Yirong Mo

List of Publications by Year in Descending Order

180 papers	6,550 citations	44 h-index	75 g-index
190 ext. papers	7,087 ext. citations	5.2 avg, IF	6.19 L-index

#	Paper	IF	Citations
180	The Block-Localized Wavefunction (BLW) Method and Its Applications **2022**,		
179	Computational Study of CO Reduction Catalyzed by Iron(I) Complex at Different Spin States: Cooperativity of Hydrogen Bonding and Auxiliary Group Effect. *ACS Omega*, **2021**, 6, 31971-31981	3.9	
178	Inter-anion chalcogen bonds: Are they anti-electrostatic in nature?. *Journal of Chemical Physics*, **2021**, 155, 234302	3.9	1
177	Classical Electrostatics Remains the Driving Force for Interanion Hydrogen and Halogen Bonding. *Journal of Physical Chemistry A*, **2021**, 125, 10428-10438	2.8	1
176	Role of Charge Transfer in Halogen Bonding. *Journal of Physical Chemistry A*, **2021**, 125, 2944-2953	2.8	9
175	Resonance-Assisted but Antielectrostatic Intramolecular Au□H-O Hydrogen Bonding in Gold(I) Complexes: A Computational Verification. *Inorganic Chemistry*, **2021**, 60, 460-467	5.1	4
174	Metalloradical complex Co-CPh3 catalyzes the CO reduction in gas phase: a theoretical study. *Physical Chemistry Chemical Physics*, **2021**, 23, 1392-1400	3.6	
173	Rational design of porous organic molecules (POMs) based on B-heterocyclic carbenes. *Molecular Systems Design and Engineering*, **2021**, 6, 132-138	4.6	1
172	Planar Tetracoordinate Silicon in Organic Molecules As Carbenoid-Type Amphoteric Centers: A Computational Study. *Chemistry - A European Journal*, **2021**, 27, 1402-1409	4.8	6
171	Molecular magnetism in nanodomains of isoreticular MIL-88(Fe)-MOFs. *Physical Chemistry Chemical Physics*, **2021**, 23, 21677-21689	3.6	0
170	Anti-Electrostatic Main Group Metal-Metal Bonds That Activate CO. *Journal of Physical Chemistry Letters*, **2021**, 12, 7545-7552	6.4	1
169	Hydrogen and Halogen Bonding in Homogeneous External Electric Fields: Modulating the Bond Strengths. *Chemistry - A European Journal*, **2021**, 27, 14042-14050	4.8	2
168	A theoretical perspective of the agostic effect in early transition metal compounds. *Coordination Chemistry Reviews*, **2020**, 419, 213401	23.2	20
167	Electride-Sponsored Radical-Controlled CO Reduction to Organic Acids: A Computational Design. *Chemistry - A European Journal*, **2020**, 26, 6234-6239	4.8	1
166	Two Push-Pull Channels Enhance the Dinitrogen Activation by Borylene Compounds. *Chemistry - A European Journal*, **2020**, 26, 2520	4.8	
165	Two Push-Pull Channels Enhance the Dinitrogen Activation by Borylene Compounds. *Chemistry - A European Journal*, **2020**, 26, 2619-2625	4.8	15
164	Resonance-assisted/impaired anion-□nteraction: towards the design of novel anion receptors.. *RSC Advances*, **2020**, 10, 36181-36191	3.7	3

163	Explaining the Variations in Isotopic Ratios in Meteoritic Amino Acids. *Astrobiology*, **2020**, 20, 964-976	3.7	0
162	Side-On versus End-On Binding Modes between Metal Cations and (NHC)AlAl(NHC). *Organometallics*, **2020**, 39, 3240-3249	3.8	0
161	Bonding and Diels–Alder reactions of substituted 2-borabicyclo(1.1.0)but-1(3)-enes: a theoretical study. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	4
160	Astrophysical Sites that Can Produce Enantiomeric Amino Acids. *Symmetry*, **2019**, 11, 23	2.7	5
159	Tetrel bonding interaction: an analysis with the block-localized wavefunction (BLW) approach. *Physical Chemistry Chemical Physics*, **2019**, 21, 11776-11784	3.6	11
158	Classical Electrostatic Interaction Is the Origin for Blue-Shifting Halogen Bonds. *Inorganic Chemistry* , **2019**, 58, 8577-8586	5.1	6
157	Agostic Interactions in Early Transition-Metal Complexes: Roles of Hyperconjugation, Dispersion, and Steric Effect. *Chemistry - A European Journal*, **2019**, 25, 6591-6599	4.8	7
