Mark S Gordon

List of Publications by Year
in descending order

292 papers	43,715 citations	10986 71 h-index	2127 203 g-index
296 all docs	296 docs citations	296 times ranked	23521 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	The isomers of silacyclopropane. Chemical Physics Letters, 1980, 76, 163-168.	2.6	1,701
4	Self-consistent molecular-orbital methods. 22. Small split-valence basis sets for second-row elements. Journal of the American Chemical Society, 1982, 104, 2797-2803.	13.7	1,662
5	Advances in electronic structure theory. , 2005, , 1167-1189.		1,208
6	Macmolplt: a graphical user interface for GAMESS. Journal of Molecular Graphics and Modelling, 1998, 16, 133-138.	2.4	981
7	Fragmentation Methods: A Route to Accurate Calculations on Large Systems. Chemical Reviews, 2012, 112, 632-672.	47.7	945
8	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
9	THE CONSTRUCTION AND INTERPRETATION OF MCSCF WAVEFUNCTIONS. Annual Review of Physical Chemistry, 1998, 49, 233-266.	10.8	611
10	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	3.0	578
11	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
12	On the Number of Water Molecules Necessary To Stabilize the Glycine Zwitterion. Journal of the American Chemical Society, 1995, 117, 8159-8170.	13.7	419
13	Ab initio reaction paths and direct dynamics calculations. The Journal of Physical Chemistry, 1989, 93, 5107-5119.	2.9	329
14	.pi.-Bond strengths in the second and third periods. Journal of the American Chemical Society, 1987, 109, 5217-5227.	13.7	300
15	Spin-orbit coupling in molecules: Chemistry beyond the adiabatic approximation. International Reviews in Physical Chemistry, 2003, 22, 551-592.	2.3	284
16	MCSCF/6-31G(d,p) calculations of one-electron spin-orbit coupling constants in diatomic molecules. The Journal of Physical Chemistry, 1992, 96, 10768-10772.	2.9	271
17	Energy Decomposition Analyses for Many-Body Interaction and Applications to Water Complexes. The Journal of Physical Chemistry, 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). Journal of Computational Chemistry, 2004, 25, 872-880.	3.3	245

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19	Main Group Effective Nuclear Charges for Spin-Orbit Calculations. The Journal of Physical Chemistry, 1995, 99, 12764-12772.	2.9	214
20	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
21	An Ab Initio Study of Potential Energy Surfaces for N8Isomers. Journal of Physical Chemistry A, 2000, 104, 5647-5650.	2.5	189
22	Understanding the Hydrogen Bond Using Quantum Chemistry. Accounts of Chemical Research, 1996, 29, 536-543.	15.6	188
23	Accurate Methods for Large Molecular Systems. Journal of Physical Chemistry B, 2009, 113, 9646-9663.	2.6	188
24	Algorithms and accuracy requirements for computing reaction paths by the method of steepest descent. The Journal of Physical Chemistry, 1988, 92, 1476-1488.	2.9	187
25	Effective Nuclear Charges for the First- through Third-Row Transition Metal Elements in Spinâ^'Orbit Calculations. Journal of Physical Chemistry A, 1998, 102, 10430-10435.	2.5	183
26	A study of the relative importance of one and two-electron contributions to spinâ€“orbit coupling. Journal of Chemical Physics, 2000, 112, 5611-5623.	3.0	183
27	Incremental Solvation of Nonionized and Zwitterionic Glycine. Journal of the American Chemical Society, 2006, 128, 12835-12850.	13.7	183
28	The intrinsic reaction coordinate and the rotational barrier in silaethylene. Journal of the American Chemical Society, 1985, 107, 2585-2589.	13.7	181
29	Triazolium-Based Energetic Ionic Liquids. Journal of Physical Chemistry A, 2005, 109, 7285-7295.	2.5	161
30	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
31	Optimizing Conical Intersections by Spinâ^'Flip Density Functional Theory: Application to Ethylene. Journal of Physical Chemistry A, 2009, 113, 12749-12753.	2.5	155
32	Direct vibrational self-consistent field method: Applications to H2O and H2CO. Journal of Chemical Physics, 2000, 113, 1005-1017.	3.0	150
33	Accurate First Principles Model Potentials for Intermolecular Interactions. Annual Review of Physical Chemistry, 2013, 64, 553-578.	10.8	150
34	Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion. Journal of Chemical Physics, 1999, 111, 8825-8831.	3.0	146
35	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
36	The Distributed Data Interface in GAMESS. Computer Physics Communications, 2000, 128, 190-200.	7.5	140

