

# Mark S Gordon

## List of Publications by Year in descending order

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292  
papers

43,715  
citations

12597

71  
h-index

2453

203  
g-index

296  
all docs

296  
docs citations

296  
times ranked

26222  
citing authors

#	ARTICLE	IF	CITATIONS
1	General atomic and molecular electronic structure system. <i>Journal of Computational Chemistry</i> , 1993, 14, 1347-1363.	1.5	19,020
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
3	The isomers of silacyclopropane. <i>Chemical Physics Letters</i> , 1980, 76, 163-168.	1.2	1,701
4	Self-consistent molecular-orbital methods. 22. Small split-valence basis sets for second-row elements. <i>Journal of the American Chemical Society</i> , 1982, 104, 2797-2803.	6.6	1,662
5	Advances in electronic structure theory. , 2005, , 1167-1189.		1,208
6	Macmolplt: a graphical user interface for GAMESS. <i>Journal of Molecular Graphics and Modelling</i> , 1998, 16, 133-138.	1.3	981
7	Fragmentation Methods: A Route to Accurate Calculations on Large Systems. <i>Chemical Reviews</i> , 2012, 112, 632-672.	23.0	945
8	Recent developments in the general atomic and molecular electronic structure system. <i>Journal of Chemical Physics</i> , 2020, 152, 154102.	1.2	734
9	THE CONSTRUCTION AND INTERPRETATION OF MCSCF WAVEFUNCTIONS. <i>Annual Review of Physical Chemistry</i> , 1998, 49, 233-266.	4.8	611
10	An effective fragment method for modeling solvent effects in quantum mechanical calculations. <i>Journal of Chemical Physics</i> , 1996, 105, 1968-1986.	1.2	578
11	The Effective Fragment Potential Method: A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. <i>Journal of Physical Chemistry A</i> , 2001, 105, 293-307.	1.1	570
12	On the Number of Water Molecules Necessary To Stabilize the Glycine Zwitterion. <i>Journal of the American Chemical Society</i> , 1995, 117, 8159-8170.	6.6	419
13	Ab initio reaction paths and direct dynamics calculations. <i>The Journal of Physical Chemistry</i> , 1989, 93, 5107-5119.	2.9	329
14	.pi.-Bond strengths in the second and third periods. <i>Journal of the American Chemical Society</i> , 1987, 109, 5217-5227.	6.6	300
15	Spin-orbit coupling in molecules: Chemistry beyond the adiabatic approximation. <i>International Reviews in Physical Chemistry</i> , 2003, 22, 551-592.	0.9	284
16	MCSCF/6-31G(d,p) calculations of one-electron spin-orbit coupling constants in diatomic molecules. <i>The Journal of Physical Chemistry</i> , 1992, 96, 10768-10772.	2.9	271
17	Energy Decomposition Analyses for Many-Body Interaction and Applications to Water Complexes. <i>The Journal of Physical Chemistry</i> , 1996, 100, 14316-14328.	2.9	256
18	A new hierarchical parallelization scheme: Generalized distributed data interface (GDDI), and an application to the fragment molecular orbital method (FMO). <i>Journal of Computational Chemistry</i> , 2004, 25, 872-880.	1.5	245

