Mark Gordon

List of Publications by Year
in descending order

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Version: 2024-02-01

		30070	8630
152	34,242	54	146
papers	citations	h-index	g-index

152	152	152	19738
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	3.3	19,020
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	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.	2.4	981
5	Fragmentation Methods: A Route to Accurate Calculations on Large Systems. Chemical Reviews, 2012, 112, 632-672.	47.7	945
6	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
7	THE CONSTRUCTION AND INTERPRETATION OF MCSCF WAVEFUNCTIONS. Annual Review of Physical Chemistry, 1998, 49, 233-266.	10.8	611
8	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	3.0	578
9	The Effective Fragment Potential Method:Â A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. Journal of Physical Chemistry A, 2001, 105, 293-307.	2.5	570
10	Benchmarking the performance of time-dependent density functional methods. Journal of Chemical Physics, 2012, 136, 104101.	3.0	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.	3.3	245
12	Chapter 10 The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions. Annual Reports in Computational Chemistry, 2007, 3, 177-193.	1.7	193
13	Accurate Methods for Large Molecular Systems. Journal of Physical Chemistry B, 2009, 113, 9646-9663.	2.6	188
14	Incremental Solvation of Nonionized and Zwitterionic Glycine. Journal of the American Chemical Society, 2006, 128, 12835-12850.	13.7	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.	3.0	160
16	Optimizing Conical Intersections by Spinâ˜Flip Density Functional Theory: Application to Ethylene. Journal of Physical Chemistry A, 2009, 113, 12749-12753.	2.5	155
17	Accurate First Principles Model Potentials for Intermolecular Interactions. Annual Review of Physical Chemistry, 2013, 64, 553-578.	10.8	150
18	Evaluation of charge penetration between distributed multipolar expansions. Journal of Chemical Physics, 2000, 112, 7300-7306.	3.0	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. Theoretical Chemistry Accounts, 2003, 110, 233-253.	1.4	142
20	The Distributed Data Interface in GAMESS. Computer Physics Communications, 2000, 128, 190-200.	7.5	140
21	Photoisomerization of Stilbene: A Spin-Flip Density Functional Theory Approach. Journal of Physical Chemistry A, 2011, 115, 7901-7911.	2.5	129
22	Dynamic polarizability, dispersion coefficient C6and dispersion energy in the effective fragment potential method. Molecular Physics, 2005, 103, 379-387.	1.7	124
23	Density functional theory based effective fragment potential method. Journal of Chemical Physics, 2003, 118, 6725-6732.	3.0	123
24	SIMOMM:â€‰ An Integrated Molecular Orbital/Molecular Mechanics Optimization Scheme for Surfaces. Journal of Physical Chemistry A, 1999, 103, 3245-3251.	2.5	120
25	A Novel Approach to Parallel Coupled Cluster Calculations:â€‰ Combining Distributed and Shared Memory Techniques for Modern Cluster Based Systems. Journal of Chemical Theory and Computation, 2007, 3, 1312-1328.	5.3	115
26	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. Molecular Physics, 1996, 89, 1313-1325.	1.7	110
27	Exploring the effect of anharmonicity of molecular vibrations on thermodynamic properties. Journal of Chemical Physics, 2006, 125, 224102.	3.0	108
28	Electrostatic energy in the effective fragment potential method: Theory and application to benzene dimer. Journal of Computational Chemistry, 2007, 28, 276-291.	3.3	108
29	Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192.	4.6	107
30	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. II. Application to the effective fragment potential method. Journal of Chemical Physics, 1998, 108, 4772-4782.	3.0	105
31	Fully analytic energy gradient in the fragment molecular orbital method. Journal of Chemical Physics, 2011, 134, 124115.	3.0	99
32	Damping functions in the effective fragment potential method. Molecular Physics, 2009, 107, 999-1016.	1.7	98
33	Localized charge distributions. I. General theory, energy partitioning, and the internal rotation barrier in ethane. Journal of the American Chemical Society, 1971, 93, 4649-4657.	13.7	96
34	Waterâ^'Benzene Interactions: An Effective Fragment Potential and Correlated Quantum Chemistry Study. Journal of Physical Chemistry A, 2009, 113, 2092-2102.	2.5	96
35	Uncontracted Rys Quadrature Implementation of up to G Functions on Graphical Processing Units. Journal of Chemical Theory and Computation, 2010, 6, 696-704.	5.3	95
36	Structures and Fragmentations of Small Silicon Oxide Clusters by ab Initio Calculations. Journal of Physical Chemistry A, 2003, 107, 6936-6943.	2.5	94