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37	Photoisomerization of Stilbene: A Spin-Flip Density Functional Theory Approach. Journal of Physical Chemistry A, 2011, 115, 7901-7911.	2.5	129
38	Dynamic polarizability, dispersion coefficient C6and dispersion energy in the effective fragment potential method. Molecular Physics, 2005, 103, 379-387.	1.7	124
39	Density functional theory based effective fragment potential method. Journal of Chemical Physics, 2003, 118, 6725-6732.	3.0	123
40	The effective fragment model for solvation: Internal rotation in formamide. Journal of Chemical Physics, 1996, 105, 11081-11090.	3.0	122
41	SIMOMM:â€‰ An Integrated Molecular Orbital/Molecular Mechanics Optimization Scheme for Surfaces. Journal of Physical Chemistry A, 1999, 103, 3245-3251.	2.5	120
42	A combined discrete/continuum solvation model: Application to glycine. Journal of Chemical Physics, 2000, 113, 1104-1109.	3.0	119
43	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
44	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. Molecular Physics, 1996, 89, 1313-1325.	1.7	110
45	An Improved Potential Energy Surface for the H2Cl System and Its Use for Calculations of Rate Coefficients and Kinetic Isotope Effects. The Journal of Physical Chemistry, 1996, 100, 13575-13587.	2.9	108
46	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
47	Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192.	4.6	107
48	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
49	Approximate second order method for orbital optimization of SCF and MCSCF wavefunctions. Theoretical Chemistry Accounts, 1997, 97, 88-95.	1.4	102
50	Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers. Journal of Physical Chemistry A, 2010, 114, 12739-12754.	2.5	100
51	Fully analytic energy gradient in the fragment molecular orbital method. Journal of Chemical Physics, 2011, 134, 124115.	3.0	99
52	Damping functions in the effective fragment potential method. Molecular Physics, 2009, 107, 999-1016.	1.7	98
53	Waterâ‹¯Benzene Interactions: An Effective Fragment Potential and Correlated Quantum Chemistry Study. Journal of Physical Chemistry A, 2009, 113, 2092-2102.	2.5	96
54	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

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55	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
56	Solvation of Sodium Chloride:â€‰ An Effective Fragment Study of NaCl(H2O)n. Journal of Physical Chemistry A, 1999, 103, 4162-4166.	2.5	88
57	The Ground and Excited State Hydrogen Transfer Potential Energy Surface in 7-Azaindole. Journal of Physical Chemistry A, 1999, 103, 185-189.	2.5	88
58	Anab initiocluster study of the structure of the Si(001) surface. Journal of Chemical Physics, 2000, 112, 2994-3005.	3.0	85
59	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
60	Theoretical Studies of the Mechanism for the Synthesis of Silsesquioxanes. 1. Hydrolysis and Initial Condensation. Journal of the American Chemical Society, 1998, 120, 11432-11438.	13.7	83
61	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
62	Efficient and Accurate Fragmentation Methods. Accounts of Chemical Research, 2014, 47, 2786-2794.	15.6	81
63	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
64	Relativistic potential energy surfaces of XH2 (X=C, Si, Ge, Sn, and Pb) molecules: Coupling of 1A1 and 3B1 states. Journal of Chemical Physics, 1996, 104, 7988-7996.	3.0	77
65	Hydrogen Transfer in 7-Azaindole. The Journal of Physical Chemistry, 1996, 100, 3974-3979.	2.9	77
66	New Multithreaded Hybrid CPU/GPU Approach to Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2012, 8, 4166-4176.	5.3	75
67	Charge transfer interaction in the effective fragment potential method. Journal of Chemical Physics, 2006, 124, 214108.	3.0	74
68	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
69	Study of Small Water Clusters Using the Effective Fragment Potential Model. Journal of Physical Chemistry A, 1998, 102, 2650-2657.	2.5	73
70	Interfacing Electronic Structure Theory with Dynamics. The Journal of Physical Chemistry, 1996, 100, 11512-11525.	2.9	72
71	Dynamic reaction path analysis based on an intrinsic reaction coordinate. Journal of Chemical Physics, 1995, 103, 10042-10049.	3.0	71
72	1,3-Transposition of Allylic Alcohols Catalyzed by Methyltrioxorhenium. Organometallics, 1998, 17, 1835-1840.	2.3	71

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73	Cubic fuels?. International Journal of Quantum Chemistry, 2000, 76, 434-446.	2.0	71
74	Nature of the silicon-nitrogen bond in silatranes. Organometallics, 1991, 10, 2657-2660.	2.3	70
75	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
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.	2.5	65
77	Effects of Conjugation and Aromaticity on the Sulfoxide Bond1. Journal of Organic Chemistry, 1996, 61, 1275-1283.	3.2	64
78	Spinâ^'Orbit Splittings in the Third-Row Transition Elements:Â Comparison of Effective Nuclear Charge and Full Breitâ^'Pauli Calculations. Journal of Physical Chemistry A, 2001, 105, 8262-8268.	2.5	64
79	Electronic Structure Studies of Tetrazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 11110-11119.	2.6	63
80	The fragment molecular orbital and systematic molecular fragmentation methods applied to water clusters. Physical Chemistry Chemical Physics, 2012, 14, 7752.	2.8	61
81	Alanine: Then There Was Water. Journal of Physical Chemistry B, 2009, 113, 8657-8669.	2.6	59
82	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	5.3	56
83	Gradients of the polarization energy in the effective fragment potential method. Journal of Chemical Physics, 2006, 125, 194103.	3.0	55
84	Pathways for H2 elimination from ethylene: A theoretical study. Journal of Chemical Physics, 1994, 100, 1981-1987.	3.0	53
85	Exascale applications: skin in the game. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190056.	3.4	53
86	Theoretical Studies of the Mechanism for the Synthesis of Silsesquioxanes. 2. Cyclosiloxanes (D3 and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.5	52
87	Perspective: Ab initio force field methods derived from quantum mechanics. Journal of Chemical Physics, 2018, 148, .	3.0	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.	3.0	51
89	Ab Initio Multiple Spawning Method for Intersystem Crossing Dynamics: Spin-Forbidden Transitions between ³B₁ and ¹A₁ States of GeH₂. Journal of Physical Chemistry A, 2016, 120, 2911-2919.	2.5	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.	3.0	50

