Sason Shaik

List of Publications by Citations

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	Mechanism of oxidation reactions catalyzed by cytochrome p450 enzymes. *Chemical Reviews*, **2004**, 104, 3947-80	68.1	1774
460	How to conceptualize catalytic cycles? The energetic span model. *Accounts of Chemical Research*, **2011**, 44, 101-10	24.3	1014
459	Theoretical perspective on the structure and mechanism of cytochrome P450 enzymes. *Chemical Reviews*, **2005**, 105, 2279-328	68.1	999
458	Two-state reactivity as a new concept in organometallic chemistry. *Accounts of Chemical Research*, **2000**, 33, 139-45	24.3	981
457	P450 enzymes: their structure, reactivity, and selectivity-modeled by QM/MM calculations. *Chemical Reviews*, **2010**, 110, 949-1017	68.1	791
456	Reactivity of high-valent iron-oxo species in enzymes and synthetic reagents: a tale of many states. *Accounts of Chemical Research*, **2007**, 40, 532-42	24.3	454
455	A combined kinetic-quantum mechanical model for assessment of catalytic cycles: application to cross-coupling and Heck reactions. *Journal of the American Chemical Society*, **2006**, 128, 3355-65	16.4	375
454	Axial ligand tuning of a nonheme iron(IV)-oxo unit for hydrogen atom abstraction. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 19181-6	11.5	344
453	A Model "Rebound" Mechanism of Hydroxylation by Cytochrome P450: Stepwise and Effectively Concerted Pathways, and Their Reactivity Patterns. *Journal of the American Chemical Society*, **2000**, 122, 8977-8989	16.4	333
452	Two-state reactivity in alkane hydroxylation by non-heme iron-oxo complexes. *Journal of the American Chemical Society*, **2006**, 128, 8590-606	16.4	308
451	Valence Bond Diagrams and Chemical Reactivity. *Angewandte Chemie - International Edition*, **1999**, 38, 586-625	16.4	304
450	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm. *Chemistry - A European Journal*, **1998**, 4, 193-199	4.8	303
449	Two-state reactivity mechanisms of hydroxylation and epoxidation by cytochrome P-450 revealed by theory. *Current Opinion in Chemical Biology*, **2002**, 6, 556-67	9.7	299
448	A proton-shuttle mechanism mediated by the porphyrin in benzene hydroxylation by cytochrome p450 enzymes. *Journal of the American Chemical Society*, **2003**, 125, 7413-24	16.4	283
447	Two-State Reactivity in Organometallic Gas-Phase Ion Chemistry. *Helvetica Chimica Acta*, **1995**, 78, 1393-1407	2	270
446	Searching for the second oxidant in the catalytic cycle of cytochrome P450: a theoretical investigation of the iron(III)-hydroperoxo species and its epoxidation pathways. *Journal of the American Chemical Society*, **2002**, 124, 2806-17	16.4	268
445	Oriented electric fields as future smart reagents in chemistry. *Nature Chemistry*, **2016**, 8, 1091-1098	17.6	267

444	Electronic Structures and Gas-Phase Reactivities of Cationic Late-Transition-Metal Oxides. *Journal of the American Chemical Society*, **1994**, 116, 10734-10741	16.4	261
443	Charge-shift bonding and its manifestations in chemistry. *Nature Chemistry*, **2009**, 1, 443-9	17.6	258
442	What factors affect the regioselectivity of oxidation by cytochrome p450? A DFT study of allylic hydroxylation and double bond epoxidation in a model reaction. *Journal of the American Chemical Society*, **2002**, 124, 11809-26	16.4	258
441	The elusive oxidant species of cytochrome P450 enzymes: characterization by combined quantum mechanical/molecular mechanical (QM/MM) calculations. *Journal of the American Chemical Society*, **2002**, 124, 8142-51	16.4	258
440	Quantum mechanical/molecular mechanical investigation of the mechanism of C-H hydroxylation of camphor by cytochrome P450cam: theory supports a two-state rebound mechanism. *Journal of the American Chemical Society*, **2004**, 126, 4017-34	16.4	250
439	Exchange-enhanced reactivity in bond activation by metal-oxo enzymes and synthetic reagents. *Nature Chemistry*, **2011**, 3, 19-27	17.6	248
438	Kinetic-quantum chemical model for catalytic cycles: the Haber-Bosch process and the effect of reagent concentration. *Journal of Physical Chemistry A*, **2008**, 112, 6032-41	2.8	236
437	Spin□Orbit Coupling in the Oxidative Activation of H□H by FeO+. Selection Rules and Reactivity Effects. *Journal of the American Chemical Society*, **1997**, 119, 1773-1786	16.4	222
436	A different story of pi-delocalization--the distortivity of pi-electrons and its chemical manifestations. *Chemical Reviews*, **2001**, 101, 1501-39	68.1	222
435	A valence bond modeling of trends in hydrogen abstraction barriers and transition states of hydroxylation reactions catalyzed by cytochrome P450 enzymes. *Journal of the American Chemical Society*, **2008**, 130, 10128-40	16.4	213
434	Nature of the Fe-O2 bonding in oxy-myoglobin: effect of the protein. *Journal of the American Chemical Society*, **2008**, 130, 14778-90	16.4	207
433	External electric field will control the selectivity of enzymatic-like bond activations. *Journal of the American Chemical Society*, **2004**, 126, 11746-9	16.4	201
432	The directive of the protein: how does cytochrome P450 select the mechanism of dopamine formation?. *Journal of the American Chemical Society*, **2011**, 133, 7977-84	16.4	200
431	Multi-state epoxidation of ethene by cytochrome P450: a quantum chemical study. *Journal of the American Chemical Society*, **2001**, 123, 3037-47	16.4	199
430	Hydrogen-abstraction reactivity patterns from A to Y: the valence bond way. *Angewandte Chemie - International Edition*, **2012**, 51, 5556-78	16.4	198
429	A predictive pattern of computed barriers for C-h hydroxylation by compound I of cytochrome p450. *Journal of the American Chemical Society*, **2004**, 126, 8362-3	16.4	195
428	Charge-shift bonding--a class of electron-pair bonds that emerges from valence bond theory and is supported by the electron localization function approach. *Chemistry - A European Journal*, **2005**, 11, 6358-71	4.8	195
427	On The Nature of the Halogen Bond. *Journal of Chemical Theory and Computation*, **2014**, 10, 3726-37	6.4	194

426	What Makes for a Good Catalytic Cycle? A Theoretical Study of the Role of an Anionic Palladium(0) Complex in the Cross-Coupling of an Aryl Halide with an Anionic Nucleophile. *Organometallics*, **2005**, 24, 2319-2330	3.8	191
425	Classical valence bond approach by modern methods. *Chemical Reviews*, **2011**, 111, 7557-93	68.1	190
424	Automatic analysis of computed catalytic cycles. *Journal of Computational Chemistry*, **2011**, 32, 978-85	3.5	184
423	A spin-restricted ensemble-referenced Kohn–Sham method and its application to diradicaloid situations. *Chemical Physics Letters*, **1999**, 304, 429-437	2.5	183
422	A two-state reactivity rationale for counterintuitive axial ligand effects on the C-H activation reactivity of nonheme FeIV=O oxidants. *Chemistry - A European Journal*, **2008**, 14, 1740-56	4.8	181
421	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
420	**2007**,		174
419	Theoretical investigation of C--H hydroxylation by (N4Py)Fe(IV)=O(2+): an oxidant more powerful than P450?. *Journal of the American Chemical Society*, **2005**, 127, 8026-7	16.4	172
418	Structure and reactivity/selectivity control by oriented-external electric fields. *Chemical Society Reviews*, **2018**, 47, 5125-5145	58.5	170
417	Quadruple bonding in C2 and analogous eight-valence electron species. *Nature Chemistry*, **2012**, 4, 195-2006	16.4	164
416	Medium Polarization and Hydrogen Bonding Effects on Compound I of Cytochrome P450: What Kind of a Radical Is It Really?. *Journal of the American Chemical Society*, **2000**, 122, 12892-12893	16.4	158
415	A mononuclear nonheme iron(IV)-oxo complex which is more reactive than cytochrome P450 model compound I. *Chemical Science*, **2011**, 2, 1039	9.4	156
414	Active species of horseradish peroxidase (HRP) and cytochrome P450: two electronic chameleons. *Journal of the American Chemical Society*, **2003**, 125, 15779-88	16.4	153
413	Two states and two more in the mechanisms of hydroxylation and epoxidation by cytochrome P450. *Journal of the American Chemical Society*, **2005**, 127, 13007-18	16.4	146
412	Oriented electric fields accelerate Diels-Alder reactions and control the endo/exo selectivity. *ChemPhysChem*, **2010**, 11, 301-10	3.2	142
411	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
410	The Rebound Controversy: An Overview and Theoretical Modeling of the Rebound Step in C–H Hydroxylation by Cytochrome P450. *European Journal of Inorganic Chemistry*, **2004**, 2004, 207-226	2.3	138
409	Radical clock substrates, their C-H hydroxylation mechanism by cytochrome P450, and other reactivity patterns: what does theory reveal about the clocks' behavior?. *Journal of the American Chemical Society*, **2004**, 126, 1907-20	16.4	138