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19	Main Group Effective Nuclear Charges for Spin-Orbit Calculations. <i>The Journal of Physical Chemistry</i> , 1995, 99, 12764-12772.	2.9	214
20	Chapter 10 The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions. <i>Annual Reports in Computational Chemistry</i> , 2007, 3, 177-193.	0.9	193
21	An Ab Initio Study of Potential Energy Surfaces for N8Isomers. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5647-5650.	1.1	189
22	Understanding the Hydrogen Bond Using Quantum Chemistry. <i>Accounts of Chemical Research</i> , 1996, 29, 536-543.	7.6	188
23	Accurate Methods for Large Molecular Systems. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9646-9663.	1.2	188
24	Algorithms and accuracy requirements for computing reaction paths by the method of steepest descent. <i>The Journal of Physical Chemistry</i> , 1988, 92, 1476-1488.	2.9	187
25	Effective Nuclear Charges for the First- through Third-Row Transition Metal Elements in Spin-Orbit Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10430-10435.	1.1	183
26	A study of the relative importance of one and two-electron contributions to spin-orbit coupling. <i>Journal of Chemical Physics</i> , 2000, 112, 5611-5623.	1.2	183
27	Incremental Solvation of Nonionized and Zwitterionic Glycine. <i>Journal of the American Chemical Society</i> , 2006, 128, 12835-12850.	6.6	183
28	The intrinsic reaction coordinate and the rotational barrier in silaethylene. <i>Journal of the American Chemical Society</i> , 1985, 107, 2585-2589.	6.6	181
29	Triazolium-Based Energetic Ionic Liquids. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7285-7295.	1.1	161
30	A study of water clusters using the effective fragment potential and Monte Carlo simulated annealing. <i>Journal of Chemical Physics</i> , 2000, 112, 2063-2073.	1.2	160
31	Optimizing Conical Intersections by Spin-Flip Density Functional Theory: Application to Ethylene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12749-12753.	1.1	155
32	Direct vibrational self-consistent field method: Applications to H <sub>2</sub> O and H <sub>2</sub> CO. <i>Journal of Chemical Physics</i> , 2000, 113, 1005-1017.	1.2	150
33	Accurate First Principles Model Potentials for Intermolecular Interactions. <i>Annual Review of Physical Chemistry</i> , 2013, 64, 553-578.	4.8	150
34	Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion. <i>Journal of Chemical Physics</i> , 1999, 111, 8825-8831.	1.2	146
35	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
36	The Distributed Data Interface in GAMESS. <i>Computer Physics Communications</i> , 2000, 128, 190-200.	3.0	140

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37	Photoisomerization of Stilbene: A Spin-Flip Density Functional Theory Approach. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7901-7911.	1.1	129
38	Dynamic polarizability, dispersion coefficient C <sub>6</sub> and dispersion energy in the effective fragment potential method. <i>Molecular Physics</i> , 2005, 103, 379-387.	0.8	124
39	Density functional theory based effective fragment potential method. <i>Journal of Chemical Physics</i> , 2003, 118, 6725-6732.	1.2	123
40	The effective fragment model for solvation: Internal rotation in formamide. <i>Journal of Chemical Physics</i> , 1996, 105, 11081-11090.	1.2	122
41	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
42	A combined discrete/continuum solvation model: Application to glycine. <i>Journal of Chemical Physics</i> , 2000, 113, 1104-1109.	1.2	119
43	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
44	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. <i>Molecular Physics</i> , 1996, 89, 1313-1325.	0.8	110
45	An Improved Potential Energy Surface for the H <sub>2</sub> Cl System and Its Use for Calculations of Rate Coefficients and Kinetic Isotope Effects. <i>The Journal of Physical Chemistry</i> , 1996, 100, 13575-13587.	2.9	108
46	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
47	Modeling Solvent Effects on Electronic Excited States. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2184-2192.	2.1	107
48	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
49	Approximate second order method for orbital optimization of SCF and MCSCF wavefunctions. <i>Theoretical Chemistry Accounts</i> , 1997, 97, 88-95.	0.5	102
50	Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12739-12754.	1.1	100
51	Fully analytic energy gradient in the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2011, 134, 124115.	1.2	99
52	Damping functions in the effective fragment potential method. <i>Molecular Physics</i> , 2009, 107, 999-1016.	0.8	98
53	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
54	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

