Sason Shaik

List of Publications by Year in Descending Order

461 papers	31,690 citations	88 h-index	159 g-index
484 ext. papers	34,674 ext. citations	10.2 avg, IF	7.6 L-index

#	Paper	IF	Citations
461	Computational Catalysis: A Land of Opportunities. *Topics in Catalysis*, **2022**, 65, 1-5	2.3	
460	Local Electric Fields Dictate Function: The Different Product Selectivities Observed for Fatty Acid Oxidation by Two Deceptively Very Similar P450-Peroxygenases OleT and BS‡ *Journal of Chemical Information and Modeling*, **2022**,	6.1	4
459	Critical Roles of Exchange and Superexchange Interactions in Dictating Electron Transfer and Reactivity in Metalloenzymes.. *Journal of Physical Chemistry Letters*, **2022**, 2871-2877	6.4	4
458	Understanding Valence Bond Theory **2022**,		
457	Bridging Conceptual Density Functional and Valence Bond Theories **2022**, 391-415		
456	Mechanistic Conundrum of C□□ Bond Cleavage by CYP51. *ACS Catalysis*, **2022**, 12, 5673-5683	13.1	1
455	MD simulations and QM/MM calculations reveal the key mechanistic elements which are responsible for the efficient C-H amination reaction performed by a bioengineered P450 enzyme. *Chemical Science*, **2021**, 12, 14507-14518	9.4	5
454	Nature of the Trigger Linkage in Explosive Materials Is a Charge-Shift Bond. *Journal of Organic Chemistry*, **2021**, 86, 15588-15596	4.2	2
453	Exploring Dyson's Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. *Journal of Physical Chemistry Letters*, **2021**, 12, 9963-9972	6.4	2
452	The catalytic cycle of cytochrome P450: a fascinating choreography. *Trends in Chemistry*, **2021**,	14.8	4
451	Promotion Energy Analysis Predicts Reaction Modes: Nucleophilic and Electrophilic Aromatic Substitution Reactions. *Journal of the American Chemical Society*, **2021**, 143, 4367-4378	16.4	1
450	Valence Bond Theory-Its Birth, Struggles with Molecular Orbital Theory, Its Present State and Future Prospects. *Molecules*, **2021**, 26,	4.8	11
449	Deciphering the oxygen activation mechanism at the CuC site of particulate methane monooxygenase. *Nature Catalysis*, **2021**, 4, 266-273	36.5	13
448	Na???B Bond in NaBH3□Solving the Conundrum. *Angewandte Chemie*, **2021**, 133, 12833-12836	3.6	
447	Na???B Bond in NaBH : Solving the Conundrum. *Angewandte Chemie - International Edition*, **2021**, 60, 12727-12736	16.1	3
446	Resolving Entangled Reactivity Modes through External Electric Fields and Substitution: Application to E/S2 Reactions. *Journal of Organic Chemistry*, **2021**, 86, 9030-9039	4.2	3
445	H-Bonding Networks Dictate the Molecular Mechanism of H2O2 Activation by P450. *ACS Catalysis*, **2021**, 11, 8774-8785	13.1	9

444	External Electric Fields Interrupt the Concerted Cope Rearrangement of Semibullvalene. *Journal of Organic Chemistry*, **2021**, 86, 731-738	4.2	4
443	CHAPTER 2:The Impact of Electric Fields on Chemical Structure and Reactivity. *RSC Theoretical and Computational Chemistry Series*, **2021**, 12-70	1.2	5
442	Modulating the radical reactivity of phenyl radicals with the help of distonic charges: it is all about electrostatic catalysis. *Chemical Science*, **2021**, 12, 4800-4809	9.4	5
441	Spin-Regulated Electron Transfer and Exchange-Enhanced Reactivity in Fe S -Mediated Redox Reaction of the Dph2 Enzyme During the Biosynthesis of Diphthamide. *Angewandte Chemie - International Edition*, **2021**, 60, 20430-20436	16.4	6
440	Spin-Regulated Electron Transfer and Exchange-Enhanced Reactivity in Fe4S4-Mediated Redox Reaction of the Dph2 Enzyme During the Biosynthesis of Diphthamide. *Angewandte Chemie*, **2021**, 133, 20593-20599	3.6	
439	Evidence for new enantiospecific interaction force in chiral biomolecules. *CheM*, **2021**,	16.2	7
