer in a Metal-Organic Framework **2021**, 3, 1599-1604		1
148	Liquid-phase sintering of lead halide perovskites and metal-organic framework glasses. *Science*, **2021**, 374, 621-625	33.3	29
147	KoopmansRType Theorem in Kohn-Sham Theory with Optimally Tuned Long-Range-Corrected (LC) Functionals. *Journal of Physical Chemistry A*, **2021**, 125, 3489-3502	2.8	5
146	An improved SlaterR transition state approximation. *Journal of Chemical Physics*, **2021**, 155, 034101	3.9	3
145	Thermochemical stabilities of giant fullerenes using density functional tight binding theory and isodesmic-type reactions. *Journal of Computational Chemistry*, **2021**, 42, 222-230	3.5	4
144	Assessment and development of DFT with the expanded CUAGAU-2 set of group-11 cluster systems. *International Journal of Quantum Chemistry*, **2021**, 121, e26453	2.1	8
143	Applications of isodesmic-type reactions for computational thermochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1501	7.9	8
142	A cofacial metal-organic framework based photocathode for carbon dioxide reduction. *Chemical Science*, **2021**, 12, 3608-3614	9.4	5
141	Re-examining the electronic structure of fluorescent tetra-silver clusters in zeolites. *Physical Chemistry Chemical Physics*, **2021**, 23, 1984-1993	3.6	1
140	A redox-active ionic liquid manifesting charge-transfer interaction between a viologen and carbazole and its effect on the viscosity, ionic conductivity, and redox process of the viologen. *Chemical Science*, **2021**, 12, 4872-4882	9.4	5
139	Accurate Heats of Formation for Polycyclic Aromatic Hydrocarbons: A High-Level Ab Initio Perspective. *Journal of Chemical & Engineering Data*, **2021**, 66, 3453-3462	2.8	2
138	Accurate Thermochemistry for Main-Group Elements up to Xenon with the W-P34 Series of Composite Methods. *Journal of Chemical Theory and Computation*, **2021**, 17, 5704-5714	6.4	0
137	Hydride Affinities for Main-Group Hydride Reductants: Assessment of Density Functionals and Trends in Reactivities. *Journal of Physical Chemistry A*, **2021**, 125, 835-842	2.8	1
136	Substituent effects on through-space intervalence charge transfer in cofacial metal-organic frameworks. *Faraday Discussions*, **2021**, 231, 152-167	3.6	0

135	Polycyclic aromatic hydrocarbons: from small molecules through nano-sized species towards bulk graphene. *Physical Chemistry Chemical Physics*, **2021**, 23, 17713-17723	3.6	0
134	The electrochemical reduction of a flexible Mn(II) salen-based metal-organic framework. *Dalton Transactions*, **2021**, 50, 12821-12825	4.3	
133	Photo-control of bimolecular reactions: reactivity of the long-lived Rhodamine 6G triplet excited state with NO. *Physical Chemistry Chemical Physics*, **2021**, 23, 25038-25047	3.6	0
132	Methylation with Dimethyl Carbonate/Dimethyl Sulfide Mixtures: An Integrated Process without Addition of Acid/Base and Formation of Residual Salts.. *ChemSusChem*, **2021**, e202102538	8.3	1
131	Core-Level Excitation Energies of Nucleic Acid Bases Expressed as Orbital Energies of the Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 10482-10494	2.8	4
130	Excitation energies expressed as orbital energies of Kohn-Sham density functional theory with long-range corrected functionals. *Journal of Computational Chemistry*, **2020**, 41, 1368-1383	3.5	9
129	Bond initiated generation of aryl radicals from aryl diazonium salts. *Organic and Biomolecular Chemistry*, **2020**, 18, 1812-1819	3.9	13