156	A strong dependence of the CH internal rotation barrier on conformation in thioacetic acid: Microwave measurements and an energy decomposition analysis. *Journal of Chemical Physics*, **2019**, 150, 134302	3.9	4
155	Single-handed supramolecular double helix of homochiral bis(N-amidothiourea) supported by double crossed C-I⋯S halogen bonds. *Nature Communications*, **2019**, 10, 3610	17.4	29
154	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
153	How Resonance Modulates Multiple Hydrogen Bonding in Self-Assembled Systems. *Journal of Organic Chemistry*, **2019**, 84, 14805-14815	4.2	7
152	Performance of the VBSCF method for pericyclic and σ-bond shift reactions. *Journal of Computational Chemistry*, **2019**, 40, 1123-1129	3.5	2
151	Attraction between electrophilic caps: A counterintuitive case of noncovalent interactions. *Journal of Computational Chemistry*, **2019**, 40, 1015-1022	3.5	12
150	B-Heterocyclic Carbene Arising from Charge Shift: A Computational Verification. *Chemistry - A European Journal*, **2018**, 24, 10216	4.8	5
149	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
148	The Transition-Metal-Like Behavior of B (NHC) in the Activation of CO: HOMO-LUMO Swap Without Photoinduction. *Angewandte Chemie - International Edition*, **2018**, 57, 13076-13081	16.4	19
147	Tautomerism of protonated imidazoles: A perspective from ab initio valence bond theory. *Tetrahedron*, **2018**, 74, 4791-4798	2.4	6
146	The Transition-Metal-Like Behavior of B2(NHC)2 in the Activation of CO: HOMO–LUMO Swap Without Photoinduction. *Angewandte Chemie*, **2018**, 130, 13260-13265	3.6	2

145	Amino Acid Chiral Selection Via Weak Interactions in Stellar Environments: Implications for the Origin of Life. *Scientific Reports*, **2018**, 8, 8833	4.9	11
144	A Direct Proof of the Resonance-Impaired Hydrogen Bond (RIHB) Concept. *Chemistry - A European Journal*, **2018**, 24, 1053-1056	4.8	11
143	Induction, Resonance, and Secondary Electrostatic Interaction on Hydrogen Bonding in the Association of Amides and Imides. *Journal of Organic Chemistry*, **2018**, 83, 13446-13453	4.2	8
142	Role of Intramolecular Electron Delocalization in the C-X Bond Strength in CHX (n = 0-4, X = F, Cl, CN, OCH). *Journal of Physical Chemistry A*, **2018**, 122, 7716-7722	2.8	5
141	C-I Halogen Bonding Driven Supramolecular Helix of Bilateral N-Amidothioureas Bearing Turns. *Journal of the American Chemical Society*, **2017**, 139, 6605-6610	16.4	70
140	Study of proton-coupled electron transfer (PCET) with four explicit diabatic states at the ab initio level. *Computational and Theoretical Chemistry*, **2017**, 1116, 50-58	2	10
139	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
138	Halogen Bonds in Novel Polyhalogen Monoanions. *Chemistry - A European Journal*, **2017**, 23, 8719-8728	4.8	10
137	Product release mechanism and the complete enzyme catalysis cycle in yeast cytosine deaminase (yCD): A computational study. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2017**, 1865, 1020-1029	4	6
136	The Origin of the Non-Additivity in Resonance-Assisted Hydrogen Bond Systems. *Journal of Physical Chemistry A*, **2017**, 121, 8535-8541	2.8	21
135	A Critical Check for the Role of Resonance in Intramolecular Hydrogen Bonding. *Chemistry - A European Journal*, **2017**, 23, 16885-16891	4.8	28
134	Adjacent Lone Pair (ALP) Effect: A Computational Approach for Its Origin. *Chemistry - A European Journal*, **2016**, 22, 7305-7305	4.8	
133	Drastic Deprotonation Reactivity Difference of 3- and 5-Alkylpyrazole Isomers, Their I2-Catalyzed Thermal Isomerization, and Telescoping Synthesis of 3,5-Dialkylpyrazoles: The "Adjacent Lone Pair Effect" Demystified. *Journal of Organic Chemistry*, **2016**, 81, 1718-22	4.2	6
