

Mark Gordon

List of Publications by Year in descending order

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152
papers

34,242
citations

34493

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9865

146
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152
all docs

152
docs citations

152
times ranked

22029
citing authors

#	ARTICLE	IF	CITATIONS
1	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	1.5	19,020
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Advances in electronic structure theory. , 2005, , 1167-1189.		1,208
4	Macmolplt: a graphical user interface for GAMESS. Journal of Molecular Graphics and Modelling, 1998, 16, 133-138.	1.3	981
5	Fragmentation Methods: A Route to Accurate Calculations on Large Systems. Chemical Reviews, 2012, 112, 632-672.	23.0	945
6	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
7	THE CONSTRUCTION AND INTERPRETATION OF MCSCF WAVEFUNCTIONS. Annual Review of Physical Chemistry, 1998, 49, 233-266.	4.8	611
8	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	1.2	578
9	The Effective Fragment Potential Method: A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. Journal of Physical Chemistry A, 2001, 105, 293-307.	1.1	570
10	Benchmarking the performance of time-dependent density functional methods. Journal of Chemical Physics, 2012, 136, 104101.	1.2	295
11	A new hierarchical parallelization scheme: Generalized distributed data interface (GDDI), and an application to the fragment molecular orbital method (FMO). Journal of Computational Chemistry, 2004, 25, 872-880.	1.5	245
12	Chapter 10 The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions. Annual Reports in Computational Chemistry, 2007, 3, 177-193.	0.9	193
13	Accurate Methods for Large Molecular Systems. Journal of Physical Chemistry B, 2009, 113, 9646-9663.	1.2	188
14	Incremental Solvation of Nonionized and Zwitterionic Glycine. Journal of the American Chemical Society, 2006, 128, 12835-12850.	6.6	183
15	A study of water clusters using the effective fragment potential and Monte Carlo simulated annealing. Journal of Chemical Physics, 2000, 112, 2063-2073.	1.2	160
16	Optimizing Conical Intersections by Spin-Flip Density Functional Theory: Application to Ethylene. Journal of Physical Chemistry A, 2009, 113, 12749-12753.	1.1	155
17	Accurate First Principles Model Potentials for Intermolecular Interactions. Annual Review of Physical Chemistry, 2013, 64, 553-578.	4.8	150
18	Evaluation of charge penetration between distributed multipolar expansions. Journal of Chemical Physics, 2000, 112, 7300-7306.	1.2	149

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19	A derivation of the frozen-orbital unrestricted open-shell and restricted closed-shell second-order perturbation theory analytic gradient expressions. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 233-253.	0.5	142
20	The Distributed Data Interface in GAMESS. <i>Computer Physics Communications</i> , 2000, 128, 190-200.	3.0	140
21	Photoisomerization of Stilbene: A Spin-Flip Density Functional Theory Approach. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7901-7911.	1.1	129
22	Dynamic polarizability, dispersion coefficient C_6 and dispersion energy in the effective fragment potential method. <i>Molecular Physics</i> , 2005, 103, 379-387.	0.8	124
23	Density functional theory based effective fragment potential method. <i>Journal of Chemical Physics</i> , 2003, 118, 6725-6732.	1.2	123
24	SIMOMM: An Integrated Molecular Orbital/Molecular Mechanics Optimization Scheme for Surfaces. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3245-3251.	1.1	120
25	A Novel Approach to Parallel Coupled Cluster Calculations: Combining Distributed and Shared Memory Techniques for Modern Cluster Based Systems. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1312-1328.	2.3	115
26	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. <i>Molecular Physics</i> , 1996, 89, 1313-1325.	0.8	110
27	Exploring the effect of anharmonicity of molecular vibrations on thermodynamic properties. <i>Journal of Chemical Physics</i> , 2006, 125, 224102.	1.2	108
28	Electrostatic energy in the effective fragment potential method: Theory and application to benzene dimer. <i>Journal of Computational Chemistry</i> , 2007, 28, 276-291.	1.5	108
29	Modeling Solvent Effects on Electronic Excited States. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2184-2192.	2.1	107
30	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. II. Application to the effective fragment potential method. <i>Journal of Chemical Physics</i> , 1998, 108, 4772-4782.	1.2	105
31	Fully analytic energy gradient in the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2011, 134, 124115.	1.2	99
32	Damping functions in the effective fragment potential method. <i>Molecular Physics</i> , 2009, 107, 999-1016.	0.8	98
33	Localized charge distributions. I. General theory, energy partitioning, and the internal rotation barrier in ethane. <i>Journal of the American Chemical Society</i> , 1971, 93, 4649-4657.	6.6	96
34	Water-Benzene Interactions: An Effective Fragment Potential and Correlated Quantum Chemistry Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2092-2102.	1.1	96
35	Uncontracted Rys Quadrature Implementation of up to G Functions on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 696-704.	2.3	95
36	Structures and Fragmentations of Small Silicon Oxide Clusters by ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6936-6943.	1.1	94