438	Conformational Motion of Ferredoxin Enables Efficient Electron Transfer to Heme in the Full-Length P450. *Journal of the American Chemical Society*, **2021**, 143, 1005-1016	16.4	8
437	How Do Local Reactivity Descriptors Shape the Potential Energy Surface Associated with Chemical Reactions? The Valence Bond Delocalization Perspective. *Journal of the American Chemical Society*, **2020**, 142, 10102-10113	16.4	22
436	Solvent Organization and Rate Regulation of a Menshutkin Reaction by Oriented External Electric Fields are Revealed by Combined MD and QM/MM Calculations. *Journal of the American Chemical Society*, **2020**, 142, 9955-9965	16.4	32
435	Comment on "The 'Inverted Bonds' Revisited. Analysis of 'in Silico' Models and of [1.1.1]Propellane Using Orbital Forces". *Chemistry - A European Journal*, **2020**, 26, 6935-6939	4.8	2
434	Covalent vs Charge-Shift Nature of the Metal-Metal Bond in Transition Metal Complexes: A Unified Understanding. *Journal of the American Chemical Society*, **2020**, 142, 12277-12287	16.4	19
433	Electric-Field Mediated Chemistry: Uncovering and Exploiting the Potential of (Oriented) Electric Fields to Exert Chemical Catalysis and Reaction Control. *Journal of the American Chemical Society*, **2020**, 142, 12551-12562	16.4	75
432	Oriented (Local) Electric Fields Drive the Millionfold Enhancement of the H-Abstraction Catalysis Observed for Synthetic Metalloenzyme Analogues. *Angewandte Chemie - International Edition*, **2020** , 59, 7915-7920	16.4	18
431	Oriented (Local) Electric Fields Drive the Millionfold Enhancement of the H-Abstraction Catalysis Observed for Synthetic Metalloenzyme Analogues. *Angewandte Chemie*, **2020**, 132, 7989-7994	3.6	5
430	Oriented External Electric Fields and Ionic Additives Elicit Catalysis and Mechanistic Crossover in Oxidative Addition Reactions. *Journal of the American Chemical Society*, **2020**, 142, 3836-3850	16.4	35
429	Two-State Reactivity: Personal Recounting of its Conception and Future Prospects. *Israel Journal of Chemistry*, **2020**, 60, 938-956	3.4	16
428	Charge-Shift Bonding: A New and Unique Form of Bonding. *Angewandte Chemie*, **2020**, 132, 996-1013	3.6	13
427	Charge-Shift Bonding: A New and Unique Form of Bonding. *Angewandte Chemie - International Edition*, **2020**, 59, 984-1001	16.4	53

426	TITAN: A Code for Modeling and Generating Electric Fields-Features and Applications to Enzymatic Reactivity. *Journal of Computational Chemistry*, **2020**, 41, 74-82	3.5	26
425	Unifying Conceptual Density Functional and Valence Bond Theory: The Hardness-Softness Conundrum Associated with Protonation Reactions and Uncovering Complementary Reactivity Modes. *Journal of the American Chemical Society*, **2020**, 142, 20002-20013	16.4	10
424	QM/MM Calculations Reveal the Important Role of β-Heteroatom Substituents in Controlling Selectivity of Mononuclear Nonheme HppE-Catalyzed Reactions. *ACS Catalysis*, **2020**, 10, 9521-9532	13.1	5
423	A Paradigm Shift in the Catalytic Cycle of P450: The Preparatory Choreography during O2 Binding and Origins of the Necessity for Two Protonation Pathways. *ACS Catalysis*, **2020**, 10, 11481-11492	13.1	9
422	External electric field effects on chemical structure and reactivity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1438	7.9	42
421	Cytochrome P450-The Wonderful Nanomachine Revealed through Dynamic Simulations of the Catalytic Cycle. *Accounts of Chemical Research*, **2019**, 52, 389-399	24.3	71
420	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. *Angewandte Chemie*, **2019**, 131, 12460-12466	3.6	1
419	Fenton-Derived OH Radicals Enable the MPnS Enzyme to Convert 2-Hydroxyethylphosphonate to Methylphosphonate: Insights from Ab Initio QM/MM MD Simulations. *Journal of the American Chemical Society*, **2019**, 141, 9284-9291	16.4	21