132	Electron conjugation versus repulsion in substituted benzenes: why the carbon-nitrogen bond in nitrobenzene is longer than in aniline. *Physical Chemistry Chemical Physics*, **2016**, 18, 11821-8	3.6	23
131	Combined QM(DFT)/MM molecular dynamics simulations of the deamination of cytosine by yeast cytosine deaminase (yCD). *Journal of Computational Chemistry*, **2016**, 37, 1163-74	3.5	9
130	Adjacent Lone Pair (ALP) Effect: A Computational Approach for Its Origin. *Chemistry - A European Journal*, **2016**, 22, 7415-21	4.8	9
129	Mechanisms for the deamination reaction of 8-oxoguanine catalyzed by 8-oxoguanine deaminase: A combined QM/MM molecular dynamics study. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650066	1.8	1
128	The origins of the directionality of noncovalent intermolecular interactions. *Journal of Computational Chemistry*, **2016**, 37, 34-45	3.5	49

127	Intramolecular multi-bond strain: the unrecognized side of the dichotomy of conjugated systems. *Chemical Science*, **2016**, 7, 5872-5878	9.4	6
126	Why Do Enolate Anions Favor O-Alkylation over C-Alkylation in the Gas Phase? The Roles of Resonance and Inductive Effects in the Gas-Phase SN2 Reaction between the Acetaldehyde Enolate Anion and Methyl Fluoride. *Journal of Organic Chemistry*, **2016**, 81, 3711-9	4.2	7
125	Red-Shifting versus Blue-Shifting Hydrogen Bonds: Perspective from Ab Initio Valence Bond Theory. *Journal of Physical Chemistry A*, **2016**, 120, 2749-56	2.8	44
124	Protonation-Triggered Carbon-Chain Elongation in Geranyl Pyrophosphate Synthase (GPPS). *ACS Catalysis*, **2015**, 5, 4466-4478	13.1	12
123	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
122	Proton-Shuttle-Assisted Heterolytic Carbon□Carbon Bond Cleavage and Formation. *ACS Catalysis*, **2015**, 5, 2805-2813	13.1	10
121	Why is sulfuric acid a much stronger acid than ethanol? Determination of the contributions by inductive/field effects and electron-delocalization effects. *Physical Chemistry Chemical Physics*, **2015**, 17, 138-44	3.6	5
120	Electron transfer in pnicogen bonds. *Journal of Physical Chemistry A*, **2014**, 118, 8911-21	2.8	59
119	On the nature of blueshifting hydrogen bonds. *Chemistry - A European Journal*, **2014**, 20, 8444-52	4.8	36
118	How solvent influences the anomeric effect: roles of hyperconjugative versus steric interactions on the conformational preference. *Journal of Organic Chemistry*, **2014**, 79, 1571-81	4.2	27
117	Metal-binding studies of linear rigid-axle [2]pseudorotaxanes with in situ generated anionic metal halide complexes. *CrystEngComm*, **2014**, 16, 7320	3.3	6
116	Redox-active gold nanoclusters immobilized ZnO nanorod electrodes for electrochemical sensing applications. *RSC Advances*, **2014**, 4, 10766-10769	3.7	12
115	On the large □hyperconjugation in alkanes and alkenes. *Journal of Molecular Modeling*, **2014**, 20, 2228	2	7
114	On The Nature of the Halogen Bond. *Journal of Chemical Theory and Computation*, **2014**, 10, 3726-37	6.4	194
113	Deprotonation of methyl-substituted, five-membered aromatic molecules: a surprising case of mixed conjugation, rehybridization, and induction contributions. *Organic Letters*, **2014**, 16, 4680-3	6.2	8
112	The Block-Localized Wavefunction (BLW) Perspective of Chemical Bonding **2014**, 199-232		15
111	A full picture of enzymatic catalysis by hydroxynitrile lyases from Hevea brasiliensis: protonation dependent reaction steps and residue-gated movement of the substrate and the product. *Physical Chemistry Chemical Physics*, **2014**, 16, 26864-75	3.6	11
110	Two states are not enough: quantitative evaluation of the valence-bond intramolecular charge-transfer model and its use in predicting bond length alternation effects. *Chemistry - A European Journal*, **2014**, 20, 17214-21	4.8	13

