

# Wei Li

## List of Publications by Year in descending order

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80  
papers

3,975  
citations

159358

30  
h-index

123241

61  
g-index

81  
all docs

81  
docs citations

81  
times ranked

2614  
citing authors

#	ARTICLE	IF	CITATIONS
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
2	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.	1.1	254
3	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.	6.6	208
4	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	1.2	199
5	Generalized Energy-Based Fragmentation Approach and Its Applications to Macromolecules and Molecular Aggregates. Accounts of Chemical Research, 2014, 47, 2712-2720.	7.6	143
6	Homolytic Cleavage of a B $\sim$ B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. Angewandte Chemie - International Edition, 2016, 55, 5985-5989.	7.2	143
7	An efficient implementation of the "cluster-in-molecule" approach for local electron correlation calculations. Journal of Chemical Physics, 2006, 125, 074109.	1.2	126
8	Geometry Optimizations and Vibrational Spectra of Large Molecules from a Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2008, 112, 10864-10872.	1.1	121
9	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	1.1	114
10	Chemically Self-Charging Aqueous Zinc-Organic Battery. Journal of the American Chemical Society, 2021, 143, 15369-15377.	6.6	109
11	Multilevel Extension of the Cluster-in-Molecule Local Correlation Methodology: Merging Coupled-Cluster and M $\tilde{J}$ ller $\tilde{P}$ lesset Perturbation Theories. Journal of Physical Chemistry A, 2010, 114, 6721-6727.	1.1	107
12	The Cobalt $\tilde{C}$ Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations. Journal of Chemical Theory and Computation, 2012, 8, 1870-1894.	2.3	97
13	Divide-and-conquer local correlation approach to the correlation energy of large molecules. Journal of Chemical Physics, 2004, 121, 6649-6657.	1.2	95
14	Improved Design of Orbital Domains within the Cluster-in-Molecule Local Correlation Framework: Single-Environment Cluster-in-Molecule Ansatz and Its Application to Local Coupled-Cluster Approach with Singles and Doubles <sup>&lt;sup&gt;&lt;/sup&gt;</sup> . Journal of Physical Chemistry A, 2010, 114, 8644-8657.	1.1	91
15	Different Ways of Hydrogen Bonding in Water - Why Does Warm Water Freeze Faster than Cold Water?. Journal of Chemical Theory and Computation, 2017, 13, 55-76.	2.3	85
16	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H <sub>2</sub> O) <sub>20</sub> . Journal of Chemical Theory and Computation, 2014, 10, 1546-1553.	2.3	62
17	LSQC: Low scaling quantum chemistry program. International Journal of Quantum Chemistry, 2015, 115, 641-646.	1.0	57
18	A refined cluster-in-molecule local correlation approach for predicting the relative energies of large systems. Physical Chemistry Chemical Physics, 2012, 14, 7854.	1.3	50