408	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
407	The EDA Perspective of Chemical Bonding **2014**, 121-157		137
406	Breathing-orbital valence bond method a modern valence bond method that includes dynamic correlation. *Theoretical Chemistry Accounts*, **2002**, 108, 255-272	1.9	136
405	The charge-shift bonding concept. Electron-pair bonds with very large ionic-covalent resonance energies. *Journal of the American Chemical Society*, **1992**, 114, 7861-7866	16.4	133
404	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
403	Theoretical Investigation of Two-State-Reactivity Pathways of H I Activation by FeO+: Addition Elimination, Rebound, and Oxene-Insertion Mechanisms. *Journal of Physical Chemistry A* , **1998**, 102, 3835-3846	2.8	131
402	Evidence for an alternative to the oxygen rebound mechanism in C-H bond activation by non-heme Fe(IV)O complexes. *Journal of the American Chemical Society*, **2012**, 134, 20222-5	16.4	129
401	The 'push' effect of the thiolate ligand in cytochrome P450: a theoretical gauging. *Journal of Inorganic Biochemistry*, **2002**, 91, 554-67	4.2	127
400	A conversation on VB vs MO theory: a never-ending rivalry?. *Accounts of Chemical Research*, **2003**, 36, 750-6	24.3	124
399	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
398	Can a single oxidant with two spin states masquerade as two different oxidants? A study of the sulfoxidation mechanism by cytochrome p450. *Journal of the American Chemical Society*, **2003**, 125, 8698-9	16.4	111
397	One molecule, two atoms, three views, four bonds?. *Angewandte Chemie - International Edition*, **2013**, 52, 3020-33	16.4	110
396	Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I. *Angewandte Chemie - International Edition*, **2002**, 41, 1947	16.4	110
395	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
394	The fundamental role of exchange-enhanced reactivity in C-H activation by S=2 oxo iron(IV) complexes. *Angewandte Chemie - International Edition*, **2010**, 49, 3342-5	16.4	106
393	What is the active species of cytochrome P450 during camphor hydroxylation? QM/MM studies of different electronic states of compound I and of reduced and oxidized iron-oxo intermediates. *Journal of the American Chemical Society*, **2007**, 129, 8978-87	16.4	105
392	The valence bond way: reactivity patterns of cytochrome P450 enzymes and synthetic analogs. *Accounts of Chemical Research*, **2010**, 43, 1154-65	24.3	104
391	A two-state reactivity model explains unusual kinetic isotope effect patterns in C-H bond cleavage by nonheme oxoiron(IV) complexes. *Angewandte Chemie - International Edition*, **2009**, 48, 1291-5	16.4	104

390	Theoretical study of N-demethylation of substituted N,N-dimethylanilines by cytochrome P450: the mechanistic significance of kinetic isotope effect profiles. *Journal of Physical Chemistry B*, **2007**, 111, 7700-10	3.4	103
389	Chameleon States: High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analogue. *Angewandte Chemie - International Edition*, **2001**, 40, 2874-2878	16.4	103
388	Application of spin-restricted open-shell KohnSham method to atomic and molecular multiplet states. *Journal of Chemical Physics*, **1999**, 110, 116-125	3.9	102
387	Assessment of Theoretical Methods for Complexes of Gold(I) and Gold(III) with Unsaturated Aliphatic Hydrocarbon: Which Density Functional Should We Choose?. *Journal of Chemical Theory and Computation*, **2011**, 7, 4002-11	6.4	101
386	The inverted bond in [1.1.1]propellane is a charge-shift bond. *Angewandte Chemie - International Edition*, **2009**, 48, 1407-10	16.4	101
385	Multistate reactivity in styrene epoxidation by compound I of cytochrome p450: mechanisms of products and side products formation. *Chemistry - A European Journal*, **2005**, 11, 2825-35	4.8	101
384	Characterization, Orbital Description, and Reactivity Patterns of Transition-Metal Oxo Species in the Gas Phase **2000**, 91-123		101
383	Enhanced reactivities of iron(IV)-oxo porphyrin pi-cation radicals in oxygenation reactions by electron-donating axial ligands. *Chemistry - A European Journal*, **2009**, 15, 10039-46	4.8	98
382	QM/MM study of mechanisms for compound I formation in the catalytic cycle of cytochrome P450cam. *Journal of the American Chemical Society*, **2006**, 128, 13204-15	16.4	98
381	The effect of heme environment on the hydrogen abstraction reaction of camphor in P450cam catalysis: a QM/MM study. *Journal of the American Chemical Society*, **2006**, 128, 3924-5	16.4	98
380	Active anionic zero-valent palladium catalysts: characterization by density functional calculations. *Chemistry - A European Journal*, **2004**, 10, 3072-80	4.8	98
379	Exchange-Enhanced H-Abstraction Reactivity of High-Valent Nonheme Iron(IV)-Oxo from Coupled Cluster and Density Functional Theories. *Journal of Physical Chemistry Letters*, **2010**, 1, 1533-1540	6.4	96
378	Structure and quantum chemical characterization of chloroperoxidase compound 0, a common reaction intermediate of diverse heme enzymes. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 99-104	11.5	92
377	Understanding the Nature of the CH···HC Interactions in Alkanes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1977-91	6.4	90
376	The effect of a water molecule on the mechanism of formation of compound 0 in horseradish peroxidase. *Journal of the American Chemical Society*, **2007**, 129, 6346-7	16.4	90
375	Reactivity patterns of cytochrome P450 enzymes: multifunctionality of the active species, and the two states-two oxidants conundrum. *Natural Product Reports*, **2007**, 24, 533-52	15.1	89
374	Characterization of manganese(V)-oxo polyoxometalate intermediates and their properties in oxygen-transfer reactions. *Journal of the American Chemical Society*, **2006**, 128, 15451-60	16.4	89
373	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

372	Theoretical characterization of substrate access/exit channels in the human cytochrome P450 3A4 enzyme: involvement of phenylalanine residues in the gating mechanism. *Journal of Physical Chemistry B*, **2009**, 113, 13018-25	3.4	87
371	The high-valent iron-oxo species of polyoxometalate, if it can be made, will be a highly potent catalyst for C-H hydroxylation and double-bond epoxidation. *Journal of the American Chemical Society*, **2005**, 127, 17712-8	16.4	87
370	The High-Valent Compound of Cytochrome P450: The Nature of the Fe-S Bond and the Role of the Thiolate Ligand as an Internal Electron Donor. *Angewandte Chemie - International Edition*, **2000**, 39, 3851-3855	16.4	87
369	How does product isotope effect prove the operation of a two-state "rebound" mechanism in C-H hydroxylation by cytochrome P450?. *Journal of the American Chemical Society*, **2003**, 125, 13024-5	16.4	86
368	Two-State Reactivity in the Rebound Step of Alkane Hydroxylation by Cytochrome P-450: Origins of Free Radicals with Finite Lifetimes This research was sponsored by the Israeli Science Foundation (ISF) and, in part, by the German Israeli Foundation (GIF), and the VW Stiftung. S.S. thanks the Humboldt Foundation for a Senior Research Award. F.O. thanks the EU for a Marie Curie Fellowship.	16.4	85
367	Topology of electron charge density for chemical bonds from valence bond theory: a probe of bonding types. *Chemistry - A European Journal*, **2009**, 15, 2979-89	4.8	84
366	Is the avoided crossing state a good approximation for the transition state of a chemical reaction? An analysis of Menschutkin and ionic SN2 reactions. *Journal of the American Chemical Society*, **1994**, 116, 262-273	16.4	84
365	Structural characterization of the fleeting ferric peroxo species in myoglobin: experiment and theory. *Journal of the American Chemical Society*, **2007**, 129, 13394-5	16.4	83
364	Effect of external electric fields on the C-H bond activation reactivity of nonheme iron-oxo reagents. *Journal of the American Chemical Society*, **2008**, 130, 3319-27	16.4	83
363	What is the difference between the manganese porphyrin and corrole analogues of cytochrome P450's compound I?. *Chemistry - A European Journal*, **2001**, 7, 4954-60	4.8	83
362	Wasserstoffatomabstraktion von A bis Y: Reaktionsmuster nach der Valenzstrukturtheorie. *Angewandte Chemie*, **2012**, 124, 5652-5676	3.6	82
361	The Poulos-Kraut mechanism of Compound I formation in horseradish peroxidase: a QM/MM study. *Journal of Physical Chemistry B*, **2006**, 110, 10526-33	3.4	82
360	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study. *Angewandte Chemie - International Edition*, **2001**, 40, 2871-2874	16.4	82
359	One oxidant, many pathways: a theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 661-8	3.7	81
358	Electrophilic aromatic chlorination and haloperoxidation of chloride catalyzed by polyfluorinated alcohols: a new manifestation of template catalysis. *Journal of the American Chemical Society*, **2003**, 125, 12116-7	16.4	81
357	Water as an oxygen source: synthesis, characterization, and reactivity studies of a mononuclear nonheme manganese(IV) oxo complex. *Angewandte Chemie - International Edition*, **2010**, 49, 8190-4	16.4	79
356	A survey of recent developments in ab initio valence bond theory. *Journal of Computational Chemistry*, **2007**, 28, 137-51	3.5	79
355	Systematic QM/MM investigation of factors that affect the cytochrome P450-catalyzed hydrogen abstraction of camphor. *Journal of Computational Chemistry*, **2006**, 27, 1324-37	3.5	79