109	Direct evaluation of the hyperconjugative interactions in 1,1,1-trihaloethane (CH3CX3, X = F, Cl, and Br). *Journal of Physical Chemistry A*, **2014**, 118, 5743-7	2.8	7
108	Electron Transfer in Electrophilic Aromatic Nitration and Nitrosation: Computational Evidence for the Marcus Inverted Region. *Journal of Chemical Theory and Computation*, **2013**, 9, 4428-35	6.4	16
107	How the generalized anomeric effect influences the conformational preference. *Chemistry - A European Journal*, **2013**, 19, 1436-44	4.8	35
106	Elucidation of the Forces Governing the Stereochemistry of Biphenyl. *European Journal of Organic Chemistry*, **2013**, 2013, 611-616	3.2	21
105	Effects of a remote binding partner on the electric field and electric field gradient at an atom in a weakly bound trimer. *Journal of Chemical Physics*, **2013**, 139, 034320	3.9	3
104	In silico identification of EGFR-T790M inhibitors with novel scaffolds: start with extraction of common features. *Drug Design, Development and Therapy*, **2013**, 7, 789-839	4.4	12
103	Reply to comment on the paper An efficient Algorithm for Energy Gradients and Orbital Optimization in Valence Bond Theory *Journal of Computational Chemistry*, **2012**, 33, 914-915	3.5	
102	The generalized block-localized wavefunction method: a case study on the conformational preference and C-O rotational barrier of formic acid. *Journal of Chemical Physics*, **2012**, 136, 144315	3.9	9
101	Block-Localized Wavefunction (BLW) Based Two-State Approach for Charge Transfers between Phenyl Rings. *Journal of Chemical Theory and Computation*, **2012**, 8, 800-5	6.4	21
100	Origin of the SN2 Benzylic Effect: Contributions by Delocalization and Field/Inductive Effects. *European Journal of Organic Chemistry*, **2012**, 2012, 5991-6004	3.2	10
99	Why Cyclooctatetraene Is Highly Stabilized: The Importance of "Two-Way" (Double) Hyperconjugation. *Journal of Chemical Theory and Computation*, **2012**, 8, 1280-7	6.4	47
98	Is cyclobutadiene really highly destabilized by antiaromaticity?. *Chemical Communications*, **2012**, 48, 8437-9	5.9	60
97	Can QTAIM topological parameters be a measure of hydrogen bonding strength?. *Journal of Physical Chemistry A*, **2012**, 116, 5240-6	2.8	51
96	Correlation between biological activity and binding energy in systems of integrin with cyclic RGD-containing binders: a QM/MM molecular dynamics study. *Journal of Molecular Modeling*, **2012**, 18, 4917-27	2	9
95	Computer-aided drug design: lead discovery and optimization. *Combinatorial Chemistry and High Throughput Screening*, **2012**, 15, 328-37	1.3	43
94	The norbornene mystery revealed. *Chemical Communications*, **2011**, 47, 227-9	5.8	20
93	How do electron localization functions describe electron delocalization?. *Physical Chemistry Chemical Physics*, **2011**, 13, 20584-92	3.6	62
92	Energy decomposition analysis based on a block-localized wavefunction and multistate density functional theory. *Physical Chemistry Chemical Physics*, **2011**, 13, 6760-75	3.6	171

91	Rotational barriers in alkanes. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 164-171	7.9	34
90	Steric and electronic effects on the heterolytic H2-splitting by phosphine-boranes R3B/PR?3 (R = C6F5, Ph; R? = C6H2Me3, tBu, Ph, C6F5, Me, H): A computational study. *International Journal of Quantum Chemistry*, **2011**, 111, 3761-3775	2.1	10
89	Sensing or no sensing: can the anomeric effect be probed by a sensing molecule?. *Journal of the American Chemical Society*, **2011**, 133, 13731-6	16.4	34
88	Dispersion-corrected energy decomposition analysis for intermolecular interactions based on the BLW and dDXDM methods. *Journal of Physical Chemistry A*, **2011**, 115, 5467-77	2.8	38
87	Computational evidence that hyperconjugative interactions are not responsible for the anomeric effect. *Nature Chemistry*, **2010**, 2, 666-71	17.6	158
