Shu-Hua Li

List of Publications by Year
in descending order

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232 papers	8,916 citations	41344 49 h-index	56724 83 g-index
248 all docs	248 docs citations	248 times ranked	7655 citing authors

#	Article	IF	Citations
1	Generalized Energy-Based Fragmentation Approach for Computing the Ground-State Energies and Properties of Large Molecules. Journal of Physical Chemistry A, 2007, 111, 2193-2199.	2.5	254
2	Temperature Controlled Reversible Change of the Coordination Modes of the Highly Symmetrical Multitopic Ligand To Construct Coordination Assemblies: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2008, 130, 7778-7779.	13.7	254
3	Targeted tumour theranostics in mice via carbon quantum dots structurally mimicking large amino acids. Nature Biomedical Engineering, 2020, 4, 704-716.	22.5	243
4	Raman scattering study of zinc blende and wurtzite ZnS. Journal of Applied Physics, 2009, 106, .	2.5	235
5	A Large Protonated Water Cluster H+(H2O)27in a 3D Metalâ^'Organic Framework. Journal of the American Chemical Society, 2006, 128, 13318-13319.	13.7	218
6	An Efficient Fragment-Based Approach for Predicting the Ground-State Energies and Structures of Large Molecules. Journal of the American Chemical Society, 2005, 127, 7215-7226.	13.7	208
7	A Time-Dependent DFT Study on Band Gaps and Effective Conjugation Lengths of Polyacetylene, Polyphenylene, Polypentafulvene, Polycyclopentadiene, Polypyrrole, Polyfuran, Polysilole, Polyphosphole, and Polythiophene. Macromolecules, 2002, 35, 1109-1115.	4.8	205
8	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	3.0	199
9	Linear scaling local correlation approach for solving the coupled cluster equations of large systems. Journal of Computational Chemistry, 2002, 23, 237-244.	3.3	181
10	Visibleâ€Light Photoredoxâ€Catalyzed Câ^'H Difluoroalkylation of Hydrazones through an Aminyl Radical/Polar Mechanism. Angewandte Chemie - International Edition, 2016, 55, 2939-2943.	13.8	176
11	High and selective CO2 capture by two mesoporous acylamide-functionalized rht-type metalâ€“organic frameworks. Chemical Communications, 2012, 48, 7025.	4.1	174
12	Highly selective CO2 capture of an agw-type metalâ€“organic framework with inserted amides: experimental and theoretical studies. Chemical Communications, 2012, 48, 3058.	4.1	166
13	Selective Câ^'N Borylation of Alkyl Amines Promoted by Lewis Base. Angewandte Chemie - International Edition, 2018, 57, 15227-15231.	13.8	166
14	Generalized Energy-Based Fragmentation Approach and Its Applications to Macromolecules and Molecular Aggregates. Accounts of Chemical Research, 2014, 47, 2712-2720.	15.6	143
15	Homolytic Cleavage of a Bâ^'B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. Angewandte Chemie - International Edition, 2016, 55, 5985-5989.	13.8	143
16	Finely tuning MOFs towards high performance in C₂H₂ storage: synthesis and properties of a new MOF-505 analogue with an inserted amide functional group. Chemical Communications, 2016, 52, 7241-7244.	4.1	131
17	An efficient implementation of the â€œcluster-in-moleculeâ€•approach for local electron correlation calculations. Journal of Chemical Physics, 2006, 125, 074109.	3.0	126
18	Unusual Concerted Lewis Acidâ^'Lewis Base Mechanism for Hydrogen Activation by a Phosphineâ^'Borane Compound. Inorganic Chemistry, 2008, 47, 6212-6219.	4.0	123

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19	Geometry Optimizations and Vibrational Spectra of Large Molecules from a Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2008, 112, 10864-10872.	2.5	121
20	Metal-Free Synthesis of C-4 Substituted Pyridine Derivatives Using Pyridine-boryl Radicals via a Radical Addition/Coupling Mechanism: A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2017, 139, 3904-3910.	13.7	108