354	Identification of a low-spin acylperoxoiron(III) intermediate in bio-inspired non-heme iron-catalysed oxidations. *Nature Communications*, **2014**, 5, 3046	17.4	78
353	Origins of the Exalted b2u Frequency in the First Excited State of Benzene. *Journal of the American Chemical Society*, **1996**, 118, 666-671	16.4	77
352	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
351	Valence Bond Mixing and Curve Crossing Diagrams in Chemical Reactivity and Bonding. *Advances in Quantum Chemistry*, **1995**, 99-163	1.4	76
350	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
349	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
348	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
347	On the role of water in peroxidase catalysis: a theoretical investigation of HRP compound I formation. *Journal of Physical Chemistry B*, **2010**, 114, 5161-9	3.4	75
346	Kinetic isotope effect is a sensitive probe of spin state reactivity in C-H hydroxylation of N,N-dimethylaniline by cytochrome P450. *Journal of the American Chemical Society*, **2006**, 128, 394-5	16.4	75
345	The experimentally elusive oxidant of cytochrome P450: a theoretical "trapping" defining more closely the "real" species. *ChemBioChem*, **2001**, 2, 848-51	3.8	75
344	On the "Rebound" Mechanism of Alkane Hydroxylation by Cytochrome P450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step. *Angewandte Chemie - International Edition*, **1999**, 38, 3510-3512	16.4	75
343	A Kekulé Crossing Model for the Anomalous Behavior of the b2u Modes of Aromatic Hydrocarbons in the Lowest Excited 1B2u State. *Accounts of Chemical Research*, **1996**, 29, 211-218	24.3	75
342	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
341	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
340	Multireference and multiconfiguration ab initio methods in heme-related systems: what have we learned so far?. *Journal of Physical Chemistry B*, **2011**, 115, 1727-42	3.4	74
339	Principal active species of horseradish peroxidase, compound I: a hybrid quantum mechanical/molecular mechanical study. *Journal of the American Chemical Society*, **2005**, 127, 13611-21	16.4	74
338	Cytochrome P450-The Wonderful Nanomachine Revealed through Dynamic Simulations of the Catalytic Cycle. *Accounts of Chemical Research*, **2019**, 52, 389-399	24.3	71
337	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

336	Why Is Cobalt the Best Transition Metal in Transition-Metal Hangman Corroles for O-O Bond Formation during Water Oxidation?. *Journal of Physical Chemistry Letters*, **2012**, 3, 2315-9	6.4	69
335	Bonding Conundrums in the C2 Molecule: A Valence Bond Study. *Journal of Chemical Theory and Computation*, **2011**, 7, 121-30	6.4	69
334	Experiment and theory reveal the fundamental difference between two-state and single-state reactivity patterns in nonheme Fe(IV)=O versus Ru(IV)=O oxidants. *Angewandte Chemie - International Edition*, **2008**, 47, 3356-9	16.4	69
333	Sulfoxidation mechanisms catalyzed by cytochrome P450 and horseradish peroxidase models: spin selection induced by the ligand. *Biochemistry*, **2005**, 44, 8148-58	3.2	68
332	Is the ruthenium analogue of compound I of cytochrome p450 an efficient oxidant? A theoretical investigation of the methane hydroxylation reaction. *Journal of the American Chemical Society*, **2003**, 125, 2291-300	16.4	68
331	Charge-Shift Bonding in Group IVB Halides:´A Valence Bond Study of MH3□l (M = C, Si, Ge, Sn, Pb) Molecules. *Journal of the American Chemical Society*, **1999**, 121, 822-834	16.4	68
330	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
329	Oxygen economy of cytochrome P450: what is the origin of the mixed functionality as a dehydrogenase-oxidase enzyme compared with its normal function?. *Journal of the American Chemical Society*, **2004**, 126, 5072-3	16.4	67
328	A single transition state serves two mechanisms: an ab initio classical trajectory study of the electron transfer and substitution mechanisms in reactions of ketyl radical anions with alkyl halides. *Journal of the American Chemical Society*, **2001**, 123, 130-4	16.4	67
327	Theoretical Investigations into C□H Bond Activation Reaction by Nonheme MnIVO Complexes: Multistate Reactivity with No Oxygen Rebound. *Journal of Physical Chemistry Letters*, **2012**, 3, 2851-2856	6.4	66
326	Valence Bond Configuration Interaction: A Practical ab Initio Valence Bond Method That Incorporates Dynamic Correlation. *Journal of Physical Chemistry A*, **2002**, 106, 2721-2726	2.8	66
325	An anatomy of the two-state reactivity concept: Personal reminiscences in memoriam of Detlef Schr□der. *International Journal of Mass Spectrometry*, **2013**, 354-355, 5-14	1.9	64
324	A mononuclear non-heme high-spin iron(III)-hydroperoxo complex as an active oxidant in sulfoxidation reactions. *Journal of the American Chemical Society*, **2013**, 135, 8838-41	16.4	64
323	Which oxidant is really responsible for sulfur oxidation by cytochrome P450?. *Angewandte Chemie - International Edition*, **2007**, 46, 8168-70	16.4	64
322	A valence bond study of the Bergman cyclization: geometric features, resonance energy, and nucleus-independent chemical shift (NICS) values. *Chemistry - A European Journal*, **2000**, 6, 1446-54	4.8	64
321	The QTAIM Perspective of Chemical Bonding **2014**, 271-308		63
320	Computer-generated high-valent iron--oxo and manganese--oxo species with polyoxometalate ligands: how do they compare with the iron--oxo active species of heme enzymes?. *Angewandte Chemie - International Edition*, **2004**, 43, 5661-5	16.4	63
319	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