128	Aqueous-Phase Conformations of Lactose, Maltose, and Sucrose and the Assessment of Low-Cost DFT Methods with the DSCONF Set of Conformers for the Three Disaccharides. *Journal of Physical Chemistry A*, **2020**, 124, 582-590	2.8	8
127	Hydrothermal Liquefaction of O-4 Aryl Ether Linkages in Lignin. *ChemSusChem*, **2020**, 13, 2002-2006	8.3	4
126	Halogenated Metal-Organic Framework Glasses and Liquids. *Journal of the American Chemical Society*, **2020**, 142, 3880-3890	16.4	34
125	How accurate are approximate quantum chemical methods at modelling solute-solvent interactions in solvated clusters?. *Physical Chemistry Chemical Physics*, **2020**, 22, 3855-3866	3.6	13
124	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. *Chemical Physics*, **2020**, 531, 110676	2.3	3
123	Fluorination effect on electrochemistry of dibutyl viologen in aqueous solution. *Journal of Electroanalytical Chemistry*, **2020**, 856, 113691	4.1	2
122	Charge-Transfer Excitation Energies Expressed as Orbital Energies of Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 8079-8087	2.8	7
121	Rapid Prediction of Ultraviolet-Visible Spectra from Conventional (Non-Time-Dependent) Density Functional Theory Calculations. *Journal of Physical Chemistry Letters*, **2020**, 11, 7882-7885	6.4	6
120	Fullerene Thermochemical Stability: Accurate Heats of Formation for Small Fullerenes, the Importance of Structural Deformation on Reactivity, and the Special Stability of C. *Journal of Physical Chemistry A*, **2020**, 124, 6688-6698	2.8	6
119	Toward an Understanding of the Forces Behind Extractive Desulfurization of Fuels with Ionic Liquids. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 4087-4093	8.3	19
118	A Simple Model for Relative Energies of All Fullerenes Reveals the Interplay between Intrinsic Resonance and Structural Deformation Effects in Medium-Sized Fullerenes. *Journal of Chemical Theory and Computation*, **2019**, 15, 1255-1264	6.4	7

117	The CUAGAU Set of Coupled-Cluster Reference Data for Small Copper, Silver, and Gold Compounds and Assessment of DFT Methods. *Journal of Physical Chemistry A*, **2019**, 123, 5781-5788	2.8	11
116	Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. *Journal of Chemical Theory and Computation*, **2019**, 15, 3610-3622	6.4	45
115	The spectroelectrochemical behaviour of redox-active manganese salen complexes. *Dalton Transactions*, **2019**, 48, 3704-3713	4.3	15
114	G4(MP2)-XK: A Variant of the G4(MP2)-6X Composite Method with Expanded Applicability for Main-Group Elements up to Radon. *Journal of Chemical Theory and Computation*, **2019**, 15, 4478-4484	6.4	15
113	An ONIOM investigation of the effect of conformation on bond dissociation energies in peptides. *Journal of Computational Chemistry*, **2019**, 40, 82-88	3.5	4
112	The reHISS Three-Range Exchange Functional with an Optimal Variation of Hartree-Fock and Its Use in the reHISSB-D Density Functional Theory Method. *Journal of Computational Chemistry*, **2019**, 40, 29-38	3.5	5
111	Accurate Thermochemical and Kinetic Stabilities of C Isomers. *Journal of Physical Chemistry A*, **2018**, 122, 4768-4777	2.8	7
110	Interligand Charge-Transfer Interactions in Electroactive Coordination Frameworks Based on N, NRDicyanoquinonediimine (DCNQI). *Inorganic Chemistry*, **2018**, 57, 9766-9774	5.1	7
109	Effect of Hydrogen Bonding and Partial Deprotonation on the Oxidation of Peptides. *Journal of Physical Chemistry A*, **2018**, 122, 1741-1746	2.8	13
108	Ni-Catalyzed Formal Carbonyl-Ene Reaction of Terminal Alkenes via Carbon Dioxide Insertion. *Synlett*, **2018**, 29, 742-746	2.2	6