21	Cooperative Au/Ag Dual-Catalyzed Cross-Dehydrogenative Biaryl Coupling: Reaction Development and Mechanistic Insight. Journal of the American Chemical Society, 2019, 141, 3187-3197.	13.7	101
22	Divide-and-conquer local correlation approach to the correlation energy of large molecules. Journal of Chemical Physics, 2004, 121, 6649-6657.	3.0	95
23	Ab initiostudy on deactivation pathways of excited 9H-guanine. Journal of Chemical Physics, 2006, 124, 154315.	3.0	93
24	A Smart Supramolecular Hydrogel Exhibiting pH-Modulated Viscoelastic Properties. Advanced Functional Materials, 2007, 17, 1837-1843.	14.9	91
25	An Efficient Implementation of the Generalized Energy-Based Fragmentation Approach for General Large Molecules. Journal of Physical Chemistry A, 2010, 114, 8126-8134.	2.5	91
26	Theoretical Study toward Understanding Ultrafast Internal Conversion of Excited 9H-Adenine. Journal of Physical Chemistry A, 2005, 109, 8443-8446.	2.5	87
27	Regulating Circularly Polarized Luminescence Signals of Chiral Binaphthyl-Based Conjugated Polymers by Tuning Dihedral Angles of Binaphthyl Moieties. Macromolecules, 2016, 49, 5444-5451.	4.8	86
28	A Novel Addition Mechanism for the Reaction of â€œFrustrated Lewis Pairsâ€•with Olefins. European Journal of Inorganic Chemistry, 2008, 2008, 2501-2505.	2.0	85
29	Perfluoroalkylative pyridylation of alkenesvia4-cyanopyridine-boryl radicals. Chemical Science, 2019, 10, 2767-2772.	7.4	81
30	IR spectroelectrochemical study of the binding of carbon monoxide to the active site of Desulfovibrio fructosovorans Ni-Fe hydrogenase. Journal of Biological Inorganic Chemistry, 2002, 7, 318-326.	2.6	78
31	X-ray absorption spectra of graphene from first-principles simulations. Physical Review B, 2010, 82, .	3.2	78
32	Sunlight-promoted cyclization versus decarboxylation in the reaction of alkynoates with N-iodosuccinimide: easy access to 3-iodocoumarins. Green Chemistry, 2016, 18, 3935-3939.	9.0	74
33	â€œInverseâ€•Frustrated Lewis Pairs â€“ Activation of Dihydrogen with Organosuperbases and Moderate to Weak Lewis Acids. Journal of the American Chemical Society, 2016, 138, 3286-3289.	13.7	73
34	Insights into Dehydrogenative Coupling of Alcohols and Amines Catalyzed by a (PNN)â€“Ru(II) Hydride Complex: Unusual Metalâ€“Ligand Cooperation. Inorganic Chemistry, 2011, 50, 10572-10580.	4.0	72
35	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H₂O)₂₀. Journal of Chemical Theory and Computation, 2014, 10, 1546-1553.	5.3	62
36	Modeling the Active Sites of Metalloenzymes. 4. Predictions of the Unready States of [NiFe]Desulfovibrio gigasHydrogenase from Density Functional Theory. Inorganic Chemistry, 2001, 40, 18-24.	4.0	61

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37	Block-correlated coupled cluster theory:â€‰The general formulation and its application to the antiferromagnetic Heisenberg model. Journal of Chemical Physics, 2004, 120, 5017-5026.	3.0	61
38	Optical properties of rocksalt and zinc blende AlN phases: First-principles calculations. Journal of Applied Physics, 2008, 103, .	2.5	61
39	Automatic Reaction Pathway Search via Combined Molecular Dynamics and Coordinate Driving Method. Journal of Physical Chemistry A, 2017, 121, 1351-1361.	2.5	61
40	Hantzsch Ester as a Photosensitizer for the Visibleâ€Lightâ€Induced Debromination of Vicinal Dibromo Compounds. Chemistry - A European Journal, 2016, 22, 9546-9550.	3.3	60
41	Dehydrogenation of Methane by Gas-Phase Os+:Â A Density Functional Study. Organometallics, 2003, 22, 3820-3830.	2.3	57
42	LSQC: Low scaling quantum chemistry program. International Journal of Quantum Chemistry, 2015, 115, 641-646.	2.0	57