318	Barriers of hydrogen abstraction vs halogen exchange: an experimental manifestation of charge-shift bonding. *Journal of the American Chemical Society*, **2006**, 128, 2836-43	16.4	62
317	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
316	Dioxygen Activation by a Non-Heme Iron(II) Complex: Theoretical Study toward Understanding Ferric-Superoxo Complexes. *Journal of Chemical Theory and Computation*, **2012**, 8, 915-26	6.4	61
315	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
314	Multiple Low-Lying States for Compound I of P450cam and Chloroperoxidase Revealed from Multireference Ab Initio QM/MM Calculations. *Journal of Chemical Theory and Computation*, **2010**, 6, 940-53	6.4	60
313	Oxidation of tertiary amines by cytochrome p450-kinetic isotope effect as a spin-state reactivity probe. *Chemistry - A European Journal*, **2009**, 15, 8492-503	4.8	60
312	Theoretical Analysis of the Catalytic Cycle of a Nickel Cross-Coupling Process: Application of the Energetic Span Model. *Organometallics*, **2009**, 28, 1303-1308	3.8	60
311	Gauging the relative oxidative powers of compound I, ferric-hydroperoxide, and the ferric-hydrogen peroxide species of cytochrome P450 toward C-H hydroxylation of a radical clock substrate. *Journal of the American Chemical Society*, **2006**, 128, 473-84	16.4	60
310	Modeling CH Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes: What Role Do Counter Ions Play?. *Journal of Physical Chemistry Letters*, **2011**, 2, 2610-2617	6.4	59
309	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
308	External Electric Field Can Control the Catalytic Cycle of Cytochrome P450cam: A QM/MM Study. *Journal of Physical Chemistry Letters*, **2010**, 1, 2082-2087	6.4	58
307	Theoretical and experimental studies of the conversion of chromopyrrolic acid to an antitumor derivative by cytochrome P450 StaP: the catalytic role of water molecules. *Journal of the American Chemical Society*, **2009**, 131, 6748-62	16.4	58
306	NR transfer reactivity of azo-compound I of P450. How does the nitrogen substituent tune the reactivity of the species toward C-H and C=C activation?. *Journal of Physical Chemistry B*, **2007**, 111, 10288-99	3.4	58
305	Green's function methods for calculating ionization potentials, electron affinities, and excitation energies. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 377-387	7.9	57
304	Is my chemical universe localized or delocalized? is there a future for chemical concepts?. *New Journal of Chemistry*, **2007**, 31, 2015	3.6	57
303	Compound I of nitric oxide synthase: the active site protonation state. *Journal of the American Chemical Society*, **2007**, 129, 3182-8	16.4	57
302	Two-state reactivity, electromerism, tautomerism, and "surprise" isomers in the formation of compound II of the enzyme horseradish peroxidase from the principal species, compound I. *Journal of the American Chemical Society*, **2006**, 128, 8185-98	16.4	57
301	How do aldehyde side products occur during alkene epoxidation by cytochrome P450? Theory reveals a state-specific multi-state scenario where the high-spin component leads to all side products. *Journal of Inorganic Biochemistry*, **2004**, 98, 1183-93	4.2	57

300	pi bonding in second and third row molecules: testing the strength of Linus's blanket. *Chemistry - A European Journal*, **2000**, 6, 2425-34	4.8	57
299	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
298	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
297	The intrinsic axial ligand effect on propene oxidation by horseradish peroxidase versus cytochrome P450 enzymes. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 181-9	3.7	56
296	Spin□Orbit Coupling Patterns Induced by Twist and Pyramidalization Modes in C2H4:´A Quantitative Study and a Qualitative Analysis. *Journal of Physical Chemistry A*, **1998**, 102, 5923-5936	2.8	56
295	Factors Controlling the Selective Hydroformylation of Internal Alkenes to Linear Aldehydes. 1. The Isomerization Step. *Organometallics*, **2009**, 28, 3656-3665	3.8	55
294	Porphyrin traps its terminator! Concerted and stepwise porphyrin degradation mechanisms induced by heme-oxygenase and cytochrome p450. *Angewandte Chemie - International Edition*, **2004**, 43, 1129-32	16.4	55
293	Identity Hydrogen Abstraction Reactions, X□ H□□> X□ + X□X = X□= CH3, SiH3, GeH3, SnH3, PbH3):´A Valence Bond Modeling. *Journal of Physical Chemistry A*, **2001**, 105, 8226-8235	2.8	55
292	Tetramethyleneethane (TME) Diradical: Experiment and Density Functional Theory Reach an Agreement. *Journal of Physical Chemistry A*, **1999**, 103, 8885-8889	2.8	54
291	How Accurate Can a Local Coupled Cluster Approach Be in Computing the Activation Energies of Late-Transition-Metal-Catalyzed Reactions with Au, Pt, and Ir?. *Journal of Chemical Theory and Computation*, **2012**, 8, 3119-27	6.4	53
290	Silynes (RC?SiR') and Disilynes (RSi?SiR'): Why Are Less Bonds Worth Energetically More?. *Angewandte Chemie - International Edition*, **2001**, 40, 4023-4026	16.4	53
289	Charge-Shift Bonding: A New and Unique Form of Bonding. *Angewandte Chemie - International Edition*, **2020**, 59, 984-1001	16.4	53
288	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
287	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
286	An efficient proton-coupled electron-transfer process during oxidation of ferulic acid by horseradish peroxidase: coming full cycle. *Journal of the American Chemical Society*, **2006**, 128, 13940-9	16.4	52
285	What Are the Reasons for the Kinetic Stability of a Mixture of H2 and O2?. *Journal of Physical Chemistry A*, **2000**, 104, 12014-12020	2.8	52
284	Does the TauD enzyme always hydroxylate alkanes, while an analogous synthetic non-heme reagent always desaturates them?. *Journal of the American Chemical Society*, **2011**, 133, 176-9	16.4	51
283	Quantum mechanical/molecular mechanical study on the mechanisms of compound I formation in the catalytic cycle of chloroperoxidase: an overview on heme enzymes. *Journal of Physical Chemistry B*, **2008**, 112, 9490-500	3.4	51

282	Single- and Two-State Reactivity in the Gas-Phase C H Bond Activation of Norbornane by ' Bare' FeO+. *Helvetica Chimica Acta*, **1999**, 82, 1784-1797	2	51
281	Structure of fluoromethyl radicals. Conjugative and inductive effects. *Journal of the American Chemical Society*, **1978**, 100, 1352-1356	16.4	51
280	New features in the catalytic cycle of cytochrome P450 during the formation of compound I from compound 0. *Journal of Physical Chemistry B*, **2005**, 109, 19946-51	3.4	50
279	Valenzbindungsdiagramme eine Hilfe zum Verst dnis chemischer Reaktivit t. *Angewandte Chemie*, **1999**, 111, 616-657	3.6	50
278	The Nature of the Idealized Triple Bonds Between Principal Elements and the Origins of Trans-Bent Geometries-A Valence Bond Study. *Journal of Chemical Theory and Computation*, **2011**, 7, 955-68	6.4	49
277	The origins of the directionality of noncovalent intermolecular interactions. *Journal of Computational Chemistry*, **2016**, 37, 34-45	3.5	49
276	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
275	A response to the critical comments on "One molecule, two atoms, three views, four bonds?". *Angewandte Chemie - International Edition*, **2013**, 52, 5926-8	16.4	48
274	Can ferric-superoxide act as a potential oxidant in P450(cam)? QM/MM investigation of hydroxylation, epoxidation, and sulfoxidation. *Journal of the American Chemical Society*, **2011**, 133, 5444-52	16.4	48
273	Lessons on O2 and NO bonding to heme from ab initio multireference/multiconfiguration and DFT calculations. *Journal of Biological Inorganic Chemistry*, **2011**, 16, 841-55	3.7	48
272	A theoretical study of electronic factors affecting hydroxylation by model ferryl complexes of cytochrome P-450 and horseradish peroxidase. *Journal of the Chemical Society Perkin Transactions II* , **1999**, 399-410		48
271	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
270	A new mechanism for ethanol oxidation mediated by cytochrome P450 2E1: bulk polarity of the active site makes a difference. *ChemBioChem*, **2007**, 8, 277-81	3.8	47
269	A practical valence bond method: a configuration interaction method approach with perturbation theoretic facility. *Journal of Computational Chemistry*, **2004**, 25, 472-8	3.5	47
268	Valence bond calculations of hydrogen transfer reactions: a general predictive pattern derived from theory. *Journal of the American Chemical Society*, **2004**, 126, 13539-49	16.4	47
267	VB-DFT: a nonempirical hybrid method combining valence bond theory and density functional energies. *Chemical Physics Letters*, **1999**, 301, 37-42	2.5	47
266	How does the reductase help to regulate the catalytic cycle of cytochrome P450 3A4 using the conserved water channel?. *Journal of Physical Chemistry B*, **2010**, 114, 5964-70	3.4	46
265	The physical origin of large covalent-ionic resonance energies in some two-electron bonds. *Faraday Discussions*, **2007**, 135, 261-72; discussion 367-401, 503-6	3.6	46