86	A simple preparation of 2,3,4,6-tetra-o-acyl-gluco-, galacto- and mannopyranoses and relevant theoretical study. *Molecules*, **2010**, 15, 374-84	4.8	5
85	Generalized X-Pol Theory and Charge Delocalization States. *Journal of Chemical Theory and Computation*, **2010**, 6, 2402-10	6.4	23
84	A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions. *Journal of Chemical Theory and Computation*, **2010**, 6, 2242-2251	6.4	16
83	A critical analysis on the rotation barriers in butane. *Journal of Organic Chemistry*, **2010**, 75, 2733-6	4.2	32
82	Insight into the relative reactivity of "frustrated Lewis pairs" and stable carbenes in activating H2 and CH4: a comparative computational study. *Physical Chemistry Chemical Physics*, **2010**, 12, 5268-75	3.6	41
81	How to properly compute the resonance energy within the ab initio valence bond theory: a response to the ZHJVL paper. *Theoretical Chemistry Accounts*, **2010**, 127, 27-38	1.9	44
80	Transport Mechanism in the Escherichia coli Ammonia Channel AmtB: A Computational Study. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 397-429	0.7	
79	Is cyclopropane really the sigma-aromatic paradigm?. *Chemistry - A European Journal*, **2009**, 15, 9730-6	4.8	52
78	An efficient algorithm for energy gradients and orbital optimization in valence bond theory. *Journal of Computational Chemistry*, **2009**, 30, 399-406	3.5	47
77	Molecular dynamics simulations of the detoxification of paraoxon catalyzed by phosphotriesterase. *Journal of Computational Chemistry*, **2009**, 30, 2388-401	3.5	33
76	Direct assessment of electron delocalization using NMR chemical shifts. *Angewandte Chemie - International Edition*, **2009**, 48, 9828-33	16.4	46
75	Why are esters and amides weaker carbon acids than ketones and Acid fluorides? Contributions by resonance and inductive effects. *Journal of Organic Chemistry*, **2009**, 74, 7245-53	4.2	17
74	The contributions of through-bond interactions to the singlet-triplet energy difference in 1,3-dehydrobenzene. *Journal of Physical Chemistry A*, **2009**, 113, 10351-8	2.8	12

73	4n pi electrons but stable: N,N-dihydrodiazapentacenes. *Journal of Organic Chemistry*, **2009**, 74, 4343-9	4.2	71
72	Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. *Journal of Chemical Theory and Computation*, **2009**, 5, 2702-2716	6.4	91
71	Broad substrate specificity and catalytic mechanism of Pseudomonas stutzeri L-rhamnose isomerase: insights from QM/MM molecular dynamics simulations. *Journal of Physical Chemistry A*, **2009**, 113, 11595-603	2.8	7
70	The resonance energy of benzene: a revisit. *Journal of Physical Chemistry A*, **2009**, 113, 5163-9	2.8	37
69	An Effective Hamiltonian Molecular Orbital-Valence Bond (MOVB) Approach for Chemical Reactions Applied to the Nucleophilic Substitution Reaction of Hydrosulfide Ion and Chloromethane. *Journal of Chemical Theory and Computation*, **2009**, 5, 174-185	6.4	21
68	Functional role of Asp160 and the deprotonation mechanism of ammonium in the Escherichia coli ammonia channel protein AmtB. *Journal of Physical Chemistry B*, **2009**, 113, 4922-9	3.4	16
67	The B-H...H-P dihydrogen bonding in ion pair complexes [(CF(3))(3)BH(-)][HPH(3-n)(Me)(n)(+)] (n = 0-3) and its implication in H(2) elimination and activation reactions. *Journal of Physical Chemistry A*, **2009**, 113, 8108-17	2.8	41
66	Combined quantum mechanics/molecular mechanics study on the reversible isomerization of glucose and fructose catalyzed by Pyrococcus furiosus phosphoglucose isomerase. *Journal of the American Chemical Society*, **2008**, 130, 7022-31	16.4	27
65	BLOCK-LOCALIZED WAVEFUNCTION ENERGY DECOMPOSITION (BLW-ED) ANALYSIS OF π INTERACTIONS IN METAL-CARBONYL BONDING. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 639-654	1.8	20