43	Organocatalytic reductive coupling of aldehydes with 1,1-diarylethylenes using an in situ generated pyridine-boryl radical. Chemical Science, 2018, 9, 3664-3671.	7.4	56
44	Block correlated coupled cluster theory with a complete active-space self-consistent-field reference function: The formulation and test applications for single bond breaking. Journal of Chemical Physics, 2007, 127, 204108.	3.0	54
45	Chemoselective Boraneâ€Catalyzed Hydroarylation of 1,3â€Dienes with Phenols. Angewandte Chemie - International Edition, 2019, 58, 1694-1699.	13.8	54
46	Theoretical Study on the Excitation Energies of Six Tautomers of Guanine:Â Evidence for the Assignment of the Rare Tautomers. Journal of Physical Chemistry A, 2006, 110, 12360-12362.	2.5	53
47	Estimation on the Individual Hydrogen-Bond Strength in Molecules with Multiple Hydrogen Bonds. Journal of Physical Chemistry A, 2007, 111, 2941-2945.	2.5	52
48	A DFT Study toward Understanding the High Activity of Fe-Exchanged Zeolites for the â€œFastâ€•Selective Catalytic Reduction of Nitrogen Oxides with Ammonia. Journal of Physical Chemistry C, 2008, 112, 16938-16944.	3.1	50
49	A refined cluster-in-molecule local correlation approach for predicting the relative energies of large systems. Physical Chemistry Chemical Physics, 2012, 14, 7854.	2.8	50
50	Cluster-in-molecule local correlation method for post-Hartreeâ€“Fock calculations of large systems. Molecular Physics, 2016, 114, 1447-1460.	1.7	50
51	Transitionâ€Metalâ€Free Defluorosilylation of Fluoroalkenes with Silylboronates. Chinese Journal of Chemistry, 2019, 37, 1009-1014.	4.9	49
52	Metal-Induced Bâ‹¯H Bond Activation: Addition of Methyl Acetylene Monocarboxylate to CpCo Half-Sandwich Complexes Containing a Chelating 1,2-Dicarba-closo-dodecaborane-1,2-dichalcogenolate Ligand. Organometallics, 2008, 27, 334-340.	2.3	46
53	Photoredoxâ€Controlled Î²â€Regioselective Radical Hydroboration of Activated Alkenes with NHCâ€Boranes. Angewandte Chemie - International Edition, 2020, 59, 12817-12821.	13.8	46
54	Effects of Substitution on the Singletâ‹¯Triplet Energy Splittings and Ground-State Multiplicities of m-Phenylene-Based Diradicals:â€‰ A Density Functional Theory Study. Journal of Physical Chemistry A, 2003, 107, 5573-5582.	2.5	45

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55	A localized molecular-orbital assembler approach for Hartreeâ€“Fock calculations of large molecules. Journal of Chemical Physics, 2005, 122, 194109.	3.0	45
56	Accurate Prediction of Lattice Energies and Structures of Molecular Crystals with Molecular Quantum Chemistry Methods. Journal of Chemical Theory and Computation, 2015, 11, 91-98.	5.3	45
57	Circularly polarized luminescence based chirality transfer of the chiral BINOL moiety via rigid Ï€-conjugation chain backbone structures. Polymer Chemistry, 2017, 8, 1555-1561.	3.9	45
58	Rh(<scp>iii</scp>)-catalyzed double Câ€“H activation of aldehyde hydrazones: a route for functionalized 1H-indazole synthesis. Chemical Science, 2017, 8, 1303-1308.	7.4	45
59	H2 Activation by a (PNP)Ir(C6H5) Complex via the Dearomatization/Aromatization Process of the PNP Ligand: A Computational Study. Inorganic Chemistry, 2009, 48, 10257-10263.	4.0	43
60	Low-Lying Structures and Stabilities of Large Water Clusters: Investigation Based on the Combination of the AMOEBA Potential and Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2010, 114, 9253-9261.	2.5	43
61	A selenium-catalysed para-amination of phenols. Nature Communications, 2018, 9, 4293.	12.8	43
62	Selective Câ€“N Borylation of Alkyl Amines Promoted by Lewis Base. Angewandte Chemie, 2018, 130, 15447-15451.	2.0	42
63	Organocatalytic decarboxylative alkylation of N-hydroxy-phthalimide esters enabled by pyridine-boryl radicals. Chemical Communications, 2018, 54, 11534-11537.	4.1	42