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19	Cluster-in-molecule local correlation method for post-Hartree-Fock calculations of large systems. <i>Molecular Physics</i> , 2016, 114, 1447-1460.	0.8	50
20	A localized molecular-orbital assembler approach for Hartree-Fock calculations of large molecules. <i>Journal of Chemical Physics</i> , 2005, 122, 194109.	1.2	45
21	Accurate Prediction of Lattice Energies and Structures of Molecular Crystals with Molecular Quantum Chemistry Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 91-98.	2.3	45
22	Improved Cluster-in-Molecule Local Correlation Approach for Electron Correlation Calculation of Large Systems. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8996-9004.	1.1	40
23	A fragment energy assembler method for Hartree-Fock calculations of large molecules. <i>Journal of Chemical Physics</i> , 2006, 124, 154102.	1.2	39
24	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. <i>Accounts of Chemical Research</i> , 2021, 54, 169-181.	7.6	36
25	Cooperativity in Long $\alpha$ - and $3 \times 10^3$ -Helical Polyalanines: Both Electrostatic and van der Waals Interactions Are Essential. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11462-11469.	1.2	35
26	The Generalized Energy-Based Fragmentation Approach with an Improved Fragmentation Scheme: Benchmark Results and Illustrative Applications. <i>ChemPhysChem</i> , 2013, 14, 108-115.	1.0	35
27	Homolytic Cleavage of a $B\cdots B$ Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. <i>Angewandte Chemie</i> , 2016, 128, 6089-6093.	1.6	35
28	Telomerase and poly(ADP-ribose) polymerase-1 activity sensing based on the high fluorescence selectivity and sensitivity of TOTO-1 towards G bases in single-stranded DNA and poly(ADP-ribose). <i>Chemical Science</i> , 2019, 10, 3706-3714.	3.7	35
29	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2696-2704.	2.3	34
30	Cluster-in-Molecule Local Correlation Method with an Accurate Distant Pair Correction for Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 756-766.	2.3	32
31	Fragmentation-Based QM/MM Simulations: Length Dependence of Chain Dynamics and Hydrogen Bonding of Polyethylene Oxide and Polyethylene in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 7061-7070.	1.2	31
32	Molecular dynamics simulations of temperature-dependent structures and dynamics of ethylammonium nitrate protic ionic liquid: The role of hydrogen bond. <i>Chemical Physics</i> , 2016, 472, 105-111.	0.9	31
33	Linear scaling explicitly correlated MP2-F12 and ONIOM methods for the long-range interactions of the nanoscale clusters in methanol aqueous solutions. <i>Journal of Chemical Physics</i> , 2013, 138, 014106.	1.2	29
34	A multireference configuration interaction method based on the separated electron pair wave functions. <i>Journal of Computational Chemistry</i> , 2006, 27, 39-47.	1.5	28
35	Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9667-9677.	1.1	28
36	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5231-5239.	2.3	28

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37	Fully optimized implementation of the cluster-in-molecule local correlation approach for electron correlation calculations of large systems. <i>Journal of Computational Chemistry</i> , 2019, 40, 1130-1140.	1.5	24
38	Molecular-Level Insights into Size-Dependent Stabilization Mechanism of Gold Nanoparticles in 1-Butyl-3-methylimidazolium Tetrafluoroborate Ionic Liquid. <i>Journal of Physical Chemistry C</i> , 2017, 121, 523-532.	1.5	23
39	An On-the-Fly Approach to Construct Generalized Energy-Based Fragmentation Machine Learning Force Fields of Complex Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5007-5014.	1.1	23
40	Fragment energy approach to Hartree-Fock calculations of macromolecules. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2008, 104, 256.	4.4	22
41	Simulations of molecular self-assembled monolayers on surfaces: packing structures, formation processes and functions tuned by intermolecular and interfacial interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22757-22771.	1.3	22
42	Cluster-in-molecule local correlation method for large systems. <i>Science China Chemistry</i> , 2014, 57, 78-86.	4.2	20
43	Are fragment-based quantum chemistry methods applicable to medium-sized water clusters?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16491-16500.	1.3	20
44	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4072-4081.	1.3	19
45	Accurate and Efficient Prediction of NMR Parameters of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2995-3005.	2.3	19
46	Diffusion of Atomic Oxygen on the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12649-12658.	1.5	18
47	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. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13547-13557.	1.3	18
48	Building quantum mechanics quality force fields of proteins with the generalized energy-based fragmentation approach and machine learning. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1326-1337.	1.3	18
49	An efficient linear scaling procedure for constructing localized orbitals of large molecules based on the one-particle density matrix. <i>Journal of Chemical Physics</i> , 2011, 135, 134107.	1.2	17
50	Accurate Relative Energies and Binding Energies of Large Ice-Liquid Water Clusters and Periodic Structures. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4030-4038.	1.1	17
51	Utilization of generalized energy-based fragmentation method on the study of hydrogen abstraction reactions of large methyl esters. <i>Combustion and Flame</i> , 2018, 190, 467-476.	2.8	17
52	Understanding of Competitive Hydrogen Bond Behavior of Imidazolium-Based Ionic Liquid Mixture around Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6634-6645.	1.5	17
53	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning. <i>Chemical Science</i> , 2021, 12, 14987-15006.	3.7	16
54	A Quick Estimate of the Correlation Energy for Alkanes. <i>Chinese Journal of Chemistry</i> , 2003, 21, 1422-1429.	2.6	15