264	Qualitative potential energy surfaces. 3. Stereoselection rules for spin inversion in triplet photochemical reactions. *Journal of the American Chemical Society*, **1978**, 100, 18-29	16.4	46
263	A tutorial for understanding chemical reactivity through the valence bond approach. *Chemical Society Reviews*, **2014**, 43, 4968-88	58.5	45
262	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
261	Identity SN2 reactions X- + CH3X --> XCH3 + X- (X=F, Cl, Br, and I) in vacuum and in aqueous solution: a valence bond study. *Chemistry - A European Journal*, **2006**, 12, 7458-66	4.8	44
260	Does substrate oxidation determine the regioselectivity of cyclohexene and propene oxidation by cytochrome p450?. *Journal of the American Chemical Society*, **2006**, 128, 11028-9	16.4	44
259	Blended hydrogen atom abstraction and proton-coupled electron transfer mechanisms of closed-shell molecules. *Chemical Science*, **2012**, 3, 1903	9.4	43
258	Disilylfluoronium IonsSynthesis, Structure, and Bonding. *Organometallics*, **2011**, 30, 4087-4096	3.8	43
257	Electron transfer activation of chromopyrrolic acid by cytochrome p450 en route to the formation of an antitumor indolocarbazole derivative: theory supports experiment. *Journal of the American Chemical Society*, **2008**, 130, 7170-1	16.4	43
256	Structural dynamics of the cooperative binding of organic molecules in the human cytochrome P450 3A4. *Journal of the American Chemical Society*, **2007**, 129, 1602-11	16.4	43
255	The Lewis legacy: the chemical bond--a territory and heartland of chemistry. *Journal of Computational Chemistry*, **2007**, 28, 51-61	3.5	43
254	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
253	The ELF Perspective of chemical bonding **2014**, 345-382		42
252	Formation of the active species of cytochrome p450 by using iodosylbenzene: a case for spin-selective reactivity. *Chemistry - A European Journal*, **2007**, 13, 4103-15	4.8	42
251	Transition states, avoided crossing states and valence-bond mixing: fundamental reactivity paradigms. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 1631		42
250	External electric field effects on chemical structure and reactivity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1438	7.9	42
249	Valence bond modelling and density functional theory calculations of reactivity and mechanism of cytochrome P450 enzymes: thioether sulfoxidation. *Faraday Discussions*, **2010**, 145, 49-70	3.6	41
248	The Inverted Bond in [1.1.1]Propellane is a Charge-Shift Bond. *Angewandte Chemie*, **2009**, 121, 1435-1438	3.6	41
247	Proton-shuffle mechanism of O-O activation for formation of a high-valent oxo-iron species of bleomycin. *Journal of the American Chemical Society*, **2006**, 128, 16148-58	16.4	41

246	The Quadruple Bonding in C2 Reproduces the Properties of the Molecule. *Chemistry - A European Journal*, **2016**, 22, 4116-28	4.8	41
245	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
244	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
243	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
242	The NBO View of Chemical Bonding **2014**, 91-120		40
241	Perferryl Fe(V)-Oxo Nonheme Complexes: Do They Have High-Spin or Low-Spin Ground States?. *Journal of Chemical Theory and Computation*, **2011**, 7, 3049-53	6.4	40
240	Structured Electron Transfer Transition State. Valence Bond Configuration Mixing Analysis and ab Initio Calculations of the Reactions of Formaldehyde Radical Anion with Methyl Chloride. *The Journal of Physical Chemistry*, **1996**, 100, 12241-12252		40
239	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
238	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
237	Nonheme iron-oxo and -superoxo reactivities: O2 binding and spin inversion probability matter. *Chemical Communications*, **2012**, 48, 2189-91	5.8	39
236	VBPCM:´A Valence Bond Method that Incorporates a Polarizable Continuum Model. *Journal of Physical Chemistry A*, **2004**, 108, 6017-6024	2.8	39
235	Trends in Aromatic Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes: A Valence Bond Modeling. *Journal of Chemical Theory and Computation*, **2011**, 7, 327-39	6.4	38
234	First half-reaction mechanism of nitric oxide synthase: the role of proton and oxygen coupled electron transfer in the reaction by quantum mechanics/molecular mechanics. *Journal of Physical Chemistry B*, **2009**, 113, 336-46	3.4	38
233	Valence Bond Theory, Its History, Fundamentals, and Applications: A Primer. *Reviews in Computational Chemistry*, **2004**, 1-100		38
232	Which Density Functional Is the Best in Computing C-H Activation Energies by Pincer Complexes of Late Platinum Group Metals?. *Journal of Chemical Theory and Computation*, **2012**, 8, 2991-6	6.4	37
231	The Fe(III)(H2O2) Complex as a Highly Efficient Oxidant in Sulfoxidation Reactions: Revival of an Underrated Oxidant in Cytochrome P450. *Journal of Chemical Theory and Computation*, **2013**, 9, 2519-25	6.4	37
230	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
229	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

228	Quantum and molecular mechanical study of the first proton transfer in the catalytic cycle of cytochrome P450cam and its mutant D251N. *Journal of Physical Chemistry B*, **2008**, 112, 5126-38	3.4	35
227	In silico design of a mutant of cytochrome P450 containing selenocysteine. *Journal of the American Chemical Society*, **2006**, 128, 2649-53	16.4	35
226	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
225	An excursion from normal to inverted C-C bonds shows a clear demarcation between covalent and charge-shift C-C bonds. *ChemPhysChem*, **2009**, 10, 2658-69	3.2	34
224	QM/MM Study of the ProductEnzyme Complex in P450cam Catalysis. *Journal of Physical Chemistry B*, **2004**, 108, 10083-10088	3.4	34
223	The origins of dramatic axial ligand effects: closed-shell Mn(V)O complexes use exchange-enhanced open-shell States to mediate efficient H abstraction reactions. *Angewandte Chemie - International Edition*, **2012**, 51, 4421-5	16.4	33
222	Enzymatic ring-opening mechanism of verdoheme by the heme oxygenase: a combined X-ray crystallography and QM/MM study. *Journal of the American Chemical Society*, **2010**, 132, 12960-70	16.4	33
221	The Distortive Tendency of Benzene Electrons: How Is It Related to Structural Observables?. *Angewandte Chemie International Edition in English*, **1997**, 36, 2205-2208		33
220	QM/MM study of the active species of the human cytochrome P450 3A4, and the influence thereof of the multiple substrate binding. *Journal of Physical Chemistry B*, **2007**, 111, 13822-32	3.4	33
219	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
218	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
217	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
216	Compound I in heme thiolate enzymes: a comparative QM/MM study. *Journal of Physical Chemistry A*, **2008**, 112, 13128-38	2.8	32
215	The Menshutkin reaction in the gas phase and in aqueous solution: a valence bond study. *ChemPhysChem*, **2007**, 8, 2603-14	3.2	32
214	The distortive tendencies of electronic systems, their relationship to isoelectronic bonded analogs, and observables: A description free of the classical paradoxes. *Physical Chemistry Chemical Physics*, **2004**, 6, 224-231	3.6	32
213	Electron transfer vs polar mechanisms. Transition-state structures and properties for reactions of a cation radical and a nucleophile. *Journal of the American Chemical Society*, **1991**, 113, 9890-9891	16.4	31
212	DFVB: A Density-Functional-Based Valence Bond Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 1608-15	6.4	30
211	A single-site mutation (F429H) converts the enzyme CYP 2B4 into a heme oxygenase: a QM/MM study. *Journal of the American Chemical Society*, **2012**, 134, 4053-6	16.4	30