64	Lewis Acid-Catalyzed Selective Reductive Decarboxylative Pyridylation of N-Hydroxyphthalimide Esters: Synthesis of Congested Pyridine-Substituted Quaternary Carbons. ACS Catalysis, 2019, 9, 10142-10151.	11.2	42
65	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The formula for general active spaces and its applications for multibond breaking systems. Journal of Chemical Physics, 2008, 128, 224107.	3.0	41
66	Block correlated second order perturbation theory with a generalized valence bond reference function. Journal of Chemical Physics, 2013, 139, 174111.	3.0	40
67	Improved Cluster-in-Molecule Local Correlation Approach for Electron Correlation Calculation of Large Systems. Journal of Physical Chemistry A, 2014, 118, 8996-9004.	2.5	40
68	Bond Lengths, Reactivities, and Aromaticities of Benzenoid Hydrocarbons Based on Valence Bond Calculations. Journal of the American Chemical Society, 1995, 117, 8401-8406.	13.7	39
69	A fragment energy assembler method for Hartree-Fock calculations of large molecules. Journal of Chemical Physics, 2006, 124, 154102.	3.0	39
70	Transition Metal Polyhydride Complexes. 10. Intramolecular Hydrogen Exchange in the Octahedral Iridium(III) Dihydrogen Dihydride Complexes IrXH2(Î·2-H2)(PR3)2(X = Cl, Br, I). Journal of the American Chemical Society, 2000, 122, 2903-2910.	13.7	38
71	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 18. Catalytic Transfer Dehydrogenation of Alkanes by an Iridium(III) Pincer Complex. Organometallics, 2001, 20, 2153-2160.	2.3	38
72	Generalized energyâ€based fragmentation approach for modeling condensed phase systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1297.	14.6	38

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73	Tetranuclear manganese(III) clusters containing both carboxylate and phosphonate bridging ligands. Inorganica Chimica Acta, 2007, 360, 1645-1650.	2.4	36
74	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. Accounts of Chemical Research, 2021, 54, 169-181.	15.6	36
75	Cooperativity in Long Î±- and 3₁₀-Helical Polyalanines: Both Electrostatic and van der Waals Interactions Are Essential. Journal of Physical Chemistry B, 2011, 115, 11462-11469.	2.6	35
76	The Generalized Energyâ€Based Fragmentation Approach with an Improved Fragmentation Scheme: Benchmark Results and Illustrative Applications. ChemPhysChem, 2013, 14, 108-115.	2.1	35
77	Homolytic Cleavage of a Bâ^'B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. Angewandte Chemie, 2016, 128, 6089-6093.	2.0	35
78	Electroâ€Descriptors for the Performance Prediction of Electroâ€Organic Synthesis. Angewandte Chemie - International Edition, 2021, 60, 4199-4207.	13.8	35
79	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 2696-2704.	5.3	34
80	Enantioselective copper-catalysed defluorosilylation of trifluoro-methylated alkenes with silylboronates. Organic Chemistry Frontiers, 2020, 7, 2618-2627.	4.5	34
81	Strength of Spin Coupling in High-Spin Organic Molecules. Journal of Physical Chemistry A, 1997, 101, 5567-5573.	2.5	33
82	Mechanistic Insight on the Hydrogenation of Conjugated Alkenes with H2Catalyzed by Early Main-Group Metal Catalysts. Inorganic Chemistry, 2010, 49, 3361-3369.	4.0	33
83	Cluster-in-Molecule Local Correlation Method with an Accurate Distant Pair Correction for Large Systems. Journal of Chemical Theory and Computation, 2021, 17, 756-766.	5.3	32
84	Fragmentation-Based QM/MM Simulations: Length Dependence of Chain Dynamics and Hydrogen Bonding of Polyethylene Oxide and Polyethylene in Aqueous Solutions. Journal of Physical Chemistry B, 2008, 112, 7061-7070.	2.6	31
85	Terahertz spectra of DNA nucleobase crystals: A joint experimental and computational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 179, 255-260.	3.9	31