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37	Solvent effects on optical properties of molecules: A combined time-dependent density functional theory/effective fragment potential approach. Journal of Chemical Physics, 2008, 129, 144112.	3.0	91
38	Uncatalyzed peptide bond formation in the gas phase. The Journal of Physical Chemistry, 1992, 96, 8340-8351.	2.9	90
39	Dynamics Simulations with Spin-Flip Time-Dependent Density Functional Theory: Photoisomerization and Photocyclization Mechanisms of cis-Stilbene in Ï€Ï€* States. Journal of Physical Chemistry A, 2014, 118, 11987-11998.	2.5	84
40	A comprehensive analysis of molecule-intrinsic quasi-atomic, bonding, and correlating orbitals. I. Hartree-Fock wave functions. Journal of Chemical Physics, 2013, 139, 234107.	3.0	83
41	Efficient and Accurate Fragmentation Methods. Accounts of Chemical Research, 2014, 47, 2786-2794.	15.6	81
42	Solvation of the Menshutkin Reaction:Â A Rigorous Test of the Effective Fragment Method. Journal of Physical Chemistry A, 1999, 103, 1265-1273.	2.5	78
43	New Multithreaded Hybrid CPU/GPU Approach to Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2012, 8, 4166-4176.	5.3	75
44	Charge transfer interaction in the effective fragment potential method. Journal of Chemical Physics, 2006, 124, 214108.	3.0	74
45	Solvent-Induced Frequency Shifts: Configuration Interaction Singles Combined with the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2010, 114, 6742-6750.	2.5	74
46	Study of Small Water Clusters Using the Effective Fragment Potential Model. Journal of Physical Chemistry A, 1998, 102, 2650-2657.	2.5	73
47	Solvent Effects on the SN2 Reaction:â€‰ Application of the Density Functional Theory-Based Effective Fragment Potential Method. Journal of Physical Chemistry A, 2005, 109, 1629-1636.	2.5	71
48	Nature of the silicon-nitrogen bond in silatranes. Organometallics, 1991, 10, 2657-2660.	2.3	70
49	Modeling Ï€â€“Ï€ Interactions with the Effective Fragment Potential Method: The Benzene Dimer and Substituents. Journal of Physical Chemistry A, 2008, 112, 5286-5294.	2.5	70
50	Breaking bonds with the left eigenstate completely renormalized coupled-cluster method. Journal of Chemical Physics, 2007, 127, 174106.	3.0	63
51	Accurate ab initio potential energy curve of F2. I. Nonrelativistic full valence configuration interaction energies using the correlation energy extrapolation by intrinsic scaling method. Journal of Chemical Physics, 2007, 127, 164317.	3.0	61
52	Alanine: Then There Was Water. Journal of Physical Chemistry B, 2009, 113, 8657-8669.	2.6	59
53	Monotonically decreasing size distributions for one-dimensional Ga rows on Si(100). Physical Review B, 2005, 72, .	3.2	56
54	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	5.3	56

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55	Gradients of the polarization energy in the effective fragment potential method. Journal of Chemical Physics, 2006, 125, 194103.	3.0	55
56	Developments in Parallel Electronic Structure Theory. Advances in Chemical Physics, 2007, , 267-294.	0.3	55
57	Solvent-Induced Shifts in Electronic Spectra of Uracil. Journal of Physical Chemistry A, 2011, 115, 4574-4582.	2.5	54
58	Direct Gas-Phase Kinetic Studies of Silylene Addition Reactions:Â SiH2+ C3H6, SiH2+i-C4H8, and SiMe2+ C2H4. The Effects of Methyl Substitution on Strain Energies in Siliranes. Journal of Physical Chemistry A, 1998, 102, 8564-8572.	2.5	49
59	Solvent-Induced Shift of the Lowest Singlet Ï€ â†' Ï€* Charge-Transfer Excited State ofp-Nitroaniline in Water: An Application of the TDDFT/EFP1 Method. Journal of Physical Chemistry A, 2011, 115, 9801-9809.	2.5	49
60	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. II. Strongly Correlated MCSCF Wave Functions. Journal of Physical Chemistry A, 2015, 119, 10360-10367.	2.5	49
61	Structure and Energetics of Ground-State Hypericin:â€‰ Comparison of Experiment and Theory. Journal of Physical Chemistry A, 1998, 102, 1647-1651.	2.5	48
62	Fast and Flexible Coupled Cluster Implementation. Journal of Chemical Theory and Computation, 2013, 9, 3385-3392.	5.3	48
63	Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. Journal of Chemical Theory and Computation, 2012, 8, 5008-5012.	5.3	47
64	Large-Scale MP2 Calculations on the Blue Gene Architecture Using the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2012, 8, 75-79.	5.3	45
65	Intrinsic Resolution of Molecular Electronic Wave Functions and Energies in Terms of Quasi-atoms and Their Interactions. Journal of Physical Chemistry A, 2017, 121, 1086-1105.	2.5	44
66	Accurate ab initio potential energy curve of F2. III. The vibration rotation spectrum. Journal of Chemical Physics, 2007, 127, 204313.	3.0	43
67	Structure and Dynamics of the 1-Hydroxyethyl-4-amino-1,2,4-triazolium Nitrate High-Energy Ionic Liquid System. Journal of Physical Chemistry B, 2012, 116, 503-512.	2.6	38
68	Effective Fragment Potential Study of the Interaction of DNA Bases. Journal of Physical Chemistry A, 2011, 115, 11269-11276.	2.5	37
69	A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. III. The Covalent Bonding Structure of Urea. Journal of Physical Chemistry A, 2015, 119, 10368-10375.	2.5	37
70	Importance of Three-Body Interactions in Molecular Dynamics Simulations of Water Demonstrated with the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2016, 12, 1423-1435.	5.3	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. Journal of Chemical Physics, 2011, 134, 054111.	3.0	36
72	Quasi-degenerate second-order perturbation theory for occupation restricted multiple active space self-consistent field reference functions. Journal of Chemical Physics, 2011, 135, 044101.	3.0	35