210	Ein Molekül zwei Atome, drei Ansichten, vier Bindungen?. *Angewandte Chemie*, **2013**, 125, 3094-3109	3.6	30
209	A Two-State Reactivity Model Explains Unusual Kinetic Isotope Effect Patterns in C?H Bond Cleavage by Nonheme Oxoiron(IV) Complexes. *Angewandte Chemie*, **2009**, 121, 1317-1321	3.6	30
208	Alkane Hydroxylation by Cytochrome P450: Is Kinetic Isotope Effect a Reliable Probe of Transition State Structure?. *European Journal of Inorganic Chemistry*, **2000**, 2000, 2455-2458	2.3	30
207	A redox-mediated Kemp eliminase. *Nature Communications*, **2017**, 8, 14876	17.4	29
206	Theoretical analysis of the structural and electronic properties of metalloporphyrin pi-cation radicals. *Journal of Physical Chemistry A*, **2006**, 110, 6091-9	2.8	29
205	Catalysts for monooxygenations made from polyoxometalate: an iron(V)-oxo derivative of the Lindqvist anion. *Inorganic Chemistry*, **2006**, 45, 8655-63	5.1	29
204	An accurate barrier for the hydrogen exchange reaction from valence bond theory: is this theory coming of age?. *Chemistry - A European Journal*, **2003**, 9, 4540-7	4.8	28
203	No-Pair Bonding in High-Spin Lithium Clusters: Li_{n+1} (n = 2−8). *Journal of Physical Chemistry A*, **2000**, 104, 11223-11231	2.8	28
202	Towards the Definition of the Maximum Allowable Tightness of an Electron Transfer Transition State in the Reactions of Radical Anions and Alkyl Halides. *Angewandte Chemie International Edition in English*, **1996**, 35, 1098-1100		28
201	Water as biocatalyst in cytochrome P450. *Faraday Discussions*, **2011**, 148, 373-83; discussion 421-41	3.6	27
200	How can theory predict the selectivity of palladium-catalyzed cross-coupling of pristine aromatic molecules?. *Chemistry - A European Journal*, **2011**, 17, 7623-31	4.8	27
199	The Fundamental Role of Exchange-Enhanced Reactivity in C?H Activation by S=2 Oxo Iron(IV) Complexes. *Angewandte Chemie*, **2010**, 122, 3414-3417	3.6	27
198	A Density Functional Study of the Factors That Influence the Regioselectivity of Toluene Hydroxylation by Cytochrome P450 Enzymes. *European Journal of Inorganic Chemistry*, **2007**, 2007, 2966-2974	2.3	27
197	The V state of ethylene: valence bond theory takes up the challenge. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	26
196	Calculated and experimental spin state of seleno cytochrome P450. *Angewandte Chemie - International Edition*, **2009**, 48, 7193-5	16.4	26
195	Water as an Oxygen Source: Synthesis, Characterization, and Reactivity Studies of a Mononuclear Nonheme Manganese(IV) Oxo Complex. *Angewandte Chemie*, **2010**, 122, 8366-8370	3.6	26
194	The Twin-Excited State as a Probe for the Transition State in Concerted Unimolecular Reactions: The Semibullvalene Rearrangement. *Angewandte Chemie - International Edition*, **1998**, 37, 1394-1397	16.4	26
193	On the identity and reactivity patterns of the "second oxidant" of the T252A mutant of cytochrome P450cam in the oxidation of 5-methylenenylcamphor. *Journal of Inorganic Biochemistry*, **2006**, 100, 2054-68	4.3	26

192	Ferromagnetic bonding in high-spin alkali-metal clusters. How does sodium compare to lithium?. *Physical Chemistry Chemical Physics*, **2003**, 5, 158-164	3.6	26
191	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
190	Heterolytic bond dissociation in water: why is it so easy for C4H9Cl but not for C3H9SiCl?. *Journal of Physical Chemistry A*, **2008**, 112, 2988-97	2.8	25
189	Stereospecific oxidation by compound I of cytochrome P450 does not proceed in a concerted synchronous manner. *Chemical Communications*, **2001**, 2322-3	5.8	25
188	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
187	A valence bond study of the dioxygen molecule. *Journal of Computational Chemistry*, **2007**, 28, 185-97	3.5	24
186	Aromaticity and antiaromaticity: what role do ionic configurations play in delocalization and induction of magnetic properties?. *Journal of Physical Organic Chemistry*, **2003**, 16, 731-745	2.1	24
185	A Valence Bond Study of the Bonding in First Row Transition Metal Hydride Cations: What Energetic Role Does Covalency Play? *Journal of Physical Chemistry A*, **2000**, 104, 1262-1270	2.8	24
184	Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. *Journal of the American Chemical Society*, **2017**, 139, 9302-9316	16.4	23
183	Theoretical predictions of a highly reactive non-heme Fe(IV)=O complex with a high-spin ground state. *Chemical Communications*, **2010**, 46, 4511-3	5.8	23
182	Valence bond all the way: from the degenerate H-exchange to cytochrome P450. *Physical Chemistry Chemical Physics*, **2010**, 12, 8706-20	3.6	23
181	Defining the optimal inductive and steric requirements for a cross-coupling catalyst using the energetic span model?. *Journal of Molecular Catalysis A*, **2010**, 324, 120-126		23
180	VBDFT(s): a H□kel-type semi-empirical valence bond method scaled to density functional energies. Application to linear polyenes. *Chemical Physics Letters*, **1998**, 292, 7-14	2.5	23
179	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. *Inorganic Chemistry*, **2017**, 56, 3287-3301	5.1	22
178	Oxoiron(IV) Complex of the Ethylene-Bridged Dialkylcyclam Ligand Me2EBC. *Inorganic Chemistry*, **2015**, 54, 7828-39	5.1	22
177	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
176	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
175	In Defense of the Hybrid Atomic Orbitals. *Journal of Chemical Education*, **2012**, 89, 575-577	2.4	22

174	Brain chemistry: how does P450 catalyze the O-demethylation reaction of 5-methoxytryptamine to yield serotonin?. *Journal of Physical Chemistry B*, **2010**, 114, 7078-89	3.4	22
173	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
172	Nature of the Three-Electron Bond. *Journal of Physical Chemistry A*, **2018**, 122, 1873-1885	2.8	21
171	The Conceptual Density Functional Theory Perspective of Bonding **2014**, 233-270		21
170	Spin-Orbit Coupling and Outer-Core Correlation Effects in Ir- and Pt-Catalyzed C-H Activation. *Journal of Chemical Theory and Computation*, **2012**, 8, 1641-5	6.4	21
169	Myth and Reality in the Attitude toward Valence-Bond (VB) Theory: Are Its Failures Real?. *Helvetica Chimica Acta*, **2003**, 86, 1063-1084	2	21
168	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
167	Correlating DFT-calculated energy barriers to experiments in nonheme octahedral Fe(IV)O species. *Chemistry - A European Journal*, **2012**, 18, 10444-53	4.8	20
166	A Topological Study of the Ferromagnetic No-Pair Bonding in Maximum-Spin Lithium clusters: n+1Li n (n=2). *Theoretical Chemistry Accounts*, **2006**, 116, 390-397	1.9	20
165	Computational Approaches to Cytochrome P450 Function **2005**, 45-85		20
164	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
163	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
162	Which Oxidant Is Really Responsible for Sulfur Oxidation by Cytochrome P450?. *Angewandte Chemie*, **2007**, 119, 8316-8318	3.6	19
161	The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron Transfer. *Journal of Physical Chemistry C*, **2007**, 111, 7711-7719	3.8	19
160	The ground and excited states of polyenyl radicals C2n-1H2n + 1 (n = 2-13): a valence bond study. *ChemPhysChem*, **2004**, 5, 515-28	3.2	19
159	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
158	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
157	Protonated alcohols are examples of complete charge-shift bonds. *Journal of Organic Chemistry*, **2014**, 79, 9998-10001	4.2	18

156	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
155	Comment on "A low-spin ruthenium(IV)-oxo complex: does the spin state have an impact on the reactivity". *Angewandte Chemie - International Edition*, **2011**, 50, 3850-1; author reply 3852-3	16.4	18
154	Will P450cam Hydroxylate or Desaturate Alkanes? QM and QM/MM Studies. *Journal of Physical Chemistry Letters*, **2011**, 2, 2229-2235	6.4	18
153	A REKS Assessment of the Face-Diagonal Bond in 1,3-Didehydrocubane and a Comparison with Benzyne Biradicals. *European Journal of Organic Chemistry*, **2003**, 2003, 4199-4204	3.2	18
152	Some answers to frequently asked questions about the distortive tendencies of □electronic system. *Theoretical Chemistry Accounts*, **2005**, 114, 169-181	1.9	18
151	Silynes (RC?SiR?) and Disilynes (RSi?SiR?): Why Are Less Bonds Worth Energetically More?. *Angewandte Chemie*, **2001**, 113, 4146-4150	3.6	18
150	Computational prediction of the ISC rate for triplet norbornene. *Chemical Physics Letters*, **2000**, 322, 358-362	2.5	18
149	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
148	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
147	Effects of substrate, protein environment, and proximal ligand mutation on compound I and compound 0 of chloroperoxidase. *Journal of Physical Chemistry A*, **2009**, 113, 11763-71	2.8	17
146	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
145	Two-State Reactivity: Personal Recounting of its Conception and Future Prospects. *Israel Journal of Chemistry*, **2020**, 60, 938-956	3.4	16
144	The Physical Origin of Covalent Bonding **2014**, 1-68		16
143	Covalent Excited States of Polyenes C2nH2n+2 (n = 2-8) and Polyenyl Radicals C2n-1H2n+1 (n = 2-8): An Ab Initio Valence Bond Study. *Journal of Chemical Theory and Computation*, **2008**, 4, 2101-7	6.4	16
142	No-pair bonding in coinage metal dimers. *Journal of Physical Chemistry A*, **2008**, 112, 12995-3001	2.8	16
141	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
140	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. *Angewandte Chemie - International Edition*, **2019**, 58, 12332-12338	16.4	15
139	The Block-Localized Wavefunction (BLW) Perspective of Chemical Bonding **2014**, 199-232		15