418	Das Periodensystem – eine universelle Ikone: seine Entstehung vor 150 Jahren und seine Verbreitung durch Literatur, Kunst und Musik. *Angewandte Chemie*, **2019**, 131, 13328-13341	3.6	2
417	The Periodic-Table-A Universal Icon: Its Birth 150 Years Ago, and Its Popularization Through Literature Art and Music. *Angewandte Chemie - International Edition*, **2019**, 58, 13194-13206	16.4	6
416	Electrophilic Aromatic Substitution Reactions: Mechanistic Landscape, Electrostatic and Electric-Field Control of Reaction Rates, and Mechanistic Crossovers. *Journal of the American Chemical Society*, **2019**, 141, 9719-9730	16.4	32
415	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. *Angewandte Chemie - International Edition*, **2019**, 58, 12332-12338	16.4	15
414	Cross Conjugation in Polyenes and Related Hydrocarbons: What Can Be Learned from Valence Bond Theory about Single-Molecule Conductance?. *Journal of the American Chemical Society*, **2019**, 141, 6030-6047	16.4	14
413	Comment on "Decoding real space bonding descriptors in valence bond language" by A. Martín Pendás and E. Francisco, Phys. Chem. Chem. Phys., 2018, 20, 12368. *Physical Chemistry Chemical Physics*, **2019**, 21, 8170-8174	3.6	2
412	Oriented External Electric Fields: Tweezers and Catalysts for Reactivity in Halogen-Bond Complexes. *Journal of the American Chemical Society*, **2019**, 141, 7122-7136	16.4	34
411	Insights into the Trends in the Acidity Strength of Organic and Inorganic Compounds: A Valence-Bond Perspective. *Journal of Physical Chemistry A*, **2019**, 123, 1851-1860	2.8	1
410	Captodative Substitution Enhances the Diradical Character of Compounds, Reduces Aromaticity, and Controls Single-Molecule Conductivity Patterns: A Valence Bond Study. *Journal of Physical Chemistry A*, **2019**, 123, 7133-7141	2.8	6
409	Quantum-Mechanical/Molecular-Mechanical Studies of CYP11A1-Catalyzed Biosynthesis of Pregnenolone from Cholesterol Reveal a C-C Bond Cleavage Reaction That Occurs by a Compound I-Mediated Electron Transfer. *Journal of the American Chemical Society*, **2019**, 141, 20079-20088	16.4	11

408	Helmut Schwarz: A story of science and friendship. *International Journal of Mass Spectrometry*, **2019**, 435, 151-162	1.9	0
407	Intrinsic Reactivity of Diatomic 3d Transition-Metal Carbides in the Thermal Activation of Methane: Striking Electronic Structure Effects. *Journal of the American Chemical Society*, **2019**, 141, 599-610	16.4	19
406	Attraction between electrophilic caps: A counterintuitive case of noncovalent interactions. *Journal of Computational Chemistry*, **2019**, 40, 1015-1022	3.5	12
405	Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Gold-Thiolate Linkers Innocent?. *Journal of the American Chemical Society*, **2018**, 140, 4354-4362	16.4	44
404	Nature of the Three-Electron Bond. *Journal of Physical Chemistry A*, **2018**, 122, 1873-1885	2.8	21
403	Choreography of the Reductase and P450 Domains Toward Electron Transfer Is Instigated by the Substrate. *Journal of the American Chemical Society*, **2018**, 140, 683-690	16.4	22
402	QM/MM Studies into the H2O2-Dependent Activity of Lytic Polysaccharide Monooxygenases: Evidence for the Formation of a Caged Hydroxyl Radical Intermediate. *ACS Catalysis*, **2018**, 8, 1346-1351	13.1	87
401	Kinetic Isotope Effect Determination Probes the Spin of the Transition State, Its Stereochemistry, and Its Ligand Sphere in Hydrogen Abstraction Reactions of Oxoiron(IV) Complexes. *Accounts of Chemical Research*, **2018**, 51, 107-117	24.3	48
400	Hydrogen- and Halogen-Bonds between Ions of like Charges: Are They Anti-Electrostatic in Nature?. *Journal of Computational Chemistry*, **2018**, 39, 481-487	3.5	42
399	Structure and reactivity/selectivity control by oriented-external electric fields. *Chemical Society Reviews*, **2018**, 47, 5125-5145	58.5	170