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91	Open-Shell Formulation of the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2010, 6, 1-5.	5.3	50
92	Methanolâ^'Water Mixtures:Â A Microsolvation Study Using the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2006, 110, 10267-10273.	2.5	49
93	Benzeneâ^'Pyridine Interactions Predicted by the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2011, 115, 4598-4609.	2.5	49
94	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
95	Fast and Flexible Coupled Cluster Implementation. Journal of Chemical Theory and Computation, 2013, 9, 3385-3392.	5.3	48
96	Effective Fragment Method for Modeling Intermolecular Hydrogen-Bonding Effects on Quantum Mechanical Calculations. ACS Symposium Series, 1994, , 139-151.	0.5	47
97	Ab initio potential energy surface by modified Shepard interpolation: Application to the CH3+H2â†'CH4+H reaction. Journal of Chemical Physics, 1998, 109, 4281-4289.	3.0	47
98	New parallel optimal-parameter fast multipole method (OPFMM). Journal of Computational Chemistry, 2001, 22, 1484-1501.	3.3	47
99	The effective fragment potential: Small clusters and radial distribution functions. Journal of Chemical Physics, 2004, 121, 2711.	3.0	47
100	Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. Journal of Chemical Theory and Computation, 2012, 8, 5008-5012.	5.3	47
101	Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants. Inorganic Chemistry, 2016, 55, 5787-5803.	4.0	46
102	Structure and energetics of the silicon carbide clusters SiC3 and Si2C2. Journal of Chemical Physics, 2001, 115, 1795-1803.	3.0	44
103	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
104	Model space diabatization for quantum photochemistry. Journal of Chemical Physics, 2015, 142, 064106.	3.0	42
105	Cationâ^'Cation Ï€â^'Ï€ Stacking in Small Ionic Clusters of 1,2,4-Triazolium. Journal of the American Chemical Society, 2008, 130, 392-393.	13.7	41
106	Spinâ€“Orbit Coupling Constants in Atoms and Ions of Transition Elements: Comparison of Effective Core Potentials, Model Core Potentials, and All-Electron Methods. Journal of Physical Chemistry A, 2019, 123, 2325-2339.	2.5	41
107	Theoretical study of the lowest triplet potential energy surface of silasilene. The Journal of Physical Chemistry, 1988, 92, 364-367.	2.9	39
108	Adsorption of Water on the Si(100) Surface:â€‰ An Ab Initio and QM/MM Cluster Study. Journal of Physical Chemistry B, 2001, 105, 4039-4044.	2.6	39

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109	Exploring the Mechanism for the Synthesis of Silsesquioxanes. 3. The Effect of Substituents and Water. Journal of Physical Chemistry A, 2002, 106, 11347-11353.	2.5	38
110	Bond-Stretch Isomerism in Tetrasilabicyclo[1.1.0]butane Derivatives. Organometallics, 1996, 15, 2118-2124.	2.3	37
111	Reaction path Hamiltonian based on a reaction coordinate and a curvature coordinate. Journal of Chemical Physics, 1996, 104, 2834-2840.	3.0	37
112	Effective Fragment Potential Study of the Interaction of DNA Bases. Journal of Physical Chemistry A, 2011, 115, 11269-11276.	2.5	37
113	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
114	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
115	Modeling Styreneâ˜Styrene Interactionsâ€. Journal of Physical Chemistry A, 2006, 110, 519-525.	2.5	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. Journal of Chemical Physics, 2011, 134, 054111.	3.0	36
117	Insertion Mechanism of N2and O2into Tn(n= 8, 10, 12)-Silsesquioxane Framework. Journal of Physical Chemistry B, 2002, 106, 11764-11770.	2.6	35
118	A general spin-complete spin-flip configuration interaction method. Physical Chemistry Chemical Physics, 2018, 20, 2615-2626.	2.8	34
119	Enabling the Efficient Use of SMP Clusters. , 2003, , .		33
120	Pentazole-Based Energetic Ionic Liquids:Â A Computational Study. Journal of Physical Chemistry A, 2007, 111, 691-703.	2.5	33
121	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
122	Water and Alanine: From Puddles(32) to Ponds(49). Journal of Physical Chemistry B, 2009, 113, 14413-14420.	2.6	31
123	Nonlinear response time-dependent density functional theory combined with the effective fragment potential method. Journal of Chemical Physics, 2014, 140, 18A523.	3.0	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. Journal of Physical Chemistry A, 2015, 119, 10376-10389.	2.5	31
125	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
126	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

