Wei Li

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1341719/publications.pdf

Version: 2024-02-01

80	3,975	159585 30	123424 61
papers	citations	h-index	g-index

81	81	81	2614
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	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.	2.5	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.	13.7	208
4	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	3.0	199
5	Generalized Energy-Based Fragmentation Approach and Its Applications to Macromolecules and Molecular Aggregates. Accounts of Chemical Research, 2014, 47, 2712-2720.	15.6	143
6	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
7	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
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.	2.5	121
9	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	2.5	114
10	Chemically Self-Charging Aqueous Zinc-Organic Battery. Journal of the American Chemical Society, 2021, 143, 15369-15377.	13.7	109
11	Multilevel Extension of the Cluster-in-Molecule Local Correlation Methodology: Merging Coupled-Cluster and MÃ¸llerâ^'Plesset Perturbation Theories. Journal of Physical Chemistry A, 2010, 114, 6721-6727.	2.5	107
12	The Cobaltâ€“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.	5.3	97
13	Divide-and-conquer local correlation approach to the correlation energy of large molecules. Journal of Chemical Physics, 2004, 121, 6649-6657.	3.0	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^{â€}. Journal of Physical Chemistry A, 2010, 114, 8644-8657.	2.5	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.	5.3	85
16	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
17	LSQC: Low scaling quantum chemistry program. International Journal of Quantum Chemistry, 2015, 115, 641-646.	2.0	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.	2.8	50

#	Article	IF	Citations
19	Cluster-in-molecule local correlation method for post-Hartreeâ€“Fock calculations of large systems. Molecular Physics, 2016, 114, 1447-1460.	1.7	50
20	A localized molecular-orbital assembler approach for Hartreeâ€“Fock calculations of large molecules. Journal of Chemical Physics, 2005, 122, 194109.	3.0	45
21	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
22	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
23	A fragment energy assembler method for Hartree-Fock calculations of large molecules. Journal of Chemical Physics, 2006, 124, 154102.	3.0	39
24	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
25	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
26	The Generalized Energyâ€Based Fragmentation Approach with an Improved Fragmentation Scheme: Benchmark Results and Illustrative Applications. ChemPhysChem, 2013, 14, 108-115.	2.1	35
27	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
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). Chemical Science, 2019, 10, 3706-3714.	7.4	35
29	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
30	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
31	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
32	Molecular dynamics simulations of temperature-dependent structures and dynamics of ethylammonium nitrate protic ionic liquid: The role of hydrogen bond. Chemical Physics, 2016, 472, 105-111.	1.9	31
33	Linear scaling explicitly correlated MP2-F12 and ONIOM methods for the long-range interactions of the nanoscale clusters in methanol aqueous solutions. Journal of Chemical Physics, 2013, 138, 014106.	3.0	29
34	A multireference configuration interaction method based on the separated electron pair wave functions. Journal of Computational Chemistry, 2006, 27, 39-47.	3.3	28
35	Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems. Journal of Physical Chemistry A, 2016, 120, 9667-9677.	2.5	28
36	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

#	Article	IF	Citations
37	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
38	Molecular-Level Insights into Size-Dependent Stabilization Mechanism of Gold Nanoparticles in 1-Butyl-3-methylimidazolium Tetrafluoroborate Ionic Liquid. Journal of Physical Chemistry C, 2017, 121, 523-532.	3.1	23
39	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
40	Fragment energy approach to Hartreeâ€“Fock calculations of macromolecules. Annual Reports on the Progress of Chemistry Section C, 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. Physical Chemistry Chemical Physics, 2016, 18, 22757-22771.	2.8	22
42	Cluster-in-molecule local correlation method for large systems. Science China Chemistry, 2014, 57, 78-86.	8.2	20
43	Are fragment-based quantum chemistry methods applicable to medium-sized water clusters?. Physical Chemistry Chemical Physics, 2016, 18, 16491-16500.	2.8	20
44	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
45	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
46	Diffusion of Atomic Oxygen on the Si(100) Surface. Journal of Physical Chemistry C, 2010, 114, 12649-12658.	3.1	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. Physical Chemistry Chemical Physics, 2018, 20, 13547-13557.	2.8	18
48	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
49	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
50	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
51	Utilization of generalized energy-based fragmentation method on the study of hydrogen abstraction reactions of large methyl esters. Combustion and Flame, 2018, 190, 467-476.	5.2	17
52	Understanding of Competitive Hydrogen Bond Behavior of Imidazolium-Based Ionic Liquid Mixture around Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2020, 124, 6634-6645.	3.1	17
53	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
54	A Quick Estimate of the Correlation Energy for Alkanes. Chinese Journal of Chemistry, 2003, 21, 1422-1429.	4.9	15