398	Oriented-External Electric Fields Create Absolute Enantioselectivity in Diels-Alder Reactions: Importance of the Molecular Dipole Moment. *Journal of the American Chemical Society*, **2018**, 140, 13350-13359	16.4	75
397	Oriented external electric fields as mimics for probing the role of metal ions and ligands in the thermal gas-phase activation of methane. *Dalton Transactions*, **2018**, 47, 15271-15277	4.3	16
396	The Nickel-Pincer Complex in Lactate Racemase Is an Electron Relay and Sink that acts through Proton-Coupled Electron Transfer. *Angewandte Chemie - International Edition*, **2017**, 56, 10098-10102	16.4	14
395	To hybridize or not to hybridize? This is the dilemma. *Computational and Theoretical Chemistry*, **2017**, 1116, 242-249	2	14
394	A personal story on a renaissance in valence bond theory: A theory coming of age!. *Computational and Theoretical Chemistry*, **2017**, 1116, 2-31	2	11
393	The Nickel-Pincer Complex in Lactate Racemase Is an Electron Relay and Sink that acts through Proton-Coupled Electron Transfer. *Angewandte Chemie*, **2017**, 129, 10232-10236	3.6	7
392	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. *Coordination Chemistry Reviews*, **2017**, 344, 355-362	23.2	58
391	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. *Inorganic Chemistry*, **2017**, 56, 3287-3301	5.1	22

390	A Unified Theory for the Blue- and Red-Shifting Phenomena in Hydrogen and Halogen Bonds. *Journal of Chemical Theory and Computation*, **2017**, 13, 1626-1637	6.4	40
389	Halogen Bonds in Novel Polyhalogen Monoanions. *Chemistry - A European Journal*, **2017**, 23, 8719-8728	4.8	10
388	Control of Product Distribution and Mechanism by Ligation and Electric Field in the Thermal Activation of Methane. *Angewandte Chemie - International Edition*, **2017**, 56, 10219-10223	16.4	47
387	Structure and spin state of nonheme FeO complexes depending on temperature: predictive insights from DFT calculations and experiments. *Chemical Science*, **2017**, 8, 5460-5467	9.4	17
386	Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. *Journal of the American Chemical Society*, **2017**, 139, 9302-9316	16.4	23
385	MD simulations and QM/MM calculations show that single-site mutations of cytochrome P450 alter the active site's complexity and the chemoselectivity of oxidation without changing the active species. *Chemical Science*, **2017**, 8, 5335-5344	9.4	24
384	A redox-mediated Kemp eliminase. *Nature Communications*, **2017**, 8, 14876	17.4	29
383	Electrostatic and Charge-Induced Methane Activation by a Concerted Double C-H Bond Insertion. *Journal of the American Chemical Society*, **2017**, 139, 1684-1689	16.4	75
382	Kinetic Isotope Effect Probes the Reactive Spin State, As Well As the Geometric Feature and Constitution of the Transition State during H-Abstraction by Heme Compound II Complexes. *Journal of the American Chemical Society*, **2017**, 139, 11451-11459	16.4	17
381	R□ktitelbild: Steuerung der Produktverteilung und der Mechanismen der thermischen Aktivierung von Methan durch Ligandeneffekte und elektrische Felder (Angew. Chem. 34/2017). *Angewandte Chemie*, **2017**, 129, 10382-10382	3.6	
380	Steuerung der Produktverteilung und der Mechanismen der thermischen Aktivierung von Methan durch Ligandeneffekte und elektrische Felder. *Angewandte Chemie*, **2017**, 129, 10353-10357	3.6	9
379	Privileged Role of Thiolate as the Axial Ligand in Hydrogen Atom Transfer Reactions by Oxoiron(IV) Complexes in Shaping the Potential Energy Surface and Inducing Significant H-Atom Tunneling. *Journal of the American Chemical Society*, **2017**, 139, 18705-18713	16.4	20