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73	A general spin-complete spin-flip configuration interaction method. Physical Chemistry Chemical Physics, 2018, 20, 2615-2626.	2.8	34
74	Analytic Gradient for Density Functional Theory Based on the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2014, 10, 5297-5307.	5.3	32
75	Water and Alanine: From Puddles(32) to Ponds(49). Journal of Physical Chemistry B, 2009, 113, 14413-14420.	2.6	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. Journal of Physical Chemistry A, 2015, 119, 10376-10389.	2.5	31
77	Ab Initio Localized Charge Distributions: Theory and a Detailed Analysis of the Water Dimer-Hydrogen Bond. The Journal of Physical Chemistry, 1995, 99, 8091-8107.	2.9	30
78	The distributed data SCF. Computer Physics Communications, 2002, 143, 69-82.	7.5	30
79	Polarization energy gradients in combined quantum mechanics, effective fragment potential, and polarizable continuum model calculations. Journal of Chemical Physics, 2007, 126, 124112.	3.0	30
80	Optimizing conical intersections of solvated molecules: The combined spin-flip density functional theory/effective fragment potential method. Journal of Chemical Physics, 2012, 137, 034116.	3.0	30
81	Interfacing the Ab Initio Multiple Spawning Method with Electronic Structure Methods in GAMESS: Photodecay of trans-Azomethane. Journal of Physical Chemistry A, 2014, 118, 10902-10908.	2.5	30
82	The dispersion interaction between quantum mechanics and effective fragment potential molecules. Journal of Chemical Physics, 2012, 136, 244107.	3.0	29
83	Breaking Bonds of Open-Shell Species with the Restricted Open-Shell Size Extensive Left Eigenstate Completely Renormalized Coupled-Cluster Method. Journal of Physical Chemistry A, 2008, 112, 11873-11884.	2.5	28
84	Substituted silabenzenes. Organometallics, 1988, 7, 144-155.	2.3	26
85	Exchange repulsion between effective fragment potentials and ab initio molecules. Theoretical Chemistry Accounts, 2010, 125, 481-491.	1.4	26
86	Combined Fragment Molecular Orbital Cluster in Molecule Approach to Massively Parallel Electron Correlation Calculations for Large Systems.. Journal of Physical Chemistry A, 2015, 119, 3587-3593.	2.5	26
87	Hybrid Distributed/Shared Memory Model for the RI-MP2 Method in the Fragment Molecular Orbital Framework. Journal of Chemical Theory and Computation, 2019, 15, 5252-5258.	5.3	26
88	Mixed-precision evaluation of two-electron integrals by Rys quadrature. Computer Physics Communications, 2012, 183, 1563-1567.	7.5	25
89	The R^{â€“7} Dispersion Interaction in the General Effective Fragment Potential Method. Journal of Chemical Theory and Computation, 2014, 10, 1576-1587.	5.3	25
90	High-Performance, Graphics Processing Unit-Accelerated Fock Build Algorithm. Journal of Chemical Theory and Computation, 2020, 16, 7232-7238.	5.3	25