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127	The dispersion interaction between quantum mechanics and effective fragment potential molecules. Journal of Chemical Physics, 2012, 136, 244107.	3.0	29
128	Intermolecular Self-Interactions of the Titanium Tetrahalides TiX4(X = F, Cl, Br). Journal of the American Chemical Society, 1999, 121, 2552-2560.	13.7	28
129	A theoretical study of the reaction of Ti+ with ethane. Journal of Chemical Physics, 2000, 112, 10247-10258.	3.0	28
130	Diffusion energy profiles in silica mesoporous molecular sieves modelled with the fragment molecular orbital method. Molecular Physics, 2013, 111, 1622-1629.	1.7	28
131	Novel Computer Architectures and Quantum Chemistry. Journal of Physical Chemistry A, 2020, 124, 4557-4582.	2.5	27
132	Exchange repulsion between effective fragment potentials and ab initio molecules. Theoretical Chemistry Accounts, 2010, 125, 481-491.	1.4	26
133	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
134	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
135	Mixed-precision evaluation of two-electron integrals by Rys quadrature. Computer Physics Communications, 2012, 183, 1563-1567.	7.5	25
136	Lewis Base Mediated Î²-Elimination and Lewis Acid Mediated Insertion Reactions of Disilazido Zirconium Compounds. Journal of the American Chemical Society, 2013, 135, 15225-15237.	13.7	25
137	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
138	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. Angewandte Chemie - International Edition, 2019, 58, 12332-12338.	13.8	25
139	High-Performance, Graphics Processing Unit-Accelerated Fock Build Algorithm. Journal of Chemical Theory and Computation, 2020, 16, 7232-7238.	5.3	25
140	Adsorption of Acetylene on Si(100)-(2 Ã— 1). Journal of Physical Chemistry B, 2004, 108, 7820-7826.	2.6	24
141	Nature of Glycine and Its Î±-Carbon Radical in Aqueous Solution: A Theoretical Investigation. Journal of Chemical Theory and Computation, 2008, 4, 1788-1794.	5.3	24
142	MCSCF Study of Multiple Bonding between Ti and the Main-Group Elements C, Si, N, and P. Organometallics, 2003, 22, 42-46.	2.3	23
143	Parallel coupled perturbed CASSCF equations and analytic CASSCF second derivatives. Journal of Computational Chemistry, 2006, 27, 352-362.	3.3	23
144	Scalable implementation of analytic gradients for second-order Z-averaged perturbation theory using the distributed data interface. Journal of Chemical Physics, 2006, 124, 014107.	3.0	23

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145	Dispersion Interactions in QM/EFP. Journal of Physical Chemistry A, 2017, 121, 9495-9507.	2.5	23
146	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
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. Journal of Chemical Theory and Computation, 2021, 17, 4799-4822.	5.3	23
148	Faster Self-Consistent Field (SCF) Calculations on GPU Clusters. Journal of Chemical Theory and Computation, 2021, 17, 7486-7503.	5.3	23
149	Potential energy surfaces for the Al+O2 reaction. Journal of Chemical Physics, 2003, 118, 4471-4476.	3.0	22
150	Parallel Unrestricted MP2 Analytic Gradients Using the Distributed Data Interfaceâ€. Journal of Physical Chemistry A, 2004, 108, 3103-3110.	2.5	22
151	Gradients of the Exchange-repulsion Energy in the General Effective Fragment Potential Method. Theoretical Chemistry Accounts, 2006, 115, 385-390.	1.4	22
152	Ab initio QM/MM excitedâ€state molecular dynamics study of coumarin 151 in water solution. International Journal of Quantum Chemistry, 2009, 109, 2308-2318.	2.0	22
153	Quantum Chemical Calculations Using Accelerators: Migrating Matrix Operations to the NVIDIA Kepler GPU and the Intel Xeon Phi. Journal of Chemical Theory and Computation, 2014, 10, 908-912.	5.3	22
154	An ab initio study of the reaction mechanism of Co++NH3. Journal of Chemical Physics, 1997, 106, 8504-8515.	3.0	21
155	Potential Energy Surfaces for Dissociation Reactions of High-Energy Isomers of N2O2. Journal of Physical Chemistry A, 1997, 101, 4283-4289.	2.5	21
156	Experimental and Theoretical Study of Oxygen Insertion into Trialkylsilanes by Methyltrioxorhenium Catalyst. Organometallics, 1999, 18, 4753-4757.	2.3	21
157	A vibrational analysis of the 7-azaindole-water complex: Anharmonicities using the quartic force field. International Journal of Quantum Chemistry, 2005, 104, 758-772.	2.0	21
158	Analytic Gradients for the Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2016, 12, 4743-4767.	5.3	21
159	ParFit: A Python-Based Object-Oriented Program for Fitting Molecular Mechanics Parameters to ab Initio Data. Journal of Chemical Information and Modeling, 2017, 57, 391-396.	5.4	21
160	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
161	Molecular and electronic structure of TiH2. Journal of Chemical Physics, 1995, 102, 6806-6811.	3.0	20
162	Investigation of a grid-free density functional theory (DFT) approach. Journal of Chemical Physics, 1998, 108, 9959-9969.	3.0	20