378	Electronic Effects on Room-Temperature, Gas-Phase C-H Bond Activations by Cluster Oxides and Metal Carbides: The Methane Challenge. *Journal of the American Chemical Society*, **2017**, 139, 17201-17212	16.4	114
377	Oriented electric fields as future smart reagents in chemistry. *Nature Chemistry*, **2016**, 8, 1091-1098	17.6	267
376	Computation Sheds Insight into Iron Porphyrin Carbenes' Electronic Structure, Formation, and N-H Insertion Reactivity. *Journal of the American Chemical Society*, **2016**, 138, 9597-610	16.4	76
375	How do Enzymes Utilize Reactive OH Radicals? Lessons from Nonheme HppE and Fenton Systems. *Journal of the American Chemical Society*, **2016**, 138, 8489-96	16.4	39
374	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO2](+) (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. *Journal of the American Chemical Society*, **2016**, 138, 7973-81	16.4	74
373	Selective Chlorination of Substrates by the Halogenase SyrB2 Is Controlled by the Protein According to a Combined Quantum Mechanics/Molecular Mechanics and Molecular Dynamics Study. *ACS Catalysis*, **2016**, 6, 2694-2704	13.1	39

372	Interplay of Tunneling, Two-State Reactivity, and Bell-Evans-Polanyi Effects in C-H Activation by Nonheme Fe(IV)O Oxidants. *Journal of the American Chemical Society*, **2016**, 138, 2094-7	16.4	61
371	Two-State Reactivity in Low-Valent Iron-Mediated C-H Activation and the Implications for Other First-Row Transition Metals. *Journal of the American Chemical Society*, **2016**, 138, 3715-30	16.4	108
370	Molecular Dynamics and QM/MM Calculations Predict the Substrate-Induced Gating of Cytochrome P450 BM3 and the Regio- and Stereoselectivity of Fatty Acid Hydroxylation. *Journal of the American Chemical Society*, **2016**, 138, 837-45	16.4	62
369	To rebound or dissociate? This is the mechanistic question in C-H hydroxylation by heme and nonheme metal-oxo complexes. *Chemical Society Reviews*, **2016**, 45, 1197-210	58.5	137
368	The Quadruple Bonding in C2 Reproduces the Properties of the Molecule. *Chemistry - A European Journal*, **2016**, 22, 4116-28	4.8	41
367	A Response to a Comment by G. Frenking and M. Hermann on: "The Quadruple Bonding in C Reproduces the Properties of the Molecule". *Chemistry - A European Journal*, **2016**, 22, 18977-18980	4.8	17
366	The origins of the directionality of noncovalent intermolecular interactions. *Journal of Computational Chemistry*, **2016**, 37, 34-45	3.5	49
365	Theory Revealing Unusual Non-Rebound Mechanisms Responsible for the Distinct Reactivities of O?MnIV?O and [HO□MnIV□OH]2+ in C□H Bond Activation. *ACS Catalysis*, **2016**, 6, 2877-2888	13.1	8
364	Emergence of Function in P450-Proteins: A Combined Quantum Mechanical/Molecular Mechanical and Molecular Dynamics Study of the Reactive Species in the H2O2-Dependent Cytochrome P450SP□and Its Regio- and Enantioselective Hydroxylation of Fatty Acids. *Journal of the American Chemical Society*, **2016**, 138, 6786-97	16.4	41
363	On the Nature of Bonding in Parallel Spins in Monovalent Metal Clusters. *Annual Review of Physical Chemistry*, **2016**, 67, 419-39	15.7	6
362	Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions. *Journal of the American Chemical Society*, **2016**, 138, 11368-77	16.4	68
361	Oxoiron(IV) Complex of the Ethylene-Bridged Dialkylcyclam Ligand Me2EBC. *Inorganic Chemistry*, **2015**, 54, 7828-39	5.1	22
360	Acidity of the methyne group of poly(4-vinylpyridine) leads to side-chain protonation in pyridine. *New Journal of Chemistry*, **2015**, 39, 5920-5922	3.6	5
359	Interplay of Experiment and Theory in Elucidating Mechanisms of Oxidation Reactions by a Nonheme Ru(IV)O Complex. *Journal of the American Chemical Society*, **2015**, 137, 8623-32	16.4	69