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55	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
56	Solvation of Sodium Chloride: An Effective Fragment Study of NaCl(H <sub>2</sub> O) <sub>n</sub> . <i>Journal of Physical Chemistry A</i> , 1999, 103, 4162-4166.	1.1	88
57	The Ground and Excited State Hydrogen Transfer Potential Energy Surface in 7-Azaindole. <i>Journal of Physical Chemistry A</i> , 1999, 103, 185-189.	1.1	88
58	An ab initio cluster study of the structure of the Si(001) surface. <i>Journal of Chemical Physics</i> , 2000, 112, 2994-3005.	1.2	85
59	Dynamics Simulations with Spin-Flip Time-Dependent Density Functional Theory: Photoisomerization and Photocyclization Mechanisms of <i>cis</i> -Stilbene in $\tilde{\pi}\pi^*$ States. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11987-11998.	1.1	84
60	Theoretical Studies of the Mechanism for the Synthesis of Silsesquioxanes. 1. Hydrolysis and Initial Condensation. <i>Journal of the American Chemical Society</i> , 1998, 120, 11432-11438.	6.6	83
61	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
62	Efficient and Accurate Fragmentation Methods. <i>Accounts of Chemical Research</i> , 2014, 47, 2786-2794.	7.6	81
63	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
64	Relativistic potential energy surfaces of XH <sub>2</sub> (X=C, Si, Ge, Sn, and Pb) molecules: Coupling of 1A <sub>1</sub> and 3B <sub>1</sub> states. <i>Journal of Chemical Physics</i> , 1996, 104, 7988-7996.	1.2	77
65	Hydrogen Transfer in 7-Azaindole. <i>The Journal of Physical Chemistry</i> , 1996, 100, 3974-3979.	2.9	77
66	New Multithreaded Hybrid CPU/GPU Approach to Hartree-Fock. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4166-4176.	2.3	75
67	Charge transfer interaction in the effective fragment potential method. <i>Journal of Chemical Physics</i> , 2006, 124, 214108.	1.2	74
68	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
69	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
70	Interfacing Electronic Structure Theory with Dynamics. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11512-11525.	2.9	72
71	Dynamic reaction path analysis based on an intrinsic reaction coordinate. <i>Journal of Chemical Physics</i> , 1995, 103, 10042-10049.	1.2	71
72	1,3-Transposition of Allylic Alcohols Catalyzed by Methyltrioxorhenium. <i>Organometallics</i> , 1998, 17, 1835-1840.	1.1	71

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73	Cubic fuels?. International Journal of Quantum Chemistry, 2000, 76, 434-446.	1.0	71
74	Nature of the silicon-nitrogen bond in silatranes. Organometallics, 1991, 10, 2657-2660.	1.1	70
75	Modeling $\pi$ - $\pi$ Interactions with the Effective Fragment Potential Method: The Benzene Dimer and Substituents. Journal of Physical Chemistry A, 2008, 112, 5286-5294.	1.1	70
76	Systematic Fragmentation Method and the Effective Fragment Potential: An Efficient Method for Capturing Molecular Energies. Journal of Physical Chemistry A, 2009, 113, 10040-10049.	1.1	65
77	Effects of Conjugation and Aromaticity on the Sulfoxide Bond. Journal of Organic Chemistry, 1996, 61, 1275-1283.	1.7	64
78	Spin-Orbit Splittings in the Third-Row Transition Elements: A Comparison of Effective Nuclear Charge and Full Breit-Pauli Calculations. Journal of Physical Chemistry A, 2001, 105, 8262-8268.	1.1	64
79	Electronic Structure Studies of Tetrazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 11110-11119.	1.2	63
80	The fragment molecular orbital and systematic molecular fragmentation methods applied to water clusters. Physical Chemistry Chemical Physics, 2012, 14, 7752.	1.3	61
81	Alanine: Then There Was Water. Journal of Physical Chemistry B, 2009, 113, 8657-8669.	1.2	59
82	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	2.3	56
83	Gradients of the polarization energy in the effective fragment potential method. Journal of Chemical Physics, 2006, 125, 194103.	1.2	55
84	Pathways for H <sub>2</sub> elimination from ethylene: A theoretical study. Journal of Chemical Physics, 1994, 100, 1981-1987.	1.2	53
85	Exascale applications: skin in the game. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190056.	1.6	53
86	Theoretical Studies of the Mechanism for the Synthesis of Silsesquioxanes. 2. Cyclosiloxanes (D <sub>3</sub> and D <sub>5</sub> ). Journal of Physical Chemistry A, 2000, 104, 10000-10000.	1.1	52
87	Perspective: <i>Ab initio</i> force field methods derived from quantum mechanics. Journal of Chemical Physics, 2018, 148, .	1.2	52
88	Analytic energy gradients for multiconfigurational self-consistent field second-order quasidegenerate perturbation theory (MC-QDPT). Journal of Chemical Physics, 1998, 108, 5660-5669.	1.2	51
89	Ab Initio Multiple Spawning Method for Intersystem Crossing Dynamics: Spin-Forbidden Transitions between <sup>3</sup> B <sub>1</sub> and <sup>1</sup> A <sub>1</sub> States of GeH <sub>2</sub> . Journal of Physical Chemistry A, 2016, 120, 2911-2919.	1.1	51
90	An ab initio study of TiC: A comparison of different levels of theory including density functional methods. Journal of Chemical Physics, 1996, 104, 6628-6630.	1.2	50