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91	An experimental and theoretical study of the spinâ€“orbit interaction for CO+(Aâ€Š2Î3/2,1/2,â€Šv+=0â€“41) and O2+(Xâ€‰2Î3/2,1/2g,â€Šv+=0â€“38). Journal of Chemical Physics, 1999, 111, 6413-6421.	3.0	23
92	Dispersion Interactions in QM/EFP. Journal of Physical Chemistry A, 2017, 121, 9495-9507.	2.5	23
93	Identification and Characterization of Molecular Bonding Structures by ab initio Quasi-Atomic Orbital Analyses. Journal of Physical Chemistry A, 2017, 121, 8884-8898.	2.5	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. Journal of Chemical Theory and Computation, 2021, 17, 4799-4822.	5.3	23
95	Faster Self-Consistent Field (SCF) Calculations on GPU Clusters. Journal of Chemical Theory and Computation, 2021, 17, 7486-7503.	5.3	23
96	Reply to â€œComment on â€˜Monotonically decreasing size distributions for one-dimensional Ga rows on Si(100)â€™â€‰â€•. Physical Review B, 2006, 74, .	3.2	22
97	Analytic Gradients for the Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2016, 12, 4743-4767.	5.3	21
98	A Quasi-Atomic Analysis of Three-Center Two-Electron Zrâ€“Hâ€“Si Interactions. Journal of Physical Chemistry A, 2018, 122, 9653-9669.	2.5	21
99	Geometry Optimizations of Open-Shell Systems with the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2012, 116, 4965-4974.	2.5	20
100	Silanol-Assisted Carbinolamine Formation in an Amine-Functionalized Mesoporous Silica Surface: Theoretical Investigation by Fragmentation Methods. Journal of Physical Chemistry B, 2016, 120, 1660-1669.	2.6	20
101	Using a Reactive Force Field To Correlate Mobilities Obtained from Solid-State¹³C NMR on Mesoporous Silica Nanoparticle Systems. Journal of Physical Chemistry C, 2011, 115, 16333-16339.	3.1	19
102	Derivation and Implementation of the Gradient of the R^{â€“7} Dispersion Interaction in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2016, 120, 639-647.	2.5	18
103	Relativistic ab Initio Accurate Atomic Minimal Basis Sets: Quantitative LUMOs and Oriented Quasi-Atomic Orbitals for the Elements Liâ€“Xe. Journal of Physical Chemistry A, 2017, 121, 3588-3597.	2.5	18
104	Quasi-Atomic Bonding Analysis of Xe-Containing Compounds. Journal of Physical Chemistry A, 2018, 122, 3442-3454.	2.5	18
105	Quasi-Atomic Bond Analyses in the Sixth Period: II. Bond Analyses of Cerium Oxides. Journal of Physical Chemistry A, 2019, 123, 5249-5256.	2.5	18
106	SPIN ORBIT COUPLING METHODS AND APPLICATIONS TO CHEMISTRY. Recent Advances in Computational, 2004, , 107-136.	0.8	17
107	A systematic multireference perturbation-theory study of the low-lying states of SiC3. Journal of Chemical Physics, 2006, 124, 034303.	3.0	17
108	Hexamers and witchamers: Which hex do you choose?. Computational and Theoretical Chemistry, 2013, 1021, 70-83.	2.5	17