358	Determination of Spin Inversion Probability, H-Tunneling Correction, and Regioselectivity in the Two-State Reactivity of Nonheme Iron(IV)-Oxo Complexes. *Journal of Physical Chemistry Letters*, **2015**, 6, 1472-6	6.4	52
357	Comment on □Rabbit-ears hybrids, VSEPR sterics, and other orbital anachronisms□A reply to a criticism. *Chemistry Education Research and Practice*, **2015**, 16, 689-693	2.1	10
356	The Self-Association of Graphane Is Driven by London Dispersion and Enhanced Orbital Interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 1621-30	6.4	36
355	Computations Reveal a Rich Mechanistic Variation of Demethylation of N-Methylated DNA/RNA Nucleotides by FTO. *ACS Catalysis*, **2015**, 5, 7077-7090	13.1	40

354	Tuning the Ground State Symmetry of Acetylenyl Radicals. *ACS Central Science*, **2015**, 1, 270-8	16.8	5
353	How does tunneling contribute to counterintuitive H-abstraction reactivity of nonheme Fe(IV)O oxidants with alkanes?. *Journal of the American Chemical Society*, **2015**, 137, 722-33	16.4	75
352	Principles and Prospects of Spin-States Reactivity in Chemistry and Bioinorganic Chemistry **2015**, 131-156		13
351	The Lise Meitner-Minerva Center for Computational Quantum Chemistry: 18 Years of Israeli-German Collaboration. *Israel Journal of Chemistry*, **2015**, 55, 1167-1176	3.4	3
350	Response to the Comment by J. Grunenberg on "The Nature of the Fourth Bond in the Ground State of C2: The Quadruple Bond Conundrum''. *Chemistry - A European Journal*, **2015**, 21, 17127-8	4.8	10
349	A Tale of Two Mounts: The History of Chemistry at the Hebrew University of Jerusalem. *Israel Journal of Chemistry*, **2015**, 55, 781-825	3.4	2
348	Quantum mechanical/molecular mechanical calculated reactivity networks reveal how cytochrome P450cam and Its T252A mutant select their oxidation pathways. *Journal of the American Chemical Society*, **2015**, 137, 7379-90	16.4	52
347	Reply to 'entropic factors also contribute to the high melting points of polyhedral alkanes'. *Nature Chemistry*, **2015**, 7, 89-90	17.6	
346	Identification of a low-spin acylperoxoiron(III) intermediate in bio-inspired non-heme iron-catalysed oxidations. *Nature Communications*, **2014**, 5, 3046	17.4	78
345	The V state of ethylene: valence bond theory takes up the challenge. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	26
344	The nature of the fourth bond in the ground state of C2: the quadruple bond conundrum. *Chemistry - A European Journal*, **2014**, 20, 6220-32	4.8	60
343	Charge-Shift Bonding Emerges as a Distinct Electron-Pair Bonding Family from Both Valence Bond and Molecular Orbital Theories. *Journal of Chemical Theory and Computation*, **2014**, 10, 2410-8	6.4	32
342	A tutorial for understanding chemical reactivity through the valence bond approach. *Chemical Society Reviews*, **2014**, 43, 4968-88	58.5	45
341	The Physical Origin of Covalent Bonding **2014**, 1-68		16
340	The ELF Perspective of chemical bonding **2014**, 345-382		42
339	The EDA Perspective of Chemical Bonding **2014**, 121-157		137
338	Relativity and Chemical Bonding **2014**, 383-404		11
337	The NBO View of Chemical Bonding **2014**, 91-120		40

336	The Conceptual Density Functional Theory Perspective of Bonding **2014**, 233-270		21
335	The Valence Bond Perspective of the Chemical Bond **2014**, 159-198		4
334	Bridging Cultures **2014**, 69-90		5
333	Protonated alcohols are examples of complete charge-shift bonds. *Journal of Organic Chemistry*, **2014**, 79, 9998-10001	4.2	18
332	QM/MM Studies of Structure and Reactivity of Cytochrome P450 Enzymes: Methodology and Selected Applications. *Methods and Principles in Medicinal Chemistry*, **2014**, 133-178	0.4	4
331	Theory uncovers an unusual mechanism of DNA repair of a lesioned adenine by AlkB enzymes. *Journal of the American Chemical Society*, **2014**, 136, 13895-901	16.4	56