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37	Solvent effects on optical properties of molecules: A combined time-dependent density functional theory/effective fragment potential approach. <i>Journal of Chemical Physics</i> , 2008, 129, 144112.	1.2	91
38	Uncatalyzed peptide bond formation in the gas phase. <i>The Journal of Physical Chemistry</i> , 1992, 96, 8340-8351.	2.9	90
39	Dynamics Simulations with Spin-Flip Time-Dependent Density Functional Theory: Photoisomerization and Photocyclization Mechanisms of <i>cis</i> -Stilbene in $\pi\pi^*$ States. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11987-11998.	1.1	84
40	A comprehensive analysis of molecule-intrinsic quasi-atomic, bonding, and correlating orbitals. I. Hartree-Fock wave functions. <i>Journal of Chemical Physics</i> , 2013, 139, 234107.	1.2	83
41	Efficient and Accurate Fragmentation Methods. <i>Accounts of Chemical Research</i> , 2014, 47, 2786-2794.	7.6	81
42	Solvation of the Menshutkin Reaction: A Rigorous Test of the Effective Fragment Method. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1265-1273.	1.1	78
43	New Multithreaded Hybrid CPU/GPU Approach to Hartree-Fock. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4166-4176.	2.3	75
44	Charge transfer interaction in the effective fragment potential method. <i>Journal of Chemical Physics</i> , 2006, 124, 214108.	1.2	74
45	Solvent-Induced Frequency Shifts: Configuration Interaction Singles Combined with the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6742-6750.	1.1	74
46	Study of Small Water Clusters Using the Effective Fragment Potential Model. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2650-2657.	1.1	73
47	Solvent Effects on the SN2 Reaction: Application of the Density Functional Theory-Based Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1629-1636.	1.1	71
48	Nature of the silicon-nitrogen bond in silatranes. <i>Organometallics</i> , 1991, 10, 2657-2660.	1.1	70
49	Modeling $\pi\pi$ Interactions with the Effective Fragment Potential Method: The Benzene Dimer and Substituents. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5286-5294.	1.1	70
50	Breaking bonds with the left eigenstate completely renormalized coupled-cluster method. <i>Journal of Chemical Physics</i> , 2007, 127, 174106.	1.2	63
51	Accurate <i>ab initio</i> potential energy curve of F2. I. Nonrelativistic full valence configuration interaction energies using the correlation energy extrapolation by intrinsic scaling method. <i>Journal of Chemical Physics</i> , 2007, 127, 164317.	1.2	61
52	Alanine: Then There Was Water. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8657-8669.	1.2	59
53	Monotonically decreasing size distributions for one-dimensional Ga rows on Si(100). <i>Physical Review B</i> , 2005, 72, .	1.1	56
54	Fully Integrated Effective Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2235-2249.	2.3	56

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55	Gradients of the polarization energy in the effective fragment potential method. <i>Journal of Chemical Physics</i> , 2006, 125, 194103.	1.2	55
56	Developments in Parallel Electronic Structure Theory. <i>Advances in Chemical Physics</i> , 2007, , 267-294.	0.3	55
57	Solvent-Induced Shifts in Electronic Spectra of Uracil. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4574-4582.	1.1	54
58	Direct Gas-Phase Kinetic Studies of Silylene Addition Reactions: $\text{SiH}_2 + \text{C}_3\text{H}_6$, $\text{SiH}_2 + \text{i-C}_4\text{H}_8$, and $\text{SiMe}_2 + \text{C}_2\text{H}_4$. The Effects of Methyl Substitution on Strain Energies in Siliranes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8564-8572.	1.1	49
59	Solvent-Induced Shift of the Lowest Singlet $\pi \rightarrow \pi^*$ Charge-Transfer Excited State of <i>p</i> -Nitroaniline in Water: An Application of the TDDFT/EFP1 Method. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9801-9809.	1.1	49
60	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. II. Strongly Correlated MCSCF Wave Functions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10360-10367.	1.1	49
61	Structure and Energetics of Ground-State Hypericin: A Comparison of Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1647-1651.	1.1	48
62	Fast and Flexible Coupled Cluster Implementation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3385-3392.	2.3	48
63	Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5008-5012.	2.3	47
64	Large-Scale MP2 Calculations on the Blue Gene Architecture Using the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 75-79.	2.3	45
65	Intrinsic Resolution of Molecular Electronic Wave Functions and Energies in Terms of Quasi-atoms and Their Interactions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1086-1105.	1.1	44
66	Accurate <i>ab initio</i> potential energy curve of F_2 . III. The vibration rotation spectrum. <i>Journal of Chemical Physics</i> , 2007, 127, 204313.	1.2	43
67	Structure and Dynamics of the 1-Hydroxyethyl-4-amino-1,2,4-triazolium Nitrate High-Energy Ionic Liquid System. <i>Journal of Physical Chemistry B</i> , 2012, 116, 503-512.	1.2	38
68	Effective Fragment Potential Study of the Interaction of DNA Bases. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11269-11276.	1.1	37
69	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. III. The Covalent Bonding Structure of Urea. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10368-10375.	1.1	37
70	Importance of Three-Body Interactions in Molecular Dynamics Simulations of Water Demonstrated with the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1423-1435.	2.3	37
71	Implementation of the analytic energy gradient for the combined time-dependent density functional theory/effective fragment potential method: Application to excited-state molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2011, 134, 054111.	1.2	36
72	Quasi-degenerate second-order perturbation theory for occupation restricted multiple active space self-consistent field reference functions. <i>Journal of Chemical Physics</i> , 2011, 135, 044101.	1.2	35