107	Barriometry - an enhanced database of accurate barrier heights for gas-phase reactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 10732-10740	3.6	5
106	Through-Space Intervalence Charge Transfer as a Mechanism for Charge Delocalization in Metal-Organic Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 6622-6630	16.4	82
105	[Fe(C5Ar5)(CO)2Br] complexes as hydrogenase mimics for the catalytic hydrogen evolution reaction. *Applied Catalysis B: Environmental*, **2018**, 223, 234-241	21.8	23
104	Bromozincate ionic liquids in the Knoevenagel condensation reaction. *Applied Catalysis B: Environmental*, **2018**, 223, 228-233	21.8	23
103	Formulation of Small Test Sets Using Large Test Sets for Efficient Assessment of Quantum Chemistry Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 4254-4262	6.4	16
102	Modelling the Effect of Conformation on Hydrogen-Atom Abstraction from Peptides. *Australian Journal of Chemistry*, **2018**, 71, 257	1.2	4
101	Spectroscopic, electronic and computational properties of a mixed tetrachalcogenafulvalene and its charge transfer complex. *Journal of Materials Chemistry C*, **2018**, 6, 1092-1104	7.1	7
100	Construction of Challenging Proline-Proline Junctions via Diselenide-Selenoester Ligation Chemistry. *Journal of the American Chemical Society*, **2018**, 140, 13327-13334	16.4	40

99	Probing charge transfer characteristics in a donor-acceptor metal-organic framework by Raman spectroelectrochemistry and pressure-dependence studies. *Physical Chemistry Chemical Physics*, **2018**, 20, 25772-25779	3.6	19
98	Solvation of the Glycyl Radical. *Journal of Physical Chemistry A*, **2018**, 122, 7212-7217	2.8	1
97	Increasing spin crossover cooperativity in 2D Hofmann-type materials with guest molecule removal. *Chemical Science*, **2018**, 9, 5623-5629	9.4	50
96	Mechanism for Three-Component Ni-Catalyzed Carbonylene Reaction for CO2 Transformation: What Practical Lessons Do We Learn from DFT Modelling?. *Australian Journal of Chemistry*, **2018**, 71, 272	1.2	5
95	How to computationally calculate thermochemical properties objectively, accurately, and as economically as possible. *Pure and Applied Chemistry*, **2017**, 89, 699-713	2.1	19
94	N-Aryl Groups Are Ubiquitous in Cross-Dehydrogenative Couplings Because They Stabilize Reactive Intermediates. *Chemistry - A European Journal*, **2017**, 23, 9313-9318	4.8	24
93	Accelerated Protein Synthesis via One-Pot Ligation-Deselenization Chemistry. *CheM*, **2017**, 2, 703-715	16.2	45
92	Impact of Hydrogen Bonding on the Susceptibility of Peptides to Oxidation. *Chemistry - an Asian Journal*, **2017**, 12, 1485-1489	4.5	6
91	Unification of the W1X and G4(MP2)-6X Composite Protocols. *Journal of Chemical Theory and Computation*, **2017**, 13, 2642-2649	6.4	17
90	Unravelling Some of the Key Transformations in the Hydrothermal Liquefaction of Lignin. *ChemSusChem*, **2017**, 10, 2140-2144	8.3	16
89	Correlation functional in screened-exchange density functional theory procedures. *Journal of Computational Chemistry*, **2017**, 38, 2307-2315	3.5	9
88	Use of Low-Cost Quantum Chemistry Procedures for Geometry Optimization and Vibrational Frequency Calculations: Determination of Frequency Scale Factors and Application to Reactions of Large Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 6052-6060	6.4	21
87	Watson-Crick Base Pair Radical Cation as a Model for Oxidative Damage in DNA. *Journal of Physical Chemistry Letters*, **2017**, 8, 3159-3165	6.4	15