330	Investigating Superoxide Transfer through a □1,2-O2 Bridge between Nonheme Ni(III)-Peroxo and Mn(II) Species by DFT Methods to Bridge Theoretical and Experimental Views. *Journal of Physical Chemistry Letters*, **2014**, 5, 2437-42	6.4	6
329	On The Nature of the Halogen Bond. *Journal of Chemical Theory and Computation*, **2014**, 10, 3726-37	6.4	194
328	The Block-Localized Wavefunction (BLW) Perspective of Chemical Bonding **2014**, 199-232		15
327	The Experimental Density Perspective of Chemical Bonding **2014**, 309-344		3
326	Chemical Bonding of Main-Group Elements **2014**, 1-24		8
325	The Role of Recoupled Pair Bonding in Hypervalent Molecules **2014**, 49-70		0
324	Electron-Counting Rules in Cluster Bonding □Polyhedral Boranes, Elemental Boron, and Boron-Rich Solids **2014**, 113-148		1
323	Chemical Bonding in Transition Metal Compounds **2014**, 175-218		5
322	Chemical Bonding of Lanthanides and Actinides **2014**, 337-356		
321	Magnetic Properties of Aromatic Compounds and Aromatic Transition States **2014**, 383-420		3
320	Chemical Bonding in Solids **2014**, 445-476		
319	Hydrogen Bonding **2014**, 501-522		2

318	Directional Electrostatic Bonding **2014**, 523-536		2
317	Multiple Bonding of Heavy Main-Group Atoms **2014**, 25-48		1
316	Donor–Acceptor Complexes of Main-Group Elements **2014**, 71-112		6
315	Bound Triplet Pairs in the Highest Spin States of Monovalent Metal Clusters **2014**, 149-174		
314	Chemical Bonding in Open-Shell Transition-Metal Complexes **2014**, 219-252		2
313	The Quantum Chemistry of Transition Metal Surface Bonding and Reactivity **2014**, 269-336		
312	Chemical Bonding in Inorganic Aromatic Compounds **2014**, 421-444		1
311	Dispersion Interaction and Chemical Bonding **2014**, 477-500		4
310	The QTAIM Perspective of Chemical Bonding **2014**, 271-308		63
309	What is Chemistry? Von Peter Atkins.. *Angewandte Chemie*, **2014**, 126, 5104-5106	3.6	
308	Bonding with parallel spins: high-spin clusters of monovalent metal atoms. *Accounts of Chemical Research*, **2014**, 47, 417-26	24.3	14
307	Dichotomous hydrogen atom transfer vs proton-coupled electron transfer during activation of X-H bonds (X = C, N, O) by nonheme iron-oxo complexes of variable basicity. *Journal of the American Chemical Society*, **2013**, 135, 17090-104	16.4	176
306	Oxygen activation by homoprotocatechuate 2,3-dioxygenase: a QM/MM study reveals the key intermediates in the activation cycle. *Chemical Science*, **2013**, 4, 3624	9.4	56
305	Electronic structure analysis of multistate reactivity in transition metal catalyzed reactions: the case of C-H bond activation by non-heme iron(IV)-oxo cores. *Physical Chemistry Chemical Physics*, **2013**, 15, 8017-30	3.6	138
304	How Do Perfluorinated Alkanoic Acids Elicit Cytochrome P450 to Catalyze Methane Hydroxylation? An MD and QM/MM Study. *RSC Advances*, **2013**, 3, 2995-3005	3.7	18
303	Formation of Carbon-Carbon Triply Bonded Molecules from Two Free Carbyne Radicals via a Conical Intersection. *Journal of Physical Chemistry Letters*, **2013**, 4, 58-64	6.4	19
302	A theory for bioinorganic chemical reactivity of oxometal complexes and analogous oxidants: the exchange and orbital-selection rules. *Accounts of Chemical Research*, **2013**, 46, 471-82	24.3	131
301	An anatomy of the two-state reactivity concept: Personal reminiscences in memoriam of Detlef Schröder. *International Journal of Mass Spectrometry*, **2013**, 354-355, 5-14	1.9	64

300	Understanding the Nature of the CH···HC Interactions in Alkanes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1977-91	6.4	90
299	One molecule, two atoms, three views, four bonds?. *Angewandte Chemie - International Edition*, **2013**, 52, 3020-33	16.4	110
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