

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	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
2	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
3	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
4	Transition orbital projection approach for excited state tracking. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	2
5	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
6	Distinct structure assembly driven by metal-ligand binding in Au ₂₃ nanoclusters and its relation to photocatalysis. <i>Chemical Communications</i> , 2021, 57, 2176-2179.	2.2	6
7	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
8	Chemically Self-Charging Aqueous Zinc-Organic Battery. <i>Journal of the American Chemical Society</i> , 2021, 143, 15369-15377.	6.6	109
9	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
10	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
11	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
12	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
13	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
14	H ₂ 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
15	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
16	Recent developments in the general atomic and molecular electronic structure system. <i>Journal of Chemical Physics</i> , 2020, 152, 154102.	1.2	734
17	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
18	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

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19	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
20	Cluster-in-Molecule Local Correlation Approach for Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2933-2943.	2.3	14
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	Different Ways of Hydrogen Bonding in Water - Why Does Warm Water Freeze Faster than Cold Water?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 55-76.	2.3	85
31	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
32	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
33	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
34	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
35	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
36	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

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37	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
38	Homolytic Cleavage of a B $\hat{=}$ B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5985-5989.	7.2	143
39	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
40	Homolytic Cleavage of a B $\hat{=}$ 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
41	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
42	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
43	Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	15
44	Dealing with chemical reaction pathways and electronic excitations in molecular systems via renormalized and active-space coupled-cluster methods. , 2015, , .		0
45	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
46	LSQC: Low scaling quantum chemistry program. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 641-646.	1.0	57
47	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
48	The relative energies of polypeptide conformers predicted by linear scaling second-order M \ddot{u} ller-Plesset perturbation theory. <i>Science China Chemistry</i> , 2014, 57, 1393-1398.	4.2	12
49	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
50	Generalized Energy-Based Fragmentation Approach and Its Applications to Macromolecules and Molecular Aggregates. <i>Accounts of Chemical Research</i> , 2014, 47, 2712-2720.	7.6	143
51	Cluster-in-molecule local correlation method for large systems. <i>Science China Chemistry</i> , 2014, 57, 78-86.	4.2	20
52	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
53	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H ₂ O) ₂₀ . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1546-1553.	2.3	62
54	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

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55	A comprehensive theoretical study of the hydrogen bonding interactions and microscopic solvation structures of a pyridyl-urea-based hydrogelator in aqueous solution. Computational and Theoretical Chemistry, 2013, 1006, 76-84.	1.1	8
56	Linear scaling explicitly correlated MP2-F12 and ONIOM methods for the long-range interactions of the nanoscale clusters in methanol aqueous solutions. Journal of Chemical Physics, 2013, 138, 014106.	1.2	29
57	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
58	An improved localized molecular-orbital assembler approach for Hartree-Fock calculations of general large molecules. Chemical Physics Letters, 2012, 539-540, 186-190.	1.2	5
59	The Cobalt-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
60	Cooperativity in Long α - and 3α -Helical Polyalanines: Both Electrostatic and van der Waals Interactions Are Essential. Journal of Physical Chemistry B, 2011, 115, 11462-11469.	1.2	35
61	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.	1.2	17
62	Diffusion of Atomic Oxygen on the Si(100) Surface. Journal of Physical Chemistry C, 2010, 114, 12649-12658.	1.5	18
63	Multilevel Extension of the Cluster-in-Molecule Local Correlation Methodology: Merging Coupled-Cluster and Møller-Plesset Perturbation Theories. Journal of Physical Chemistry A, 2010, 114, 6721-6727.	1.1	107
64	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. Journal of Physical Chemistry A, 2010, 114, 8644-8657.	1.1	91
65	Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods. , 2009, , .		9
66	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	1.2	199
67	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	1.1	114
68	Linear Scaling Local Correlation Extensions of the Standard and Renormalized Coupled-Cluster Methods. Progress in Theoretical Chemistry and Physics, 2009, , 131-195.	0.2	5
69	Fragment energy approach to Hartree-Fock calculations of macromolecules. Annual Reports on the Progress of Chemistry Section C, 2008, 104, 256.	4.4	22
70	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.	1.2	31
71	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
72	Relative Energies of Proteins and Water Clusters Predicted with the Generalized Energy-Based Fragmentation Approach. Progress in Theoretical Chemistry and Physics, 2008, , 289-299.	0.2	3

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73	Generalized Energy-Based Fragmentation Approach for Computing the Ground-State Energies and Properties of Large Molecules. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2193-2199.	1.1	254
74	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
75	An efficient implementation of the "cluster-in-molecule" approach for local electron correlation calculations. <i>Journal of Chemical Physics</i> , 2006, 125, 074109.	1.2	126
76	A fragment energy assembler method for Hartree-Fock calculations of large molecules. <i>Journal of Chemical Physics</i> , 2006, 124, 154102.	1.2	39
77	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
78	An Efficient Fragment-Based Approach for Predicting the Ground-State Energies and Structures of Large Molecules. <i>Journal of the American Chemical Society</i> , 2005, 127, 7215-7226.	6.6	208
79	Divide-and-conquer local correlation approach to the correlation energy of large molecules. <i>Journal of Chemical Physics</i> , 2004, 121, 6649-6657.	1.2	95
80	A Quick Estimate of the Correlation Energy for Alkanes. <i>Chinese Journal of Chemistry</i> , 2003, 21, 1422-1429.	2.6	15