86	Hydrogen-adduction to open-shell graphene fragments: spectroscopy, thermochemistry and astrochemistry. *Chemical Science*, **2017**, 8, 1186-1194	9.4	4
85	Restricted-Open-Shell G4(MP2)-Type Procedures. *Journal of Physical Chemistry A*, **2016**, 120, 9299-9304	2.8	11
84	On the inclusion of post-MP2 contributions to double-hybrid density functionals. *Journal of Computational Chemistry*, **2016**, 37, 183-93	3.5	25
83	Preparation of an ion with the highest calculated proton affinity: -diethynylbenzene dianion. *Chemical Science*, **2016**, 7, 6245-6250	9.4	14
82	Beyond the Halogen Bond: Examining the Limits of Extended Polybromide Networks through Quantum-Chemical Investigations. *Chemistry - an Asian Journal*, **2016**, 11, 682-6	4.5	8

81	From C60 to Infinity: Large-Scale Quantum Chemistry Calculations of the Heats of Formation of Higher Fullerenes. *Journal of the American Chemical Society*, **2016**, 138, 1420-9	16.4	23
80	Factors influencing the formation of polybromide monoanions in solutions of ionic liquid bromide salts. *Physical Chemistry Chemical Physics*, **2016**, 18, 7251-60	3.6	32
79	Redox tunable viologen-based porous organic polymers. *Journal of Materials Chemistry C*, **2016**, 4, 2535-2544	7.1	44
78	Hydrogen-atom attack on phenol and toluene is ortho-directed. *Physical Chemistry Chemical Physics* , **2016**, 18, 8625-36	3.6	8
77	Hydrogen Abstraction by OH and SH Radicals from Amino Acids and Their Peptide Derivatives. *Journal of Chemical Theory and Computation*, **2016**, 12, 1606-13	6.4	14
76	Performance of the OP correlation functional in relation to its formulation: Influence of the exchange component and the effect of incorporating same-spin correlations. *Journal of Computational Chemistry*, **2016**, 37, 1306-12	3.5	5
75	Reactivity of disulfide bonds is markedly affected by structure and environment: implications for protein modification and stability. *Scientific Reports*, **2016**, 6, 38572	4.9	68
74	Role of Hydrogen Bonding on the Reactivity of Thiyl Radicals: A Mass Spectrometric and Computational Study Using the Distonic Radical Ion Approach. *Journal of Physical Chemistry A*, **2016** , 120, 8184-8189	2.8	9
73	Frequency Scale Factors for Some Double-Hybrid Density Functional Theory Procedures: Accurate Thermochemical Components for High-Level Composite Protocols. *Journal of Chemical Theory and Computation*, **2016**, 12, 3774-80	6.4	31
72	Hydrogen from Formic Acid via Its Selective Disproportionation over Nanodomain-Modified Zeolites. *ACS Catalysis*, **2015**, 5, 4353-4362	13.1	14
71	Gas-phase structure and reactivity of the keto tautomer of the deoxyguanosine radical cation. *Physical Chemistry Chemical Physics*, **2015**, 17, 25837-44	3.6	12
70	H and D attachment to naphthalene: spectra and thermochemistry of cold gas-phase 1-C10H9 and 1-C10H8D radicals and cations. *Journal of Physical Chemistry A*, **2015**, 119, 3225-32	2.8	6
69	Outcome-changing effect of polarity reversal in hydrogen-atom-abstraction reactions. *Journal of Physical Chemistry A*, **2015**, 119, 3843-7	2.8	16
68	The electronic, optical and magnetic consequences of delocalization in multifunctional donor-acceptor organic polymers. *Physical Chemistry Chemical Physics*, **2015**, 17, 11252-9	3.6	17
67	Toward the complete range separation of non-hybrid exchange-correlation functional. *Journal of Computational Chemistry*, **2015**, 36, 871-7	3.5	6
66	W2X and W3X-L: Cost-Effective Approximations to W2 and W4 with kJ mol(-1) Accuracy. *Journal of Chemical Theory and Computation*, **2015**, 11, 2109-19	6.4	80