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91	Open-Shell Formulation of the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1-5.	2.3	50
92	Methanol-Water Mixtures: A Microsolvation Study Using the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10267-10273.	1.1	49
93	Benzene-Pyridine Interactions Predicted by the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4598-4609.	1.1	49
94	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
95	Fast and Flexible Coupled Cluster Implementation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3385-3392.	2.3	48
96	Effective Fragment Method for Modeling Intermolecular Hydrogen-Bonding Effects on Quantum Mechanical Calculations. <i>ACS Symposium Series</i> , 1994, , 139-151.	0.5	47
97	Ab initio potential energy surface by modified Shepard interpolation: Application to the CH <sub>3</sub> +H <sup>+</sup> CH <sub>4</sub> +H reaction. <i>Journal of Chemical Physics</i> , 1998, 109, 4281-4289.	1.2	47
98	New parallel optimal-parameter fast multipole method (OPFMM). <i>Journal of Computational Chemistry</i> , 2001, 22, 1484-1501.	1.5	47
99	The effective fragment potential: Small clusters and radial distribution functions. <i>Journal of Chemical Physics</i> , 2004, 121, 2711.	1.2	47
100	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
101	Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants. <i>Inorganic Chemistry</i> , 2016, 55, 5787-5803.	1.9	46
102	Structure and energetics of the silicon carbide clusters SiC <sub>3</sub> and Si <sub>2</sub> C <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2001, 115, 1795-1803.	1.2	44
103	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
104	Model space diabaticization for quantum photochemistry. <i>Journal of Chemical Physics</i> , 2015, 142, 064106.	1.2	42
105	Cation-Cation $\pi$ - $\pi$ Stacking in Small Ionic Clusters of 1,2,4-Triazolium. <i>Journal of the American Chemical Society</i> , 2008, 130, 392-393.	6.6	41
106	Spin-Orbit Coupling Constants in Atoms and Ions of Transition Elements: Comparison of Effective Core Potentials, Model Core Potentials, and All-Electron Methods. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2325-2339.	1.1	41
107	Theoretical study of the lowest triplet potential energy surface of silasilene. <i>The Journal of Physical Chemistry</i> , 1988, 92, 364-367.	2.9	39
108	Adsorption of Water on the Si(100) Surface: An Ab Initio and QM/MM Cluster Study. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4039-4044.	1.2	39

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109	Exploring the Mechanism for the Synthesis of Silsesquioxanes. 3. The Effect of Substituents and Water. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11347-11353.	1.1	38
110	Bond-Stretch Isomerism in Tetrasilabicyclo[1.1.0]butane Derivatives. <i>Organometallics</i> , 1996, 15, 2118-2124.	1.1	37
111	Reaction path Hamiltonian based on a reaction coordinate and a curvature coordinate. <i>Journal of Chemical Physics</i> , 1996, 104, 2834-2840.	1.2	37
112	Effective Fragment Potential Study of the Interaction of DNA Bases. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11269-11276.	1.1	37
113	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
114	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
115	Modeling Styrene $\pi$ -Styrene Interactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 519-525.	1.1	36
116	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
117	Insertion Mechanism of N <sub>2</sub> and O <sub>2</sub> into T <sub>n</sub> (n = 8, 10, 12)-Silsesquioxane Framework. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11764-11770.	1.2	35
118	A general spin-complete spin-flip configuration interaction method. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2615-2626.	1.3	34
119	Enabling the Efficient Use of SMP Clusters. , 2003, , .		33
120	Pentazole-Based Energetic Ionic Liquids: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 691-703.	1.1	33
121	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
122	Water and Alanine: From Puddles(32) to Ponds(49). <i>Journal of Physical Chemistry B</i> , 2009, 113, 14413-14420.	1.2	31
123	Nonlinear response time-dependent density functional theory combined with the effective fragment potential method. <i>Journal of Chemical Physics</i> , 2014, 140, 18A523.	1.2	31
124	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
125	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
126	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