86	Theoretical Study toward Understanding the Catalytic Mechanism of Pyruvate Decarboxylase. Journal of Physical Chemistry B, 2005, 109, 18664-18672.	2.6	30
87	Performance of Block Correlated Coupled Cluster Method with the CASSCF Reference Function for the Prediction of Activation Barriers, Spectroscopic Constants in Diatomic Molecules, and Singletâ^'Triplet Gaps in Diradicals. Journal of Physical Chemistry A, 2008, 112, 12518-12525.	2.5	29
88	Is Ferromagnetic Spin Coupling Constant within Homologous Di- and Triradicals?. The Journal of Physical Chemistry, 1996, 100, 4775-4780.	2.9	28
89	A multireference configuration interaction method based on the separated electron pair wave functions. Journal of Computational Chemistry, 2006, 27, 39-47.	3.3	28
90	Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems. Journal of Physical Chemistry A, 2016, 120, 9667-9677.	2.5	28

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91	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 5231-5239.	5.3	28
92	Density Functional Study on the Mechanisms of the Reactions of Gas-Phase OsOn+ (n = 1â^'4) with Methane. Organometallics, 2004, 23, 3656-3667.	2.3	27
93	New insight into selective catalytic reduction of nitrogen oxides by ammonia over H-form zeolites: a theoretical study. Physical Chemistry Chemical Physics, 2007, 9, 3304.	2.8	27
94	Energetics and Mechanism of Dinitrogen Cleavage at a Mononuclear Surface Tantalum Center: A New Way of Dinitrogen Reduction. Angewandte Chemie - International Edition, 2008, 47, 8040-8043.	13.8	27
95	Block correlated coupled cluster method with the complete active-space self-consistent-field reference function: Applications for low-lying electronic excited states. Journal of Chemical Physics, 2009, 131, 174101.	3.0	27
96	Vibrational Spectra of Molecular Crystals with the Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2016, 120, 2700-2711.	2.5	27
97	Selective Quadruple C(sp3)-F Functionalization of Polyfluoroalkyl Ketones. IScience, 2020, 23, 101259.	4.1	27
98	Transition Metal Polyhydride Complexes. 11. Mechanistic Studies of the Cis to Trans Isomerization of the Iridium(III) Dihydride Ir(H)2(CO)L (L = C6H3(CH2P(H)2)2). Organometallics, 1999, 18, 5682-5687.	2.3	26
99	Refinement of DNA Structures through Near-Edge X-ray Absorption Fine Structure Analysis: Applications on Guanine and Cytosine Nucleobases, Nucleosides, and Nucleotides. Journal of Physical Chemistry B, 2010, 114, 13214-13222.	2.6	25
100	Macrospirocyclic Oligomer Based on Triphenylamine and Diphenylphosphine Oxide as a Bipolar Host for Efficient Blue Electrophosphorescent Organic Light-Emitting Diodes (OLEDs). Organic Letters, 2015, 17, 1413-1416.	4.6	25
101	Spectroscopic Constants of Single-Bond Diatomic Molecules and Singletâ^'Triplet Gaps of Diradicals by the Block-Correlated Coupled Cluster Theory. Journal of Physical Chemistry A, 2008, 112, 4703-4709.	2.5	24
102	Understanding the Role of Intra- and Intermolecular Interactions in the Formation of Single- and Double-Helical Structures of Aromatic Oligoamides: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 1335-1342.	2.5	24
103	Systematic Study of Soft X-ray Spectra of Poly(Dg)Â·Poly(Dc) and Poly(Da)Â·Poly(Dt) DNA Duplexes. Journal of Physical Chemistry B, 2010, 114, 7016-7021.	2.6	24
104	Fully optimized implementation of the clusterâ€inâ€molecule local correlation approach for electron correlation calculations of large systems. Journal of Computational Chemistry, 2019, 40, 1130-1140.	3.3	24
105	Metal-free reductive coupling of aliphatic aldehydes/ketones with 4-cyanopyridines: expanded scope and mechanistic studies. Organic Chemistry Frontiers, 2020, 7, 2744-2751.	4.5	24