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73	A general spin-complete spin-flip configuration interaction method. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2615-2626.	1.3	34
74	Analytic Gradient for Density Functional Theory Based on the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5297-5307.	2.3	32
75	Water and Alanine: From Puddles(32) to Ponds(49). <i>Journal of Physical Chemistry B</i> , 2009, 113, 14413-14420.	1.2	31
76	A Comprehensive Analysis in Terms of Molecule-Intrinsic Quasi-Atomic Orbitals. IV. Bond Breaking and Bond Forming along the Dissociative Reaction Path of Dioxetane. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10376-10389.	1.1	31
77	Ab Initio Localized Charge Distributions: Theory and a Detailed Analysis of the Water Dimer-Hydrogen Bond. <i>The Journal of Physical Chemistry</i> , 1995, 99, 8091-8107.	2.9	30
78	The distributed data SCF. <i>Computer Physics Communications</i> , 2002, 143, 69-82.	3.0	30
79	Polarization energy gradients in combined quantum mechanics, effective fragment potential, and polarizable continuum model calculations. <i>Journal of Chemical Physics</i> , 2007, 126, 124112.	1.2	30
80	Optimizing conical intersections of solvated molecules: The combined spin-flip density functional theory/effective fragment potential method. <i>Journal of Chemical Physics</i> , 2012, 137, 034116.	1.2	30
81	Interfacing the Ab Initio Multiple Spawning Method with Electronic Structure Methods in GAMESS: Photodecay of <i>trans</i> -Azomethane. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10902-10908.	1.1	30
82	The dispersion interaction between quantum mechanics and effective fragment potential molecules. <i>Journal of Chemical Physics</i> , 2012, 136, 244107.	1.2	29
83	Breaking Bonds of Open-Shell Species with the Restricted Open-Shell Size Extensive Left Eigenstate Completely Renormalized Coupled-Cluster Method. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11873-11884.	1.1	28
84	Substituted silabenzenes. <i>Organometallics</i> , 1988, 7, 144-155.	1.1	26
85	Exchange repulsion between effective fragment potentials and ab initio molecules. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 481-491.	0.5	26
86	Combined Fragment Molecular Orbital Cluster in Molecule Approach to Massively Parallel Electron Correlation Calculations for Large Systems.. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3587-3593.	1.1	26
87	Hybrid Distributed/Shared Memory Model for the RI-MP2 Method in the Fragment Molecular Orbital Framework. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5252-5258.	2.3	26
88	Mixed-precision evaluation of two-electron integrals by Rys quadrature. <i>Computer Physics Communications</i> , 2012, 183, 1563-1567.	3.0	25
89	The R^7 Dispersion Interaction in the General Effective Fragment Potential Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1576-1587.	2.3	25
90	High-Performance, Graphics Processing Unit-Accelerated Fock Build Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7232-7238.	2.3	25