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55	Factor Analysis of Conformations and NMR Signals of Rotaxanes: AIMD and Polarizable MD Simulations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 490-502.	1.1	15
56	Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	15
57	Cluster-in-Molecule Local Correlation Approach for Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2933-2943.	2.3	14
58	Theoretical Study on Conformation Dynamics of Three-Station Molecular Shuttle in Different Environments and its Influence on NMR Chemical Shifts and Binding Interactions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9032-9044.	1.1	13
59	The relative energies of polypeptide conformers predicted by linear scaling second-order Møller-Plesset perturbation theory. <i>Science China Chemistry</i> , 2014, 57, 1393-1398.	4.2	12
60	Analytical Energy Gradients for the Cluster-in-Molecule MP2 Method and Its Application to Geometry Optimizations of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3623-3634.	2.3	11
61	Understanding of structures, dynamics, and hydrogen bonds of imidazolium-based ionic liquid mixture from molecular dynamics simulation. <i>Chemical Physics</i> , 2019, 525, 110391.	0.9	10
62	Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods. , 2009, , .		9
63	A comprehensive theoretical study of the hydrogen bonding interactions and microscopic solvation structures of a pyridyl-urea-based hydrogelator in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2013, 1006, 76-84.	1.1	8
64	Syntheses, crystal structures and photophysical properties of $d^{10}$ transition-metal ( $Ag^{+}$ , $Cu^{+}$ , $Cd^{2+}$ and $Zn^{2+}$ ) coordination complexes based on a thiophene-containing heterocyclic thioamide. <i>Journal of Coordination Chemistry</i> , 2017, 70, 2900-2915.	0.8	8
65	Understanding the polymorphism-dependent emission properties of molecular crystals using a refined QM/MM approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17516-17520.	1.3	8
66	Structures and properties of large supramolecular coordination complexes predicted with the generalized energy-based fragmentation method. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28894-28902.	1.3	8
67	Improved generalized energy-based fragmentation approach and its applications to the binding energies of supramolecular complexes. <i>Electronic Structure</i> , 2019, 1, 044003.	1.0	8
68	Generalized energy-based fragmentation approach for calculations of solvation energies of large systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19394-19401.	1.3	8
69	Distinct structure assembly driven by metal-ligand binding in Au <sub>23</sub> nanoclusters and its relation to photocatalysis. <i>Chemical Communications</i> , 2021, 57, 2176-2179.	2.2	6
70	Structures and properties of ionic crystals and condensed phase ionic liquids predicted with the generalized energy-based fragmentation method. <i>Journal of Computational Chemistry</i> , 2022, 43, 704-716.	1.5	6
71	An improved localized molecular-orbital assembler approach for Hartree-Fock calculations of general large molecules. <i>Chemical Physics Letters</i> , 2012, 539-540, 186-190.	1.2	5
72	Understanding the Boron-Nitrogen Interaction and Its Possible Implications in Drug Design. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14393-14401.	1.2	5

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73	H <sub>2</sub> Activation by Heterobimetallic Gold(I)/Platinum(0) Complex: Theoretical Understanding of Electronic Processes and Prediction on More Active Species. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4525-4533.	1.5	5
74	Linear Scaling Local Correlation Extensions of the Standard and Renormalized Coupled-Cluster Methods. <i>Progress in Theoretical Chemistry and Physics</i> , 2009, , 131-195.	0.2	5
75	Fast quantum chemistry calculations for large molecules and condensed-phase systems: The developments and applications of generalized energy-based fragmentation approach. <i>Chinese Science Bulletin</i> , 2018, 63, 3427-3441.	0.4	5
76	Controlled Fluorescence Enhancement of DNA-Binding Dye Through Chain Length Match between Oligoguanine and TOTO. <i>Journal of Physical Chemistry B</i> , 2021, 125, 518-527.	1.2	4
77	Relative Energies of Proteins and Water Clusters Predicted with the Generalized Energy-Based Fragmentation Approach. <i>Progress in Theoretical Chemistry and Physics</i> , 2008, , 289-299.	0.2	3
78	Generalized energy-based fragmentation approach for accurate binding energies and Raman spectra of methane hydrate clusters. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 167-176.	0.6	3
79	Transition orbital projection approach for excited state tracking. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	2
80	Dealing with chemical reaction pathways and electronic excitations in molecular systems via renormalized and active-space coupled-cluster methods. , 2015, , .		0