106	Pair-correlated coupled cluster theory: An alternative multireference coupled cluster method. Journal of Chemical Physics, 2003, 118, 5736-5745.	3.0	23
107	Insight into the reaction between a primary amine and a cavitand with an introverted aldehyde group: an enzyme-like mechanism. Chemical Communications, 2013, 49, 1542.	4.1	23
108	Charge-Transfer-Induced para-Selective sp² Câ€“H Bond Activation of Arenes by Use of a Hypervalent Iodine Compound: A Theoretical Study. Journal of Organic Chemistry, 2017, 82, 2984-2991.	3.2	23

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109	â€œInverseâ€•Frustrated Lewis Pairs: An Inverse FLP Approach to the Catalytic Metal Free Hydrogenation of Ketones. Chemistry - A European Journal, 2018, 24, 16526-16531.	3.3	23
110	An On-the-Fly Approach to Construct Generalized Energy-Based Fragmentation Machine Learning Force Fields of Complex Systems. Journal of Physical Chemistry A, 2020, 124, 5007-5014.	2.5	23
111	An MP2 study of linear polarizabilities and second-order hyperpolarizabilities for centrosymmetric squaraines. Chemical Physics Letters, 2002, 354, 316-323.	2.6	22
112	Fragment energy approach to Hartreeâ€“Fock calculations of macromolecules. Annual Reports on the Progress of Chemistry Section C, 2008, 104, 256.	4.4	22
113	Theoretical Study on the Mechanism of the Petasisâ€type Boronic Mannich Reaction of Organoboronic Acids, Amines, and Î±â€Hydroxy Aldehydes. Chinese Journal of Chemistry, 2010, 28, 41-49.	4.9	22
114	A coupled cluster approach with a hybrid treatment of connected triple excitations for bond-breaking potential energy surfaces. Journal of Chemical Physics, 2010, 132, 114115.	3.0	22
115	Metal complexes formed by metal-assisted solvolysis of di-pyridylketone azine: structures and magnetic properties. Dalton Transactions, 2007, , 1838.	3.3	21
116	Theoretical study on the mechanism of H₂activation mediated by two transition metal thiolate complexes: Homolytic for Ir, heterolytic for Rh. Dalton Transactions, 2010, 39, 857-863.	3.3	21
117	Circularly Polarized Luminescence of Chiral Perylene Diimide Based Enantiomers Triggered by Supramolecular Selfâ€Assembly. Chemistry - A European Journal, 2016, 22, 12910-12915.	3.3	21
118	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. Journal of Chemical Theory and Computation, 2018, 14, 5787-5796.	5.3	21
119	Assessment of density functionals on intramolecular dispersion interaction in large normal alkanes. Chemical Physics Letters, 2012, 541, 7-11.	2.6	20
120	Mechanistic Insight on the Dielsâ€“Alder Reaction Catalyzed by a Self-Assembled Molecular Capsule. Journal of Organic Chemistry, 2013, 78, 3577-3582.	3.2	20
121	Cluster-in-molecule local correlation method for large systems. Science China Chemistry, 2014, 57, 78-86.	8.2	20
122	Multireference Second Order Perturbation Theory with a Simplified Treatment of Dynamical Correlation. Journal of Chemical Theory and Computation, 2015, 11, 4634-4643.	5.3	20
123	Are fragment-based quantum chemistry methods applicable to medium-sized water clusters?. Physical Chemistry Chemical Physics, 2016, 18, 16491-16500.	2.8	20
124	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases. Physical Chemistry Chemical Physics, 2019, 21, 4072-4081.	2.8	19
125	Automatic Construction of the Initial Orbitals for Efficient Generalized Valence Bond Calculations of Large Systems. Journal of Chemical Theory and Computation, 2019, 15, 141-153.	5.3	19
126	Accurate and Efficient Prediction of NMR Parameters of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2020, 16, 2995-3005.	5.3	19

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127	Accurate prediction of the structure and vibrational spectra of ionic liquid clusters with the generalized energy-based fragmentation approach: critical role of ion-pair-based fragmentation. Physical Chemistry Chemical Physics, 2018, 20, 13547-13557.	2.8	18