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163	Towards multireference equivalents of the G2 and G3 methods. Journal of Chemical Physics, 2001, 115, 8758-8772.	3.0	20
164	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
165	Gradient of the ZAPT2 energy. Theoretical Chemistry Accounts, 2002, 107, 57-70.	1.4	19
166	Can Orbitals Really Be Observed in Scanning Tunneling Microscopy Experiments?. Journal of Physical Chemistry A, 2017, 121, 4851-4852.	2.5	19
167	Why is Si₂H₂ Not Linear? An Intrinsic Quasi-Atomic Bonding Analysis. Journal of the American Chemical Society, 2020, 142, 13729-13742.	13.7	19
168	The Catalyzed Hydrosilation Reaction. Journal of the American Chemical Society, 1998, 120, 1552-1555.	13.7	18
169	Structures and Stabilities of Titanium Silsesquioxanes. Journal of Physical Chemistry A, 2001, 105, 11276-11284.	2.5	18
170	An ab initio study of the structure of two-, three- and five-dimersilicon clusters: An approach to the Si(100) surface. Theoretical Chemistry Accounts, 2003, 109, 268-273.	1.4	18
171	Theoretical Investigations of Acetylcholine (ACh) and Acetylthiocholine (ATCh) Using ab Initio and Effective Fragment Potential Methods. Journal of Physical Chemistry A, 2004, 108, 11419-11432.	2.5	18
172	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
173	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
174	Quasi-Atomic Bonding Analysis of Xe-Containing Compounds. Journal of Physical Chemistry A, 2018, 122, 3442-3454.	2.5	18
175	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
176	Theoretical study of Van der Waals complexes of Al atom with N2. Journal of Chemical Physics, 1997, 107, 2160-2161.	3.0	17
177	Hexamers and witchamers: Which hex do you choose?. Computational and Theoretical Chemistry, 2013, 1021, 70-83.	2.5	17
178	The Decomposition of Hydrazine in the Gas Phase and over an Iridium Catalyst. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	2.8	17
179	Charge transfer interaction using quasiatomic minimal-basis orbitals in the effective fragment potential method. Journal of Chemical Physics, 2013, 139, 194104.	3.0	17
180	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

#	Article	IF	Citations
181	Energy-Efficient Computational Chemistry: Comparison of x86 and ARM Systems. Journal of Chemical Theory and Computation, 2015, 11, 5055-5061.	5.3	17
182	Predictive Beyond-Mean-Field Rate Equations for Multisite Latticeâ€“Gas Models of Catalytic Surface Reactions: CO Oxidation on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28639-28653.	3.1	17
183	Many-Body Dispersion in Molecular Clusters. Journal of Physical Chemistry A, 2019, 123, 8406-8416.	2.5	17
184	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
185	The effect of spin-orbit coupling on the magnetic properties of H2Ti(Î¼â€“H)2TiH2. Journal of Chemical Physics, 1998, 109, 919-927.	3.0	16
186	Fast computation of analytical second derivatives with effective core potentials: Application to Si8C12, Ge8C12, and Sn8C12. Journal of Chemical Physics, 1999, 111, 8778-8784.	3.0	16
187	On the Electronic Structure of Bis(Î·5-cyclopentadienyl) Titanium. Journal of Physical Chemistry A, 2002, 106, 7921-7926.	2.5	16
188	Conformations of Organophosphine Oxides. Journal of Physical Chemistry A, 2015, 119, 8765-8773.	2.5	16
189	Threshold Ionization and Spinâ€“Orbit Coupling of Ceracyclopropene Formed by Ethylene Dehydrogenation. Journal of Physical Chemistry A, 2016, 120, 6963-6969.	2.5	16
190	Ab Initio Investigation of Cation Proton Affinity and Proton Transfer Energy for Energetic Ionic Liquids. Journal of Physical Chemistry A, 2016, 120, 6059-6063.	2.5	16
191	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
192	Many-Body Dispersion. Chemical Reviews, 2020, 120, 12343-12356.	47.7	16
193	Multiple Bonding in Rhodium Monoboride. Quasi-atomic Analyses of the Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 2021, 125, 4836-4846.	2.5	16
194	Ab initio study of cyclic siloxanes (H2SiO)n:n = 3, 4, 5. Journal of Computational Chemistry, 1996, 17, 1163-1170.	3.3	15
195	Molecular Electronic Structure and Energetics of the Isomers of Ti2H6. Journal of the American Chemical Society, 1998, 120, 3846-3857.	13.7	15
196	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
197	Structure and Stability of Mâ”H2Complexes. The Journal of Physical Chemistry, 1996, 100, 95-99.	2.9	14
198	Perspective on "The physical nature of the chemical bond". Theoretical Chemistry Accounts, 2000, 103, 248-251.	1.4	14