65	Rapid additive-free selenocystine-selenoester peptide ligation. *Journal of the American Chemical Society*, **2015**, 137, 14011-4	16.4	131
64	Bio-inspired transition metal-organic hydride conjugates for catalysis of transfer hydrogenation: experiment and theory. *Chemistry - A European Journal*, **2015**, 21, 2821-34	4.8	9

63	Hydrogen-atom abstraction from a model amino acid: dependence on the attacking radical. *Journal of Physical Chemistry B*, **2015**, 119, 783-8	3.4	29
62	Accurate quadruple-ζ basis-set approximation for double-hybrid density functional theory with an order of magnitude reduction in computational cost. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	18
61	Synthesis of (+)-luzofuran and (-)-ancistrofuran. *Journal of Organic Chemistry*, **2014**, 79, 880-7	4.2	17
60	Controlling charge separation in a novel donor–acceptor metal–organic framework via redox modulation. *Chemical Science*, **2014**, 5, 4724-4728	9.4	124
59	Thiosquaramides: pH switchable anion transporters. *Chemical Science*, **2014**, 5, 3617-3626	9.4	88
58	Effect of protonation state and interposed connector groups on bond dissociation enthalpies of alcohols and related systems. *Journal of Physical Chemistry A*, **2014**, 118, 2810-9	2.8	26
57	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3777-83	6.4	37
56	Hydrogen from formic acid through its selective disproportionation over sodium germanate--a non-transition-metal catalysis system. *Angewandte Chemie - International Edition*, **2014**, 53, 11275-9	16.4	9
55	Ethylene Trimerisation with Cr-PNP Catalysts: A Theoretical Benchmarking Study and Assessment of Catalyst Oxidation State. *Australian Journal of Chemistry*, **2014**, 67, 1481	1.2	22
54	Experimental and computational studies of a multi-electron donor-acceptor ligand containing the thiazolo[5,4-d]thiazole core and its incorporation into a metal-organic framework. *Chemistry - A European Journal*, **2014**, 20, 17597-605	4.8	27
53	Hydrogen from Formic Acid through Its Selective Disproportionation over Sodium Germanate—A Non-Transition-Metal Catalysis System. *Angewandte Chemie*, **2014**, 126, 11457-11461	3.6	2
52	W3X: A Cost-Effective Post-CCSD(T) Composite Procedure. *Journal of Chemical Theory and Computation*, **2013**, 9, 4769-78	6.4	47
51	Accurate Computation of Cohesive Energies for Small to Medium-Sized Gold Clusters. *Journal of Chemical Theory and Computation*, **2013**, 9, 1964-70	6.4	37
50	Electronic, optical, and computational studies of a redox-active napthalenediimide-based coordination polymer. *Inorganic Chemistry*, **2013**, 52, 14246-52	5.1	33
49	Evaluation of the heats of formation of corannulene and C60 by means of high-level theoretical procedures. *Journal of Physical Chemistry A*, **2013**, 117, 1834-42	2.8	42
48	Gas-phase infrared spectrum and acidity of the radical cation of 9-methylguanine. *Chemical Communications*, **2013**, 49, 7343-5	5.8	25
47	A Benchmark Ab Initio and DFT Study of the Structure and Binding of Methane in the σ-Alkane Complex CpRe(CO)2(CH4). *Journal of Chemical Theory and Computation*, **2013**, 9, 2199-208	6.4	35
46	Hierarchy of relative bond dissociation enthalpies and their use to efficiently compute accurate absolute bond dissociation enthalpies for C-H, C-C, and C-F bonds. *Journal of Physical Chemistry A*, **2013**, 117, 3666-75	2.8	26

45	Chemoselective Peptide Ligation–Desulfurization at Aspartate. *Angewandte Chemie*, **2013**, 125, 9905-9909	3.6	19