128	Building quantum mechanics quality force fields of proteins with the generalized energy-based fragmentation approach and machine learning. Physical Chemistry Chemical Physics, 2022, 24, 1326-1337.	2.8	18
129	Electron Correlation and Magnetism:Â A Simple Molecular Orbital Approach for Predicting Ground-State Spins of Conjugated Hydrocarbons. Journal of Physical Chemistry A, 1997, 101, 5587-5592.	2.5	17
130	An efficient linear scaling procedure for constructing localized orbitals of large molecules based on the one-particle density matrix. Journal of Chemical Physics, 2011, 135, 134107.	3.0	17
131	Tuning Charge Balance in Solution-Processable Bipolar Triphenylamine-diazafluorene Host Materials for Phosphorescent Devices. ACS Applied Materials & Interfaces, 2015, 7, 9445-9452.	8.0	17
132	Accurate Relative Energies and Binding Energies of Large Iceâ€“Liquid Water Clusters and Periodic Structures. Journal of Physical Chemistry A, 2017, 121, 4030-4038.	2.5	17
133	Biofumigation with volatile organic compounds from Streptomyces alboflavus TDâ€1 and pure chemicals to control Aspergillus ochraceus. Annals of Applied Biology, 2018, 173, 313-322.	2.5	17
134	Theoretical Study on the Dielsâ^'Alder Reaction between 2-Methylacrolein and Cyclopentadiene Catalyzed by a Cationic Oxazaborolidine Lewis Acid. Journal of Physical Chemistry A, 2006, 110, 9225-9230.	2.5	16
135	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The implementation for low-lying excited states. Journal of Chemical Physics, 2008, 129, 234106.	3.0	16
136	New coupled cluster approaches based on the unrestricted Hartreeâ€“Fock reference for treating molecules with multireference character. Physical Chemistry Chemical Physics, 2011, 13, 8795.	2.8	16
137	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning. Chemical Science, 2021, 12, 14987-15006.	7.4	16
138	A coupled cluster approach with a hybrid treatment of connected triple excitations: Implementation and applications for open-shell systems. Journal of Chemical Physics, 2010, 133, 234106.	3.0	15
139	A Quick Estimate of the Correlation Energy for Alkanes. Chinese Journal of Chemistry, 2003, 21, 1422-1429.	4.9	15
140	The coupled cluster approach with a hybrid treatment of connected triple excitations based on the restricted Hartreeâ€“Fock reference. Journal of Chemical Physics, 2011, 134, 044134.	3.0	15
141	Mechanistic insights into the full hydrogenation of 2,6-substituted pyridine catalyzed by the Lewis acid C₆F₅(CH₂)₂B(C₆F₅)₂. Dalton Transactions, 2015, 44, 9200-9208.	3.3	15
142	Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	15
143	Mechanism of Ruthenium-Catalyzed Alder Ene-Type Reaction:â€‰ A Theoretical Study. Organometallics, 2005, 24, 872-884.	2.3	14
144	Interfacial Charge Transfer and Transport in Polyacetylene-Based Heteroionic Junctions:Â Quantum Chemistry Calculations and Molecular Dynamics Simulations. Macromolecules, 2007, 40, 4363-4369.	4.8	14

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145	THz spectra and corresponding vibrational modes of DNA base pair cocrystals and polynucleotides. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 200, 195-201.	3.9	14
146	Cluster-in-Molecule Local Correlation Approach for Periodic Systems. Journal of Chemical Theory and Computation, 2019, 15, 2933-2943.	5.3	14
147	Automatic Selection of Active Orbitals from Generalized Valence Bond Orbitals. Journal of Physical Chemistry A, 2020, 124, 8321-8329.	2.5	14
148	A Density Functional Theory Study on the Intramolecular Proton Transfer in the Enzyme Carbonic Anhydrase. Journal of Physical Chemistry A, 2003, 107, 4652-4660.	2.5	13
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