138	A primer on qualitative valence bond theory – a theory coming of age. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 18-29	7.9	15
137	Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I. *Angewandte Chemie*, **2002**, 114, 2027	3.6	15
136	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study. *Angewandte Chemie*, **2001**, 113, 2955-2958	3.6	15
135	Comparative Study of Identity Proton-Transfer Reactions between Simple Atoms or Groups by VB Methods. *Journal of Physical Chemistry A*, **2002**, 106, 11616-11622	2.8	15
134	Quantitative valence-bond computations of curve crossing diagrams for a gas-phase SN2 reaction: F⁻ CH3F -> FCH3+ F⁻ *Journal of the Chemical Society Perkin Transactions II*, **1992**, 1019-1025		15
133	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
132	To hybridize or not to hybridize? This is the dilemma. *Computational and Theoretical Chemistry*, **2017**, 1116, 242-249	2	14
131	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
130	Bonding with parallel spins: high-spin clusters of monovalent metal atoms. *Accounts of Chemical Research*, **2014**, 47, 417-26	24.3	14
129	Intramolecular gas-phase reactions of synthetic nonheme oxoiron(IV) ions: proximity and spin-state reactivity rules. *Chemistry - A European Journal*, **2012**, 18, 11747-60	4.8	14
128	A Response to the Critical Comments on "One Molecule, Two Atoms, Three Views, Four Bonds?" *Angewandte Chemie*, **2013**, 125, 6040-6042	3.6	14
127	An acyl group makes a difference in the reactivity patterns of cytochrome P450 catalyzed N-demethylation of substituted N,N-dimethylbenzamides-high spin selective reactions. *Journal of Physical Chemistry B*, **2010**, 114, 2964-70	3.4	14
126	Reply to Comment on "Identity Hydrogen Abstraction Reactions, X· + HX'> XH + X'(X = X'= CH3, SiH3, GeH3, SnH3, PbH3): A Valence Bond Modeling" *Journal of Physical Chemistry A*, **2002**, 106, 5043-5045	2.8	14
125	VBDFT(s): semi-empirical valence bond method: Application to linear polyenes containing oxygen and nitrogen heteroatoms. *Physical Chemistry Chemical Physics*, **2001**, 3, 5459-5465	3.6	14
124	Electron Transfer and Polar Reactions of Cyclizable Anion Radicals: Structural Consequences of Orbital Selection Rules and Chain-Length Constraints. *Angewandte Chemie International Edition in English*, **1995**, 34, 1495-1497		14
123	Principles and Prospects of Spin-States Reactivity in Chemistry and Bioinorganic Chemistry **2015**, 131-156		13
122	The reaction mechanism of allene oxide synthase: Interplay of theoretical QM/MM calculations and experimental investigations. *Archives of Biochemistry and Biophysics*, **2011**, 507, 14-25	4.1	13
121	Inner-sphere electron transfer in metal-cation chemistry. *International Journal of Mass Spectrometry* , **2000**, 200, 163-173	1.9	13

120	Charge-Shift Bonding: A New and Unique Form of Bonding. *Angewandte Chemie*, **2020**, 132, 996-1013	3.6	13
119	Deciphering the oxygen activation mechanism at the CuC site of particulate methane monooxygenase. *Nature Catalysis*, **2021**, 4, 266-273	36.5	13
118	Bound Triplet Pairs in the Highest Spin States of Coinage Metal Clusters. *Journal of Chemical Theory and Computation*, **2010**, 6, 1479-89	6.4	12
117	Radical cations of non-alternant systems as probes of theShaikPross VB configuration mixing model. *Journal of the Chemical Society Perkin Transactions II*, **1997**, 463-472		12
116	Chameleon States: High-Valent MetalOxo Species of Cytochrome P450 and Its Ruthenium Analogue. *Angewandte Chemie*, **2001**, 113, 2958-2962	3.6	12
115	Origins of non-perfect synchronization in the lowest energy path of the identity proton transfer reaction of allyl anion + propene: a VBSCF study. *Journal of Physical Organic Chemistry*, **1999**, 12, 259-262	2.1	12
114	Attraction between electrophilic caps: A counterintuitive case of noncovalent interactions. *Journal of Computational Chemistry*, **2019**, 40, 1015-1022	3.5	12
113	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
112	Relativity and Chemical Bonding **2014**, 383-404		11
111	An efficient algorithm for complete active space valence bond self-consistent field calculation. *Journal of Computational Chemistry*, **2013**, 34, 38-48	3.5	11
110	The High-Valent Compound of Cytochrome P450: The Nature of the Fe Bond and the Role of the Thiolate Ligand as an Internal Electron Donor. *Angewandte Chemie*, **2000**, 112, 4009-4013	3.6	11
109	er den Neuanbindungs-Mechanismus der Alkanhydroxylierung durch Cytochrom P450: elektronische Struktur der Zwischenstufe und Charakter des Elektronentransfers bei der Neuanbindung. *Angewandte Chemie*, **1999**, 111, 3730-3733	3.6	11
108	Reactions of tellurium(IV) halides with anthracene and other organic compounds. *Journal of the Chemical Society Perkin Transactions 1*, **1975**, 1223		11
107	Valence Bond Theory-Its Birth, Struggles with Molecular Orbital Theory, Its Present State and Future Prospects. *Molecules*, **2021**, 26,	4.8	11
106	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
105	Halogen Bonds in Novel Polyhalogen Monoanions. *Chemistry - A European Journal*, **2017**, 23, 8719-8728	4.8	10
104	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
103	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

102	QM/MM theoretical study of the pentacoordinate Mn(III) and resting states of manganese-reconstituted cytochrome P450(cam). *Journal of Biological Inorganic Chemistry*, **2008**, 13, 521-30	3.7	10
101	Experiment and Theory Reveal the Fundamental Difference between Two-State and Single-State Reactivity Patterns in Nonheme FeIV?O versus RuIV?O Oxidants. *Angewandte Chemie*, **2008**, 120, 3404-3407	3.6	10
100	Porphyrin Traps Its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450. *Angewandte Chemie*, **2004**, 116, 1149-1152	3.6	10
99	A primer for valence bond mixing and avoided crossing: General paradigms in chemical reactivity. *Journal of Molecular Liquids*, **1994**, 61, 49-79	6	10
98	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
97	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
96	Computer-Generated High-Valent Iron□Oxo and Manganese□Oxo Species with Polyoxometalate Ligands: How do they Compare with the Iron□Oxo Active Species of Heme Enzymes?. *Angewandte Chemie*, **2004**, 116, 5779-5783	3.6	9
95	Zwei Reaktionswege beim „Wiederanbindungs"-Mechanismus der Alkanhydroxylierung durch Cytochrom P450: Entstehung freier Radikale mit begrenzter Lebensdauer. *Angewandte Chemie*, **2000**, 112, 2070-2074	3.6	9
94	Identification of tellurium-containing compounds by means of mass spectrometry. *Journal of Organometallic Chemistry*, **1975**, 91, 307-313	2.3	9
93	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
92	H-Bonding Networks Dictate the Molecular Mechanism of H2O2 Activation by P450. *ACS Catalysis*, **2021**, 11, 8774-8785	13.1	9
91	Valence Bond Diagrams and Chemical Reactivity **1999**, 38, 586		9
90	Chemical Bonding of Main-Group Elements **2014**, 1-24		8
89	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
88	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
87	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
86	Facile Monolayer Formation on SiO2 Surfaces via Organoboron Functionalities. *Angewandte Chemie* , **2013**, 125, 7563-7566	3.6	7
85	Chemistry--a central pillar of human culture. *Angewandte Chemie - International Edition*, **2003**, 42, 3208-15	16.4	7