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127	The dispersion interaction between quantum mechanics and effective fragment potential molecules. <i>Journal of Chemical Physics</i> , 2012, 136, 244107.	1.2	29
128	Intermolecular Self-Interactions of the Titanium Tetrahalides TiX <sub>4</sub> (X = F, Cl, Br). <i>Journal of the American Chemical Society</i> , 1999, 121, 2552-2560.	6.6	28
129	A theoretical study of the reaction of Ti <sup>+</sup> with ethane. <i>Journal of Chemical Physics</i> , 2000, 112, 10247-10258.	1.2	28
130	Diffusion energy profiles in silica mesoporous molecular sieves modelled with the fragment molecular orbital method. <i>Molecular Physics</i> , 2013, 111, 1622-1629.	0.8	28
131	Novel Computer Architectures and Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4557-4582.	1.1	27
132	Exchange repulsion between effective fragment potentials and ab initio molecules. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 481-491.	0.5	26
133	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
134	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
135	Mixed-precision evaluation of two-electron integrals by Rys quadrature. <i>Computer Physics Communications</i> , 2012, 183, 1563-1567.	3.0	25
136	Lewis Base Mediated $\beta$ -Elimination and Lewis Acid Mediated Insertion Reactions of Disilazido Zirconium Compounds. <i>Journal of the American Chemical Society</i> , 2013, 135, 15225-15237.	6.6	25
137	The $\langle i \rangle R \langle i \rangle \langle \sup \hat{\epsilon}^7 \langle /sup \rangle$ Dispersion Interaction in the General Effective Fragment Potential Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1576-1587.	2.3	25
138	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12332-12338.	7.2	25
139	High-Performance, Graphics Processing Unit-Accelerated Fock Build Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7232-7238.	2.3	25
140	Adsorption of Acetylene on Si(100)-(2 $\times$ 1). <i>Journal of Physical Chemistry B</i> , 2004, 108, 7820-7826.	1.2	24
141	Nature of Glycine and Its $\dot{\pm}$ -Carbon Radical in Aqueous Solution: A Theoretical Investigation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1788-1794.	2.3	24
142	MCSCF Study of Multiple Bonding between Ti and the Main-Group Elements C, Si, N, and P. <i>Organometallics</i> , 2003, 22, 42-46.	1.1	23
143	Parallel coupled perturbed CASSCF equations and analytic CASSCF second derivatives. <i>Journal of Computational Chemistry</i> , 2006, 27, 352-362.	1.5	23
144	Scalable implementation of analytic gradients for second-order Z-averaged perturbation theory using the distributed data interface. <i>Journal of Chemical Physics</i> , 2006, 124, 014107.	1.2	23

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145	Dispersion Interactions in QM/EFP. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9495-9507.	1.1	23
146	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
147	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
148	Faster Self-Consistent Field (SCF) Calculations on GPU Clusters. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7486-7503.	2.3	23
149	Potential energy surfaces for the Al+O2 reaction. <i>Journal of Chemical Physics</i> , 2003, 118, 4471-4476.	1.2	22
150	Parallel Unrestricted MP2 Analytic Gradients Using the Distributed Data Interface. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3103-3110.	1.1	22
151	Gradients of the Exchange-repulsion Energy in the General Effective Fragment Potential Method. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 385-390.	0.5	22
152	Ab initio QM/MM excited-state molecular dynamics study of coumarin 151 in water solution. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2308-2318.	1.0	22
153	Quantum Chemical Calculations Using Accelerators: Migrating Matrix Operations to the NVIDIA Kepler GPU and the Intel Xeon Phi. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 908-912.	2.3	22
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