#	Article	IF	Citations
199	Ab Initio Study of the Catalytic Reactivity of Titanosilsesquioxanes and Titanosiloxanes. Journal of Physical Chemistry A, 2003, 107, 8756-8762.	2.5	14
200	Modeling Systems with Ï€â€“Ï€ Interactions Using the Hartreeâ€“Fock Method with an Empirical Dispersion Correction. Journal of Physical Chemistry A, 2015, 119, 5377-5385.	2.5	14
201	Editorial: Modern Architectures and Their Impact on Electronic Structure Theory. Chemical Reviews, 2020, 120, 9015-9020.	47.7	14
202	A Theoretical Study of the Reaction Paths for Cobalt Cation + Propane. Journal of Physical Chemistry A, 2000, 104, 2253-2260.	2.5	13
203	Coupling of Large-Amplitude Side Chain Motions to the Excited-State H-Atom Transfer of Perylene Quinones:â€‰ Application of Theory and Experiment to Calphostin C. Journal of Physical Chemistry A, 2001, 105, 1057-1060.	2.5	13
204	Molecular Structures for Azatitanatranes. Organometallics, 1997, 16, 158-162.	2.3	12
205	Multiterminal Nanowire Junctions of Silicon:Â A Theoretical Prediction of Atomic Structure and Electronic Properties. Nano Letters, 2007, 7, 2063-2067.	9.1	12
206	Analytic second derivative of the energy for density functional theory based on the three-body fragment molecular orbital method. Journal of Chemical Physics, 2015, 142, 124101.	3.0	12
207	Performance and energy efficiency analysis of 64-bit ARM using GAMESS. , 2015, , .		12
208	Ab initio calculation of anion proton affinity and ionization potential for energetic ionic liquids. Journal of Computational Chemistry, 2015, 36, 597-600.	3.3	12
209	Analytic non-adiabatic couplings for the spin-flip ORMAS method. Physical Chemistry Chemical Physics, 2020, 22, 1475-1484.	2.8	12
210	Auxiliary basis sets for grid-free density functional theory. Journal of Chemical Physics, 2000, 112, 10738-10745.	3.0	11
211	Chemistry on Silicon Surfaces. , 0, , 821-851.		11
212	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
213	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
214	Core and Uncore Joint Frequency Scaling Strategy. Journal of Computer and Communications, 2018, 06, 184-201.	0.9	11
215	Theoretical Study of Addition Reactions of SiX2to Acetylene (X = H, CH3, t-Bu, Cl, F). Organometallics, 1999, 18, 4881-4883.	2.3	10
216	Simultaneous etching and oxidation of vicinal Si(100) surfaces: Atomistic lattice-gas modeling of morphological evolution. Physical Review B, 2005, 72, .	3.2	10

#	Article	IF	Citations
217	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. Journal of Chemical Theory and Computation, 2014, 10, 90-101.	5.3	10
218	The Melting Temperature of Liquid Water with the Effective Fragment Potential. Journal of Physical Chemistry Letters, 2015, 6, 3555-3559.	4.6	10
219	Nontotally symmetric trifurcation of an S N 2 reaction pathway. Journal of Computational Chemistry, 2016, 37, 487-493.	3.3	10
220	Dispersion Interactions in Water Clusters. Journal of Physical Chemistry A, 2017, 121, 3736-3745.	2.5	10
221	Ionic liquids from a fragmented perspective. Physical Chemistry Chemical Physics, 2019, 21, 16878-16888.	2.8	10
222	Compressing the Four-Index Two-Electron Repulsion Integral Matrix using the Resolution-of-the-Identity Approximation Combined with the Rank Factorization Approximation. Journal of Chemical Theory and Computation, 2019, 15, 2254-2264.	5.3	10
223	Scaling the Hartree-Fock Matrix Build on Summit. , 2020, , .		10
224	Symmetry in Spin-Orbit Coupling. ACS Symposium Series, 2002, , 276-297.	0.5	9
225	Molecular Structures and Potential Energy Surfaces for IHI-Â·Arn(n= 1â^'7). Journal of Physical Chemistry A, 2004, 108, 11042-11048.	2.5	9
226	A theoretical study of the reaction of Ti+ with propane. Theoretical Chemistry Accounts, 2008, 120, 243-261.	1.4	9
227	Structure, Bonding, and Heats of Formation of Silatitanacyclobutanes. Journal of Physical Chemistry A, 1997, 101, 8714-8719.	2.5	8
228	Electronic Structure and Magnetic Properties of Y2Ti(Ì¼-X)2TiY2 (X, YH, F, Cl, Br) Isomers. Journal of Physical Chemistry A, 2003, 107, 104-114.	2.5	8
229	Theoretical Study of the Bis-Silylation Reaction of Ethylene Catalyzed by Titanium Dichloride. Organometallics, 2003, 22, 4111-4117.	2.3	8
230	Potential Energy Surfaces for the Reactions Si + O2. Journal of Physical Chemistry A, 2004, 108, 8395-8399.	2.5	8
231	A new approach for secondâ€order perturbation theory. Journal of Computational Chemistry, 2016, 37, 1274-1282.	3.3	8
232	An efficient MPI/openMP parallelization of the Hartree-Fock method for the second generation of Intel ^{Â®} Xeon Phi ^{â„¢} processor. , 2017, , .		8
233	Nodal variational principle for excited states. Physical Review A, 2018, 98, .	2.5	8
234	A New Kid on the Block: Application of Julia to Hartreeâ€“Fock Calculations. Journal of Chemical Theory and Computation, 2020, 16, 5006-5013.	5.3	8