84	Evidence for new enantiospecific interaction force in chiral biomolecules. *CheM*, **2021**,	16.2	7
83	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
82	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
81	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
80	Donor□Acceptor Complexes of Main-Group Elements **2014**, 71-112		6
79	The Origins of Dramatic Axial Ligand Effects: Closed-Shell MnVO Complexes Use Exchange-Enhanced Open-Shell States to Mediate Efficient H Abstraction Reactions. *Angewandte Chemie*, **2012**, 124, 4497-4501	3.6	6
78	On the Nature of Bonding in Parallel Spins in Monovalent Metal Clusters. *Annual Review of Physical Chemistry*, **2016**, 67, 419-39	15.7	6
77	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
76	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
75	Tuning the Ground State Symmetry of Acetylenyl Radicals. *ACS Central Science*, **2015**, 1, 270-8	16.8	5
74	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
73	Bridging Cultures **2014**, 69-90		5
72	Chemical Bonding in Transition Metal Compounds **2014**, 175-218		5
71	The valence bond workshop in Paris: the phoenix rises from the ashes or, has a love story with MO-based theories begun?. *ChemPhysChem*, **2012**, 13, 4029-30	3.2	5
70	The valence bond diagram approach: A paradigm for chemical reactivity **2005**, 635-668		5
69	The High-Valent Compound of Cytochrome P450: The Nature of the Fe□ Bond and the Role of the Thiolate Ligand as an Internal Electron Donor. *Angewandte Chemie - International Edition*, **2001**, 40, 647-647	16.4	5
68	Polare und Elektronentransferreaktionen cyclisierbarer Radikalanionen: strukturelle Konsequenzen aus Orbitalauswahlregeln und Beschr□kungen aufgrund der C-Kettenl□nge. *Angewandte Chemie*, **1995**, 107, 1619-1621	3.6	5
67	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. *Journal of Chemical Education*,	2.4	5

66	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
65	QM/MM Calculations Reveal the Important Role of Heteroatom Substituents in Controlling Selectivity of Mononuclear Nonheme HppE-Catalyzed Reactions. *ACS Catalysis*, **2020**, 10, 9521-9532	13.1	5
64	Na???B Bond in NaBH : Solving the Conundrum. *Angewandte Chemie - International Edition*, **2021**, 60, 12725-12726	15.1	5
63	CHAPTER 2:The Impact of Electric Fields on Chemical Structure and Reactivity. *RSC Theoretical and Computational Chemistry Series*, **2021**, 12-70	1.2	5
62	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
61	The Valence Bond Perspective of the Chemical Bond **2014**, 159-198		4
60	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
59	Dispersion Interaction and Chemical Bonding **2014**, 477-500		4
58	Comment on A Low-Spin Ruthenium(IV)Oxo Complex: Does the Spin State Have an Impact on the Reactivity*Angewandte Chemie*, **2011**, 123, 3934-3935	3.6	4
57	Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?. *Angewandte Chemie - International Edition*, **2008**, 47, 8148-8148	16.4	4
56	Die Chemie eine zentrale Sule der menschlichen Kultur. *Angewandte Chemie*, **2003**, 115, 3326-3333	3.6	4
55	Chameleon States: High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analogue The research in HU was sponsored by the Binational German Israeli Foundation (GIF) and by the Israeli Ministry of Science, Culture and Sport. Partial support by the US National Science Foundation (CHE-9811301) to J.T.G. is acknowledged. E.G. thanks the EU for a Marie Curie	16.4	4
54	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
53	The catalytic cycle of cytochrome P450: a fascinating choreography. *Trends in Chemistry*, **2021**,	14.8	4
52	A Conversation on New Types of Chemical Bonds. *Israel Journal of Chemistry*,	3.4	4
51	External Electric Fields Interrupt the Concerted Cope Rearrangement of Semibullvalene. *Journal of Organic Chemistry*, **2021**, 86, 731-738	4.2	4
50	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
49	The Experimental Density Perspective of Chemical Bonding **2014**, 309-344		3

48	Magnetic Properties of Aromatic Compounds and Aromatic Transition States **2014**, 383-420		3
47	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
46	L sich die Frage nach der Tendenz des Elektronensystems von Benzol zur Abweichung von der D6h-Symmetrie mit Hilfe von Strukturobservablen beantworten?. *Angewandte Chemie*, **1997**, 109, 2322-2324	3.6	3
45	Silynes (RC?SiR?) and Disilynes (RSi?SiR?): Why Are Less Bonds Worth Energetically More?. *Angewandte Chemie - International Edition*, **2004**, 43, 141-141	16.4	3
44	Silynes (RC?SiR?) and Disilynes (RSi?SiR?): Why Are Less Bonds Worth Energetically More?. *Angewandte Chemie*, **2004**, 116, 143-143	3.6	3
43	Chameleon States: High-Valent Metal Oxo Species of Cytochrome P450 and Its Ruthenium Analogue. *Angewandte Chemie*, **2001**, 113, 3612-3612	3.6	3
42	Zu einer Definition der maximal zul sigen Ann erung von Radikalanion und Alkylhalogenid im bergangszustand der Elektronentransferreaktion. *Angewandte Chemie*, **1996**, 108, 1208-1211	3.6	3
41	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
40	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
39	Comment on "Decoding real space bonding descriptors in valence bond language" by A. Mart Pend and E. Francisco, Phys. Chem. Chem. Phys., 2018, 20, 12368. *Physical Chemistry Chemical Physics*, **2019**, 21, 8170-8174	3.6	2
38	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
37	Hydrogen Bonding **2014**, 501-522		2
36	Directional Electrostatic Bonding **2014**, 523-536		2
35	Chemical Bonding in Open-Shell Transition-Metal Complexes **2014**, 219-252		2
34	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
33	Der angeregte Zwillingszustand als Sonde f r den bergangszustand in konzertierten unimolekularen Reaktionen: die Semibullvalen-Umlagerung. *Angewandte Chemie*, **1998**, 110, 1470-1473	3.6	2
32	Autobiography of Sason Shaik. *Journal of Physical Chemistry A*, **2008**, 112, 12724-36	2.8	2
31	Theoretical Perspective on the Structure and Mechanism of Cytochrome P450 Enzymes. *ChemInform*, **2005**, 36, no		2

30	Nature of the Trigger Linkage in Explosive Materials Is a Charge-Shift Bond. *Journal of Organic Chemistry*, **2021**, 86, 15588-15596	4.2	2
29	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
28	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm		2
27	Valence Bond Diagrams and Chemical Reactivity **1999**, 38, 586		2
26	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. *Angewandte Chemie*, **2019**, 131, 12460-12466	3.6	1
25	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
24	Electron-Counting Rules in Cluster Bonding Polyhedral Boranes, Elemental Boron, and Boron-Rich Solids **2014**, 113-148		1
23	Multiple Bonding of Heavy Main-Group Atoms **2014**, 25-48		1
22	Chemical Bonding in Inorganic Aromatic Compounds **2014**, 421-444		1
21	Mechanism of Oxidation Reactions Catalyzed by Cytochrome P450 Enzyme. *ChemInform*, **2004**, 35, no		1
20	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
19	Mechanistic Conundrum of C Bond Cleavage by CYP51. *ACS Catalysis*, **2022**, 12, 5673-5683	13.1	1
18	The Role of Recoupled Pair Bonding in Hypervalent Molecules **2014**, 49-70		0
17	Helmut Schwarz A story of science and friendship. *International Journal of Mass Spectrometry*, **2019**, 435, 151-162	1.9	0
16	Chemical Bonding of Lanthanides and Actinides **2014**, 337-356		
15	Chemical Bonding in Solids **2014**, 445-476		
14	Bound Triplet Pairs in the Highest Spin States of Monovalent Metal Clusters **2014**, 149-174		
13	The Quantum Chemistry of Transition Metal Surface Bonding and Reactivity **2014**, 269-336		

12	What is Chemistry? Von Peter Atkins.. *Angewandte Chemie*, **2014**, 126, 5104-5106	3.6
11	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
10	Reply to 'entropic factors also contribute to the high melting points of polyhedral alkanes'. *Nature Chemistry*, **2015**, 7, 89-90	17.6
9	Modern Ab Initio Valence Bond Methods **2011**, 201-235	
8	Computational Inorganic and Bioinorganic Chemistry. Herausgegeben von Edward I. Solomon, Robert A. Scott und R. Bruce King.. *Angewandte Chemie*, **2010**, 122, 3177-3179	3.6
7	Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?. *Angewandte Chemie*, **2008**, 120, 8267-8267	3.6
6	The High-Valent Compound of Cytochrome P450: The Nature of the Fe□ Bond and the Role of the Thiolate Ligand as an Internal Electron Donor. *Angewandte Chemie*, **2001**, 113, 667-667	3.6
5	Computational Catalysis: A Land of Opportunities. *Topics in Catalysis*, **2022**, 65, 1-5	2.3
4	Na???B Bond in NaBH3□Solving the Conundrum. *Angewandte Chemie*, **2021**, 133, 12833-12836	3.6
3	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
2	Understanding Valence Bond Theory **2022**,	
1	Bridging Conceptual Density Functional and Valence Bond Theories **2022**, 391-415	