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109	Charge transfer interaction using quasiatomic minimal-basis orbitals in the effective fragment potential method. Journal of Chemical Physics, 2013, 139, 194104.	3.0	17
110	Dispersion Correction Derived from First Principles for Density Functional Theory and Hartreeâ€“Fock Theory. Journal of Physical Chemistry A, 2015, 119, 2161-2168.	2.5	17
111	Development of the FMO/RI-MP2 Fully Analytic Gradient Using a Hybrid-Distributed/Shared Memory Programming Model. Journal of Chemical Theory and Computation, 2020, 16, 1039-1054.	5.3	17
112	Ab initio molecular orbital study of the insertion of H2 into POSS compounds. Theoretical Chemistry Accounts, 2008, 120, 155-166.	1.4	16
113	An Accurate Quantum-Based Approach to Explicit Solvent Effects: Interfacing the General Effective Fragment Potential Method with Ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2019, 123, 8460-8475.	2.5	16
114	On the question of empirical corrections in ab initio model chemistries. Journal of Chemical Physics, 1999, 110, 6154-6157.	3.0	15
115	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
116	Editorial: Modern Architectures and Their Impact on Electronic Structure Theory. Chemical Reviews, 2020, 120, 9015-9020.	47.7	14
117	Analytic non-adiabatic couplings for the spin-flip ORMAS method. Physical Chemistry Chemical Physics, 2020, 22, 1475-1484.	2.8	12
118	Quasi-Atomic Bond Analyses in the Sixth Period: I. Relativistic Accurate Atomic Minimal Basis Sets for the Elements Cesium to Radon. Journal of Physical Chemistry A, 2019, 123, 5242-5248.	2.5	11
119	Analytic Gradients for the Spin-Flip ORMAS-CI Method: Optimizing Minima, Saddle Points, and Conical Intersections. Journal of Physical Chemistry A, 2019, 123, 1260-1272.	2.5	11
120	Core and Uncore Joint Frequency Scaling Strategy. Journal of Computer and Communications, 2018, 06, 184-201.	0.9	11
121	Dispersion Interactions in Water Clusters. Journal of Physical Chemistry A, 2017, 121, 3736-3745.	2.5	10
122	Ionic liquids from a fragmented perspective. Physical Chemistry Chemical Physics, 2019, 21, 16878-16888.	2.8	10
123	Scaling the Hartree-Fock Matrix Build on Summit. , 2020, , .		10
124	Theoretical study of spin-orbit coupling constants for O2+ (Aâ€Š2Î3/2,1/2u, v+=0â€“17 and aâ€Š4Î5/2,3/2,1/2,â^'1/2u,) Tj ETQq0 0 0 rgE	3.0	9
125	A new approach for secondâ€order perturbation theory. Journal of Computational Chemistry, 2016, 37, 1274-1282.	3.3	8
126	Nodal variational principle for excited states. Physical Review A, 2018, 98, .	2.5	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.	0.9	8
128	Application of a semiâ€empirical dispersion correction for modeling water clusters. Journal of Computational Chemistry, 2019, 40, 310-315.	3.3	7
129	Bonding analysis of water clusters using quasi-atomic orbitals. Physical Chemistry Chemical Physics, 2021, 23, 18734-18743.	2.8	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.	2.5	6
132	Computation of hostâ€“guest binding free energies with a new quantum mechanics based mining minima algorithm. Journal of Chemical Physics, 2021, 154, 104122.	3.0	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.	1.3	5
135	Effective Fragment Potential-Based Molecular Dynamics Studies of Diffusion in Acetone and Hexane. Journal of Physical Chemistry A, 2021, 125, 3398-3405.	2.5	5
136	Intramolecular hydrogen bonding analysis. Journal of Chemical Physics, 2022, 156, 174302.	3.0	5
137	Development of a combined quantum monte carlo-effective fragment molecular orbital method. Molecular Physics, 2019, 117, 1532-1540.	1.7	4
138	Benchmarking the Effective Fragment Potential Dispersion Correction on the S22 Test Set. Journal of Physical Chemistry A, 2018, 122, 4076-4084.	2.5	3
139	PDG: A Composite Method Based on the Resolution of the Identity. Journal of Physical Chemistry A, 2021, 125, 9421-9429.	2.5	3
140	A Task-Based Approach to Parallel Restricted Hartreeâ€“Fock Calculations. Journal of Chemical Theory and Computation, 2022, , .	5.3	3
141	Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles. Physical Chemistry Chemical Physics, 2022, 24, 10475-10487.	2.8	3
142	Benchmarking of the R^{â€“7} Anisotropic Dispersion Energy Term on the S22 Dimer Test Set. Journal of Physical Chemistry A, 2018, 122, 6100-6108.	2.5	2
143	Combined quantum Monte Carlo â€“ effective fragment molecular orbital method: fragmentation across covalent bonds. Physical Chemistry Chemical Physics, 2021, 23, 14308-14314.	2.8	2
144	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	2

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145	Excited states of lutetium oxide and its singly charged cation. Journal of Chemical Physics, 2022, 156, 084303.	3.0	2
146	Synthesis of Hydroxy and Methoxy Perylene Quinones, Their Spectroscopic and Computational Characterization, and Their Antiviral Activity^{Â¶}. Photochemistry and Photobiology, 2005, 81, 924-933.	2.5	1
147	Identification of a Vibrational Frequency Corresponding to H-atom Translocation in HypericinÂ¶. Photochemistry and Photobiology, 2007, 74, 157-163.	2.5	1
148	Model protein excited states: MRCI calculations with large active spaces vs CC2 method. Journal of Chemical Physics, 2021, 154, 214105.	3.0	1
149	Electronic Structure Theory Calculations Using Modern Architectures: KNL vs Haswell. Journal of Chemical Theory and Computation, 2021, 17, 6910-6917.	5.3	1
150	Rotational and translational diffusion of liquid n-hexane: EFP-based molecular dynamics analysis. Journal of Chemical Physics, 2022, 156, 114503.	3.0	1
151	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	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.	3.0	0