#	Article	IF	Citations
235	On the structure and stability of geometrical isomers of N3F. Journal of Chemical Physics, 1995, 103, 7983-7989.	3.0	7
236	A Computational Study of the Proton-Transfer Chemistry of the Silaformyl Anion. Journal of the American Chemical Society, 1998, 120, 2124-2130.	13.7	7
237	Ab Initio Molecular Orbital Study of TiH2O and TiH3OH. Journal of Physical Chemistry A, 1998, 102, 6967-6972.	2.5	7
238	Integrating Performance Tools with Large-Scale Scientific Software. , 2007, , .		7
239	Multipole Moments in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2017, 121, 2056-2067.	2.5	7
240	Effect of Boron Clusters on the Ignition Reaction of HNO₃ and Dicynanamide-Based Ionic Liquids. Journal of Physical Chemistry A, 2017, 121, 8003-8011.	2.5	7
241	Application of a semiâ€empirical dispersion correction for modeling water clusters. Journal of Computational Chemistry, 2019, 40, 310-315.	3.3	7
242	Bonding analysis of water clusters using quasi-atomic orbitals. Physical Chemistry Chemical Physics, 2021, 23, 18734-18743.	2.8	7
243	Enabling large-scale correlated electronic structure calculations. , 2021, , .		7
244	Evaluation of gradient corrections in grid-free density functional theory. Journal of Chemical Physics, 1999, 110, 6580-6582.	3.0	6
245	The catalyzed hydrosilation reaction: substituent effects. Theoretical Chemistry Accounts, 1999, 102, 366-376.	1.4	6
246	Addition of POSSâ˜T₈to the Si(100) Surface. Journal of Physical Chemistry C, 2008, 112, 754-761.	3.1	6
247	Stability and Dissociation of Ethylenedione (OCCO). Journal of Physical Chemistry A, 2020, 124, 8209-8222.	2.5	6
248	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
249	Parallel Implementation of the Electronic Structure Code GAMESS. ACS Symposium Series, 1995, , 16-28.	0.5	5
250	Isomers on the Si2CH4+ Potential Energy Surface. Organometallics, 1996, 15, 5391-5398.	2.3	5
251	Perspective on â€œThe restricted active space selfâ€consistentâ€field method, implemented with a splitâ€graph unitary group approachâ€• International Journal of Quantum Chemistry, 2011, 111, 3280-3283.	2.0	5
252	Outcomes of OpenMP Hackathon: OpenMP Application Experiences with the Offloading Model (Part II). Lecture Notes in Computer Science, 2021, , 81-95.	1.3	5