44	Chemoselective peptide ligation-desulfurization at aspartate. *Angewandte Chemie - International Edition*, **2013**, 52, 9723-7	16.4	98
43	Proton-bound homodimers involving second-row atoms. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	3
42	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. *Journal of Chemical Theory and Computation*, **2012**, 8, 4899-906	6.4	12
41	Heteroatomic deprotonation of substituted methanes and methyl radicals: theoretical insights into structure, stability, and thermochemistry. *Journal of Physical Chemistry A*, **2012**, 116, 12381-7	2.8	19
40	Reactivities of amino acid derivatives toward hydrogen abstraction by Cl• and OH•. *Journal of Organic Chemistry*, **2012**, 77, 9807-12	4.2	39
39	W1X-1 and W1X-2: W1-Quality Accuracy with an Order of Magnitude Reduction in Computational Cost. *Journal of Chemical Theory and Computation*, **2012**, 8, 4259-69	6.4	59
38	BDE261: a comprehensive set of high-level theoretical bond dissociation enthalpies. *Journal of Physical Chemistry A*, **2012**, 116, 4975-86	2.8	58
37	Heats of Formation for CrO, CrO2, and CrO3: An Extreme Challenge for Black-Box Composite Procedures. *Journal of Chemical Theory and Computation*, **2012**, 8, 3159-66	6.4	22
36	Determination of Barrier Heights for Proton Exchange in Small Water, Ammonia, and Hydrogen Fluoride Clusters with G4(MP2)-Type, MPn, and SCS-MPn Procedures-A Caveat. *Journal of Chemical Theory and Computation*, **2012**, 8, 3128-36	6.4	50
35	Approaches for obtaining accurate rate constants for hydrogen abstraction by a chlorine atom. *Journal of Physical Chemistry A*, **2012**, 116, 3745-52	2.8	24
34	Comment on the ionization energy of B2F4. *Journal of Physical Chemistry A*, **2012**, 116, 9214-5	2.8	3
33	The outcome of the oxidations of unusual enediamide motifs is governed by the stabilities of the intermediate iminium ions. *PLoS ONE*, **2012**, 7, e47224	3.7	3
32	Proton-bound homodimers involving second-row atoms. *Highlights in Theoretical Chemistry*, **2012**, 15-22		
31	Hydrogen abstraction by chlorine atom from amino acids: remarkable influence of polar effects on regioselectivity. *Journal of the American Chemical Society*, **2011**, 133, 16553-9	16.4	43
30	Obtaining Good Performance With Triple-ζ Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. *Journal of Chemical Theory and Computation*, **2011**, 7, 2852-63	6.4	52
29	A Palladium-Catalyzed Multicascade Reaction: Facile Low-Temperature Hydrogenolysis of Activated Nitriles and Related Functional Groups. *ChemCatChem*, **2011**, 3, 1496-1502	5.2	17
28	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. *Theoretical Chemistry Accounts*, **2011**, 130, 251-260	1.9	34

27	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). *Journal of Chemical Theory and Computation*, **2011**, 7, 112-20	6.4	119
26	O - H Bond Dissociation Energies. *Australian Journal of Chemistry*, **2011**, 64, 394	1.2	18
25	G4-SP, G4(MP2)-SP, G4-sc, and G4(MP2)-sc: Modifications to G4 and G4(MP2) for the Treatment of Medium-Sized Radicals. *Journal of Chemical Theory and Computation*, **2010**, 6, 2647-53	6.4	34
24	A computational study of methanol-to-hydrocarbon conversion Towards the design of a low-barrier process. *Canadian Journal of Chemistry*, **2010**, 88, 866-876	0.9	15
23	Gas-Phase Synthesis and Reactivity of Lithium Acetylide Ion, Li?C?C *Angewandte Chemie*, **2010**, 122, 5287-5290	3.6	1
22	Gas-phase synthesis and reactivity of lithium acetylide ion, Li-C[triple bond]C-. *Angewandte Chemie - International Edition*, **2010**, 49, 5161-4	16.4	8