#	Article	IF	Citations
55	Factor Analysis of Conformations and NMR Signals of Rotaxanes: AIMD and Polarizable MD Simulations. Journal of Physical Chemistry A, 2016, 120, 490-502.	2.5	15
56	Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	15
57	Cluster-in-Molecule Local Correlation Approach for Periodic Systems. Journal of Chemical Theory and Computation, 2019, 15, 2933-2943.	5.3	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. Journal of Physical Chemistry A, 2014, 118, 9032-9044.	2.5	13
59	The relative energies of polypeptide conformers predicted by linear scaling second-order MÃ¸ller-Plesset perturbation theory. Science China Chemistry, 2014, 57, 1393-1398.	8.2	12
60	Analytical Energy Gradients for the Cluster-in-Molecule MP2 Method and Its Application to Geometry Optimizations of Large Systems. Journal of Chemical Theory and Computation, 2019, 15, 3623-3634.	5.3	11
61	Understanding of structures, dynamics, and hydrogen bonds of imidazolium-based ionic liquid mixture from molecular dynamics simulation. Chemical Physics, 2019, 525, 110391.	1.9	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. Computational and Theoretical Chemistry, 2013, 1006, 76-84.	2.5	8
64	Syntheses, crystal structures and photophysical properties of d¹⁰ transition-metal (Ag⁺, Cu⁺, Cd²⁺ and Zn²⁺) coordination complexes based on a thiophene-containing heterocyclic thioamide. Journal of Coordination Chemistry, 2017, 70, 2900-2915.	2.2	8
65	Understanding the polymorphism-dependent emission properties of molecular crystals using a refined QM/MM approach. Physical Chemistry Chemical Physics, 2017, 19, 17516-17520.	2.8	8
66	Structures and properties of large supramolecular coordination complexes predicted with the generalized energy-based fragmentation method. Physical Chemistry Chemical Physics, 2018, 20, 28894-28902.	2.8	8
67	Improved generalized energy-based fragmentation approach and its applications to the binding energies of supramolecular complexes. Electronic Structure, 2019, 1, 044003.	2.8	8
68	Generalized energy-based fragmentation approach for calculations of solvation energies of large systems. Physical Chemistry Chemical Physics, 2021, 23, 19394-19401.	2.8	8
69	Distinct structure assembly driven by metalâ€“ligand binding in Au23 nanoclusters and its relation to photocatalysis. Chemical Communications, 2021, 57, 2176-2179.	4.1	6
70	Structures and properties of ionic crystals and condensed phase ionic liquids predicted with the generalized energyâ€based fragmentation method. Journal of Computational Chemistry, 2022, 43, 704-716.	3.3	6
71	An improved localized molecular-orbital assembler approach for Hartreeâ€“Fock calculations of general large molecules. Chemical Physics Letters, 2012, 539-540, 186-190.	2.6	5
72	Understanding the Boronâ€“Nitrogen Interaction and Its Possible Implications in Drug Design. Journal of Physical Chemistry B, 2015, 119, 14393-14401.	2.6	5

#	Article	IF	Citations
73	H₂ Activation by Heterobimetallic Gold(I)/Platinum(0) Complex: Theoretical Understanding of Electronic Processes and Prediction on More Active Species. Journal of Physical Chemistry C, 2020, 124, 4525-4533.	3.1	5
74	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
75	Fast quantum chemistry calculations for large molecules and condensed-phase systems: The developments and applications of generalized energy-based fragmentation approach. Chinese Science Bulletin, 2018, 63, 3427-3441.	0.7	5
76	Controlled Fluorescence Enhancement of DNA-Binding Dye Through Chain Length Match between Oligoguanine and TOTO. Journal of Physical Chemistry B, 2021, 125, 518-527.	2.6	4
77	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
78	Generalized energy-based fragmentation approach for accurate binding energies and Raman spectra of methane hydrate clusters. Chinese Journal of Chemical Physics, 2022, 35, 167-176.	1.3	3
79	Transition orbital projection approach for excited state tracking. Journal of Chemical Physics, 2022, 156, .	3.0	2
80	Dealing with chemical reaction pathways and electronic excitations in molecular systems via renormalized and active-space coupled-cluster methods. , 2015, , .		0