#	Article	IF	Citations
253	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
254	Outcomes of OpenMP Hackathon: OpenMP Application Experiences with the Offloading Model (Part I). Lecture Notes in Computer Science, 2021, , 67-80.	1.3	5
255	Intramolecular hydrogen bonding analysis. Journal of Chemical Physics, 2022, 156, 174302.	3.0	5
256	Adsorption and Diffusion of Gallium Adatoms on the Si(100)-2 Ã— 1 Reconstructed Surface: A Multiconfiguration Self-Consistent Field Study Utilizing Molecular Surface Clusters. Journal of Physical Chemistry C, 2011, 115, 23488-23500.	3.1	4
257	MAIN GROUP ORGANOMETALLIC CHEMISTRY: BONDING, STRUCTURE AND REACTIVITY. Advanced Series in Physical Chemistry, 1995, , 311-344.	1.5	3
258	Potential Energy Surfaces for the Bis-Silylation of Ethylene. Journal of Physical Chemistry A, 1998, 102, 4666-4668.	2.5	3
259	Thermodynamics and kinetics of graphene chemistry: a graphene hydrogenation prototype study. Physical Chemistry Chemical Physics, 2016, 18, 33274-33281.	2.8	3
260	Spin-Free [2]_{R12} Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference Average Coupled Pair Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 3176-3184.	5.3	3
261	Excited state properties of 5-formylcytosine and 5-hydroxymethylcytosine. Molecular Physics, 2017, 115, 2721-2730.	1.7	3
262	Benchmarking the Effective Fragment Potential Dispersion Correction on the S22 Test Set. Journal of Physical Chemistry A, 2018, 122, 4076-4084.	2.5	3
263	Solvation of the Glycyl Radical. Journal of Physical Chemistry A, 2018, 122, 7212-7217.	2.5	3
264	Effect of frequency scaling granularity on energy-saving strategies. International Journal of High Performance Computing Applications, 2019, 33, 590-601.	3.7	3
265	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. Angewandte Chemie, 2019, 131, 12460-12466.	2.0	3
266	PDG: A Composite Method Based on the Resolution of the Identity. Journal of Physical Chemistry A, 2021, 125, 9421-9429.	2.5	3
267	A Task-Based Approach to Parallel Restricted Hartreeâ€“Fock Calculations. Journal of Chemical Theory and Computation, 2022, , .	5.3	3
268	Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles. Physical Chemistry Chemical Physics, 2022, 24, 10475-10487.	2.8	3
269	Applications of Parallel GAMESS. ACS Symposium Series, 1995, , 29-46.	0.5	2
270	The uncatalyzed hydrosilation reaction. Theoretica Chimica Acta, 1995, 91, 83-90.	0.8	2

#	Article	IF	Citations
271	Theoretical Study of the Interaction of Fe+with Silene. Organometallics, 1997, 16, 27-33.	2.3	2
272	Hyperfine coupling tensors for multi-configurational quasi-degenerate perturbation theory. Journal of Chemical Physics, 2003, 118, 40-45.	3.0	2
273	Cycloaddition Reactions of Dienes on the SI(100)-2 Ã— 1 Surface. International Journal of Modern Physics B, 2003, 17, 1205-1210.	2.0	2
274	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
275	Anharmonic vibrational computations with a quartic force field for curvilinear coordinates. Journal of Chemical Physics, 2019, 151, 064104.	3.0	2
276	Runtime power allocation approach for GAMESS hybrid CPUâ€€GPU implementation. Concurrency Computation Practice and Experience, 2020, 32, e5917.	2.2	2
277	Excited states of lutetium oxide and its singly charged cation. Journal of Chemical Physics, 2022, 156, 084303.	3.0	2
278	Catalysis of the Hydrosilation and Bis-Silylation Reactions. ACS Symposium Series, 1999, , 128-137.	0.5	1
279	Full configuration interaction and multiconfigurational spin density in boron and carbon atoms. Journal of Chemical Physics, 2000, 113, 4238-4241.	3.0	1
280	Runtime Power Limiting in GAMESS on Dual-Socket Nodes. , 2017, , .		1
281	Proton Transfer in 1,2,4-Triazolium Dinitramide: Effect of Aqueous Microsolvation. Journal of Physical Chemistry A, 2018, 122, 7443-7454.	2.5	1
282	Model protein excited states: MRCI calculations with large active spaces vs CC2 method. Journal of Chemical Physics, 2021, 154, 214105.	3.0	1
283	Cubic fuels?. International Journal of Quantum Chemistry, 2000, 76, 434.	2.0	1
284	Electronic Structure Theory Calculations Using Modern Architectures: KNL vs Haswell. Journal of Chemical Theory and Computation, 2021, 17, 6910-6917.	5.3	1
285	Rotational and translational diffusion of liquid n-hexane: EFP-based molecular dynamics analysis. Journal of Chemical Physics, 2022, 156, 114503.	3.0	1
286	Competitive Etching and Oxidation of Vicinal Si(100) Surfaces. Materials Research Society Symposia Proceedings, 2004, 859, 34.	0.1	0
287	Electronic Polarization Effect of the Water Environment in Charge-Separated Donorâ€“Acceptor Systems: An Effective Fragment Potential Model Study. Journal of Physical Chemistry A, 2016, 120, 10273-10280.	2.5	0
288	Ab initio Molecular Dynamics Study of H2 Formation inside POSS Compounds. 2. The Effect of an Encapsulated Hydrogen Molecule. Journal of Physical Chemistry A, 2016, 120, 8699-8715.	2.5	0

#	Article	IF	Citations
289	Energy components in spin-density functional theory. Physical Review A, 2021, 104, .	2.5	0
290	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
291	Anomalous Kinetics of Catalytic Conversion Reactions in Linear Nanopores Mediated by Inhibited Transport: Multiscale Modeling. , 2019, , 173-190.		0
292	Coarse-Grained Water Model Development for Accurate Dynamics and Structure Prediction. ACS Omega, 0, , .	3.5	0