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91	An experimental and theoretical study of the spin-orbit interaction for $\text{CO}^+(\text{A}^2\Sigma^+_{1/2,1/2}, \text{v}^+=0)$ and $\text{O}_2^+(\text{X}^2\Sigma^+_{g,1/2g}, \text{v}^+=0)$. <i>Journal of Chemical Physics</i> , 1999, 111, 6413-6421.	1.2	23
92	Dispersion Interactions in QM/EFP. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9495-9507.	1.1	23
93	Identification and Characterization of Molecular Bonding Structures by ab initio Quasi-Atomic Orbital Analyses. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8884-8898.	1.1	23
94	A Massively Parallel Implementation of the CCSD(T) Method Using the Resolution-of-the-Identity Approximation and a Hybrid Distributed/Shared Memory Parallelization Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4799-4822.	2.3	23
95	Faster Self-Consistent Field (SCF) Calculations on GPU Clusters. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7486-7503.	2.3	23
96	Reply to "Comment on "Monotonically decreasing size distributions for one-dimensional Ga rows on Si(100)". <i>Physical Review B</i> , 2006, 74, .	1.1	22
97	Analytic Gradients for the Effective Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4743-4767.	2.3	21
98	A Quasi-Atomic Analysis of Three-Center Two-Electron Zr-H-Si Interactions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9653-9669.	1.1	21
99	Geometry Optimizations of Open-Shell Systems with the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4965-4974.	1.1	20
100	Silanol-Assisted Carbinolamine Formation in an Amine-Functionalized Mesoporous Silica Surface: Theoretical Investigation by Fragmentation Methods. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1660-1669.	1.2	20
101	Using a Reactive Force Field To Correlate Mobilities Obtained from Solid-State ^{13}C NMR on Mesoporous Silica Nanoparticle Systems. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16333-16339.	1.5	19
102	Derivation and Implementation of the Gradient of the R^7 Dispersion Interaction in the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2016, 120, 639-647.	1.1	18
103	Relativistic ab Initio Accurate Atomic Minimal Basis Sets: Quantitative LUMOs and Oriented Quasi-Atomic Orbitals for the Elements Li-Xe. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3588-3597.	1.1	18
104	Quasi-Atomic Bonding Analysis of Xe-Containing Compounds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3442-3454.	1.1	18
105	Quasi-Atomic Bond Analyses in the Sixth Period: II. Bond Analyses of Cerium Oxides. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5249-5256.	1.1	18
106	SPIN ORBIT COUPLING METHODS AND APPLICATIONS TO CHEMISTRY. <i>Recent Advances in Computational</i> , 2004, , 107-136.	0.8	17
107	A systematic multireference perturbation-theory study of the low-lying states of SiC_3 . <i>Journal of Chemical Physics</i> , 2006, 124, 034303.	1.2	17
108	Hexamers and witchamers: Which hex do you choose?. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 70-83.	1.1	17

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109	Charge transfer interaction using quasiatomic minimal-basis orbitals in the effective fragment potential method. <i>Journal of Chemical Physics</i> , 2013, 139, 194104.	1.2	17
110	Dispersion Correction Derived from First Principles for Density Functional Theory and Hartree-Fock Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2161-2168.	1.1	17
111	Development of the FMO/RI-MP2 Fully Analytic Gradient Using a Hybrid-Distributed/Shared Memory Programming Model. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1039-1054.	2.3	17
112	Ab initio molecular orbital study of the insertion of H ₂ into POSS compounds. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 155-166.	0.5	16
113	An Accurate Quantum-Based Approach to Explicit Solvent Effects: Interfacing the General Effective Fragment Potential Method with <i>Ab Initio</i> Electronic Structure Theory. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8460-8475.	1.1	16
114	On the question of empirical corrections in ab initio model chemistries. <i>Journal of Chemical Physics</i> , 1999, 110, 6154-6157.	1.2	15
115	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. <i>Journal of Chemical Physics</i> , 2021, 155, 204801.	1.2	15
116	Editorial: Modern Architectures and Their Impact on Electronic Structure Theory. <i>Chemical Reviews</i> , 2020, 120, 9015-9020.	23.0	14
117	Analytic non-adiabatic couplings for the spin-flip ORMAS method. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1475-1484.	1.3	12
118	Quasi-Atomic Bond Analyses in the Sixth Period: I. Relativistic Accurate Atomic Minimal Basis Sets for the Elements Cesium to Radon. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5242-5248.	1.1	11
119	Analytic Gradients for the Spin-Flip ORMAS-CI Method: Optimizing Minima, Saddle Points, and Conical Intersections. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1260-1272.	1.1	11
120	Core and Uncore Joint Frequency Scaling Strategy. <i>Journal of Computer and Communications</i> , 2018, 06, 184-201.	0.6	11
121	Dispersion Interactions in Water Clusters. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3736-3745.	1.1	10
122	Ionic liquids from a fragmented perspective. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16878-16888.	1.3	10
123	Scaling the Hartree-Fock Matrix Build on Summit. , 2020, , .		10
124	Theoretical study of spin-orbit coupling constants for O ₂ ⁺ ($A\tilde{3}/2, 1/2_u, v+=0\tilde{17}$ and $a\tilde{4}5/2, 3/2, 1/2, \tilde{1}1/2_u$). <i>Tj ETQq0 0 0 rgt</i>	1.2	9
125	A new approach for second-order perturbation theory. <i>Journal of Computational Chemistry</i> , 2016, 37, 1274-1282.	1.5	8
126	Nodal variational principle for excited states. <i>Physical Review A</i> , 2018, 98, .	1.0	8