21	Low barrier hydrogenolysis of the carbon-heteroatom bond as catalyzed by HAlF(4). *Organic Letters* , **2009**, 11, 749-51	6.2	17
20	What factors determine whether a proton-bound homodimer has a symmetric or an asymmetric hydrogen bond?. *Molecular Physics*, **2009**, 107, 1095-1105	1.7	22
19	Structures and thermochemistry of the alkali metal monoxide anions, monoxide radicals, and hydroxides. *Journal of Physical Chemistry A*, **2009**, 113, 9501-10	2.8	12
18	Zeolite-catalyzed hydrogenation of carbon dioxide and ethene. *Journal of the American Chemical Society*, **2008**, 130, 9790-9	16.4	63
17	Lithium monoxide anion: a ground-state triplet with the strongest base to date. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 7647-51	11.5	34
16	Modelling the interaction of molecular hydrogen with lithium-doped hydrogen storage materials. *Chemical Physics Letters*, **2008**, 467, 126-130	2.5	57
15	Proton-bound homodimers: how are the binding energies related to proton affinities?. *Journal of the American Chemical Society*, **2007**, 129, 12197-9	16.4	38
14	Uncatalyzed transfer hydrogenation of quinones and related systems: a theoretical mechanistic study. *Journal of Physical Chemistry A*, **2007**, 111, 6456-67	2.8	16
13	Uncatalyzed 1,4-hydrogenation of polycyclic aromatic hydrocarbons: A computational study. *Computational and Theoretical Chemistry*, **2007**, 811, 13-17		10
12	Hydrogenation of simple aromatic molecules: a computational study of the mechanism. *Journal of the American Chemical Society*, **2007**, 129, 924-33	16.4	40
11	Transfer hydrogenation between ethane and ethene: a critical assessment of theoretical procedures. *Molecular Physics*, **2006**, 104, 777-794	1.7	11
10	Design of effective zeolite catalysts for the complete hydrogenation of CO2. *Journal of the American Chemical Society*, **2006**, 128, 5322-3	16.4	57

9	Base-catalyzed hydrogenation: rationalizing the effects of catalyst and substrate structures and solvation. *Journal of the American Chemical Society*, **2005**, 127, 2443-54	16.4	43
8	On the relationship between the preferred site of hydrogen bonding and protonation. *Journal of Physical Chemistry A*, **2005**, 109, 5509-17	2.8	50
7	Electrical detection of DNA hybridization with multilayer gold nanoparticles between nanogap electrodes. *Microsystem Technologies*, **2005**, 11, 91-96	1.7	16
6	Understanding Metal-Free Catalytic Hydrogenation: A Systematic Theoretical Study of the Hydrogenation of Ethene. *Australian Journal of Chemistry*, **2004**, 57, 659	1.2	16
5	Effect of structural character of gold nanoparticles in nanofluid on heat pipe thermal performance. *Materials Letters*, **2004**, 58, 1461-1465	3.3	274
4	Shrinking gold nanoparticles: dramatic effect of a cryogenic process on tannic acid/sodium citrate-generated gold nanoparticles. *Materials Letters*, **2004**, 58, 2023-2026	3.3	17
3	A polar effects controlled enantioselective 1,2-chlorine atom migration via a chlorine-bridged radical intermediate. *Journal of the American Chemical Society*, **2002**, 124, 2078-9	16.4	13
2	(+)-(2R,3S)-3-Bromo-2-chloro-N,N-diisopropyl-3-phenylpropanamide and (+)-(2R,3S)-3-bromo-2-chloro-N-(4-nitrophenyl)-3-phenylpropanamide. *Acta Crystallographica Section C: Crystal Structure Communications*, **2000**, 56, e354-e355		
1	Stereoselective radical bromination of □chloro hydrocinnamic acid derivatives. *Tetrahedron Letters*, **2000**, 41, 2671-2674	2	2