64	COMPUTATIONAL CHARACTERIZATION OF THE ELUSIVE C-CLUSTER OF CARBON MONOXIDE DEHYDROGENASE. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 473-484	1.8	4
63	Block-localized wavefunction (BLW) method at the density functional theory (DFT) level. *Journal of Physical Chemistry A*, **2007**, 111, 8291-301	2.8	218
62	The concept of protobranching and its many paradigm shifting implications for energy evaluations. *Chemistry - A European Journal*, **2007**, 13, 7731-44	4.8	173
61	Deprotonation mechanism of NH4+ in the Escherichia coli ammonium transporter AmtB: insight from QM and QM/MM calculations. *Angewandte Chemie - International Edition*, **2007**, 46, 6811-5	16.4	25
60	Deprotonation Mechanism of NH4+ in the Escherichia coli Ammonium Transporter AmtB: Insight from QM and QM/MM Calculations. *Angewandte Chemie*, **2007**, 119, 6935-6939	3.6	4
59	How resonance assists hydrogen bonding interactions: an energy decomposition analysis. *Journal of Computational Chemistry*, **2007**, 28, 455-66	3.5	85
58	Two-state model based on the block-localized wave function method. *Journal of Chemical Physics*, **2007**, 126, 224104	3.9	17
57	Theoretical analysis of the rotational barrier of ethane. *Accounts of Chemical Research*, **2007**, 40, 113-9	24.3	159
56	An energetic measure of aromaticity and antiaromaticity based on the Pauling-Wheland resonance energies. *Chemistry - A European Journal*, **2006**, 12, 2009-20	4.8	130

55	Molecular dynamics simulations on the Escherichia coli ammonia channel protein AmtB: mechanism of ammonia/ammonium transport. *Journal of the American Chemical Society*, **2006**, 128, 10876-84	16.4	67
54	Why is the linking C-C bond in tetrahedranyltetrahedrane so short?. *Organic Letters*, **2006**, 8, 535-8	6.2	15
53	Polarization and charge-transfer effects in aqueous solution via ab initio QM/MM simulations. *Journal of Physical Chemistry B*, **2006**, 110, 2976-80	3.4	46
52	Amine-hydrogen halide complexes: experimental electric dipole moments and a theoretical decomposition of dipole moments and binding energies. *Journal of Physical Chemistry A*, **2006**, 110, 10025-34	2.8	23
51	Intramolecular Electron Transfer: Computational Study Based on the Orbital Deletion Procedure (ODP). *Current Organic Chemistry*, **2006**, 10, 779-790	1.7	12
50	Probing the nature of hydrogen bonds in DNA base pairs. *Journal of Molecular Modeling*, **2006**, 12, 665-72	2	61
49	Origins of Rotational Barriers in Hydrogen Peroxide and Hydrazine. *Journal of Chemical Theory and Computation*, **2005**, 1, 394-402	6.4	31
48	Steric strain versus hyperconjugative stabilization in ethane congeners. *Journal of Physical Chemistry A*, **2005**, 109, 2310-6	2.8	43
47	Y-aromaticity: why is the trimethylenemethane dication more stable than the butadienyl dication?. *Journal of Organic Chemistry*, **2005**, 70, 7605-16	4.2	24
46	Density functional study on dihydrogen activation at the H cluster in Fe-only hydrogenases. *Inorganic Chemistry*, **2005**, 44, 4941-6	5.1	28
45	XMVB: a program for ab initio nonorthogonal valence bond computations. *Journal of Computational Chemistry*, **2005**, 26, 514-21	3.5	187
44	Doping and Undoping of OH[sup]during Redox Processes of Poly(vinyl ferrocene). *Journal of the Electrochemical Society*, **2005**, 152, E94	3.9	6
43	Resonance effect in the allyl cation and anion: a revisit. *Journal of Organic Chemistry*, **2004**, 69, 5563-7	4.2	38
42	Applications of graphic method to C20, C60, and achiral single-wall nanotubes. *International Journal of Quantum Chemistry*, **2004**, 98, 51-58	2.1	1
41	The magnitude of hyperconjugation in ethane: a perspective from ab initio valence bond theory. *Angewandte Chemie - International Edition*, **2004**, 43, 1986-90	16.4	131