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127	Maximizing Performance under a Power Constraint on Modern Multicore Systems. Journal of Computer and Communications, 2019, 07, 252-266.	0.6	8
128	Application of a semi-empirical dispersion correction for modeling water clusters. Journal of Computational Chemistry, 2019, 40, 310-315.	1.5	7
129	Bonding analysis of water clusters using quasi-atomic orbitals. Physical Chemistry Chemical Physics, 2021, 23, 18734-18743.	1.3	7
130	Enabling large-scale correlated electronic structure calculations. , 2021, , .		7
131	Stability and Dissociation of Ethylenedione (OCCO). Journal of Physical Chemistry A, 2020, 124, 8209-8222.	1.1	6
132	Computation of host-guest binding free energies with a new quantum mechanics based mining minima algorithm. Journal of Chemical Physics, 2021, 154, 104122.	1.2	6
133	Hypericin and Its Perylene Quinone Analogs: Probing Structure, Dynamics, and Interactions with the Environment. Advances in Photochemistry, 2005, , 1-26.	0.4	5
134	Outcomes of OpenMP Hackathon: OpenMP Application Experiences with the Offloading Model (Part II). Lecture Notes in Computer Science, 2021, , 81-95.	1.0	5
135	Effective Fragment Potential-Based Molecular Dynamics Studies of Diffusion in Acetone and Hexane. Journal of Physical Chemistry A, 2021, 125, 3398-3405.	1.1	5
136	Intramolecular hydrogen bonding analysis. Journal of Chemical Physics, 2022, 156, 174302.	1.2	5
137	Development of a combined quantum monte carlo-effective fragment molecular orbital method. Molecular Physics, 2019, 117, 1532-1540.	0.8	4
138	Benchmarking the Effective Fragment Potential Dispersion Correction on the S22 Test Set. Journal of Physical Chemistry A, 2018, 122, 4076-4084.	1.1	3
139	PDG: A Composite Method Based on the Resolution of the Identity. Journal of Physical Chemistry A, 2021, 125, 9421-9429.	1.1	3
140	A Task-Based Approach to Parallel Restricted Hartree-Fock Calculations. Journal of Chemical Theory and Computation, 2022, , .	2.3	3
141	Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles. Physical Chemistry Chemical Physics, 2022, 24, 10475-10487.	1.3	3
142	Benchmarking of the $\langle r^{-7} \rangle$ Anisotropic Dispersion Energy Term on the S22 Dimer Test Set. Journal of Physical Chemistry A, 2018, 122, 6100-6108.	1.1	2
143	Combined quantum Monte Carlo effective fragment molecular orbital method: fragmentation across covalent bonds. Physical Chemistry Chemical Physics, 2021, 23, 14308-14314.	1.3	2
144	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	0.6	2

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145	Excited states of lutetium oxide and its singly charged cation. Journal of Chemical Physics, 2022, 156, 084303.	1.2	2
146	Synthesis of Hydroxy and Methoxy Perylene Quinones, Their Spectroscopic and Computational Characterization, and Their Antiviral Activity [†] . Photochemistry and Photobiology, 2005, 81, 924-933.	1.3	1
147	Identification of a Vibrational Frequency Corresponding to H-atom Translocation in Hypericin [†] . Photochemistry and Photobiology, 2007, 74, 157-163.	1.3	1
148	Model protein excited states: MRCI calculations with large active spaces vs CC2 method. Journal of Chemical Physics, 2021, 154, 214105.	1.2	1
149	Electronic Structure Theory Calculations Using Modern Architectures: KNL vs Haswell. Journal of Chemical Theory and Computation, 2021, 17, 6910-6917.	2.3	1
150	Rotational and translational diffusion of liquid n-hexane: EFP-based molecular dynamics analysis. Journal of Chemical Physics, 2022, 156, 114503.	1.2	1
151	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	0.6	0
152	Scalable ab initio fragmentation methods based on a truncated expansion of the non-orthogonal molecular orbital model. Journal of Chemical Physics, 2021, 155, 154101.	1.2	0