40	The Magnitude of Hyperconjugation in Ethane: A Perspective from Ab Initio Valence Bond Theory. *Angewandte Chemie*, **2004**, 116, 2020-2024	3.6	45
39	Studies of Solvation Free Energies of Methylammoniums and Irregular Basicity Ordering of Methylamines in Aqueous Solution by a Combined Discrete-Continuum Model. *Journal of Physical Chemistry A*, **2004**, 108, 4277-4282	2.8	22
38	Enzymatic mechanism of Fe-only hydrogenase: density functional study on H-H making/breaking at the diiron cluster with concerted proton and electron transfers. *Inorganic Chemistry*, **2004**, 43, 923-30	5.1	65

37	Hyperconjugation effect in substituted methyl boranes: an orbital deletion procedure analysis. *Journal of Organic Chemistry*, **2004**, 69, 3493-9	4.2	22
36	Charge transfer in the electron donor-acceptor complex BH3NH3. *Journal of the American Chemical Society*, **2004**, 126, 3974-82	16.4	87
35	Importance of Electronic Delocalization on the C□N Bond Rotation in HCX(NH2) (X = O, NH, CH2, S, and Se). *Journal of Physical Chemistry A*, **2003**, 107, 10011-10018	2.8	59
34	Geometrical optimization for strictly localized structures. *Journal of Chemical Physics*, **2003**, 119, 1300-1306	3.9	93
33	Study of intramolecular electron transfer with a two-state model based on the orbital deletion procedure. *Journal of Chemical Physics*, **2003**, 119, 6448-6456	3.9	18
32	ELECTRONIC DELOCALIZATION: A QUANTITATIVE STUDY FROM MODERN AB INITIO VALENCE BOND THEORY. *Journal of Theoretical and Computational Chemistry*, **2002**, 01, 137-151	1.8	21
31	A spin□free approach for valence bond theory and its applications. *Theoretical and Computational Chemistry*, **2002**, 143-185		33
30	Cation-pi interactions: an energy decomposition analysis and its implication in delta-opioid receptor-ligand binding. *Journal of the American Chemical Society*, **2002**, 124, 4832-7	16.4	129
29	Paired-permanent approach for VB theory (II). *Science in China Series B: Chemistry*, **2001**, 44, 561-570		4
28	Polarization and Charge-Transfer Effects in Lewis Acid□Base Complexes. *Journal of Physical Chemistry A*, **2001**, 105, 6530-6536	2.8	79
27	New insight on the origin of the unusual acidity of Meldrum's acid from ab initio and combined QM/MM simulation study. *Journal of the American Chemical Society*, **2001**, 123, 3974-9	16.4	78
26	Ab initio QM/MM simulations with a molecular orbital-valence bond (MOVB) method: application to an SN2 reaction in water. *Journal of Computational Chemistry*, **2000**, 21, 1458-1469	3.5	137
25	Sequential Mechanism of Methane Dehydrogenation over Metal (Mo or W) Oxide and Carbide Catalysts. *Journal of Physical Chemistry A*, **2000**, 104, 4505-4513	2.8	22
24	An Ab Initio Molecular Orbital□Valence Bond (MOVB) Method for Simulating Chemical Reactions in Solution. *Journal of Physical Chemistry A*, **2000**, 104, 3012-3020	2.8	116
23	Energy decomposition analysis of intermolecular interactions using a block-localized wave function approach. *Journal of Chemical Physics*, **2000**, 112, 5530-5538	3.9	312
22	Ab initio QM/MM simulations with a molecular orbital-valence bond (MOVB) method: application to an SN2 reaction in water **2000**, 21, 1458		8
21	Theoretical analysis of the internal rotation in aminoborane and borylphosphine. *Theoretical Chemistry Accounts*, **1999**, 101, 311-318	1.9	10
20	Orbital deletion procedure and its applications. *Science in China Series B: Chemistry*, **1999**, 42, 253-260		2

19	A new theory for symmetry orbital and tensor (II). *Science in China Series B: Chemistry*, **1999**, 42, 34-42		
18	General method for symmetry orbitals and tensors in electronic structure calculations. *Journal of Computational Chemistry*, **1999**, 20, 305-321	3.5	
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