H Bernhard Schlegel

List of Publications by Year
in descending order

222 papers	34,171 citations	22099 59 h-index	3563 181 g-index
227 all docs	227 docs citations	227 times ranked	18259 citing authors

#	Article	IF	Citations
1	Calculations of pK_a Values for a Series of Naturally Occurring Modified Nucleobases. Journal of Physical Chemistry A, 2022, 126, 1518-1529.	1.1	16
2	Distinct Bimetallic Cooperativity Among Water Reduction Catalysts Containing [Co ^{III} Co ^{III}], [Ni ^{II} Ni ^{II}], and [Zn ^{II} Zn ^{II}] Cores. Chemistry - A European Journal, 2022, , .	1.7	1
3	Stereoselective 1,2-cis Furanosylations Catalyzed by Phenanthroline. Journal of the American Chemical Society, 2022, 144, 7441-7456.	6.6	15
4	Ionization of HCCI Neutral and Cations by Strong Laser Fields Simulated With Time Dependent Configuration Interaction. Frontiers in Chemistry, 2022, 10, 866137.	1.8	3
5	Phenanthroline-Catalyzed Stereoselective Formation of Î±-1,2-cis 2-Deoxy-2-Fluoro Glycosides. ACS Catalysis, 2021, 11, 2108-2120.	5.5	12
6	The Bond Dissociation Energy of the Nâ€“O Bond. Journal of Physical Chemistry A, 2021, 125, 5014-5021.	1.1	30
7	Alkyl Radical-Free Cu(I) Photocatalytic Cross-Coupling: A Theoretical Study of Anomerically Specific Photocatalyzed Glycosylation of Pyranosyl Bromide. Inorganic Chemistry, 2021, 60, 12801-12812.	1.9	2
8	Sequential double ionization of molecules by strong laser fields simulated with time-dependent configuration interaction. Journal of Chemical Physics, 2021, 155, 114103.	1.2	7
9	Ab Initio Direct Dynamics. Accounts of Chemical Research, 2021, 54, 3749-3759.	7.6	3
10	Ellipticity controlled dissociative double ionization of ethane by strong fields. Physical Chemistry Chemical Physics, 2021, 23, 23537-23543.	1.3	7
11	Mechanism of Orbital Interactions in the Sharpless Epoxidation with Ti(IV) Peroxides: A DFT Study. Journal of Physical Chemistry A, 2021, 125, 10541-10556.	1.1	4
12	Ascorbic acid: The chemistry underlying its antioxidant properties. Free Radical Biology and Medicine, 2020, 159, 37-43.	1.3	224
13	Angular Dependence of Strong Field Ionization of 2-Phenylethyl-N,N-dimethylamine (PENNA) Using Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2020, 124, 4777-4781.	1.1	9
14	Bond Dissociation Energy of Peroxides Revisited. Journal of Physical Chemistry A, 2020, 124, 4742-4751.	1.1	37
15	Computational Investigation into the Oxidation of Guanine to Form Imidazolone (Iz) and Related Degradation Products. Chemical Research in Toxicology, 2020, 33, 1010-1027.	1.7	5
16	Angular dependence of strong field sequential double ionization for neon and acetylene simulated with time-dependent configuration interaction using CIS and CISD-IP. Journal of Chemical Physics, 2020, 152, 064106.	1.2	12
17	Diastereoselective sp³ Câ€“O Bond Formation via Visible Light-Induced, Copper-Catalyzed Cross-Couplings of Glycosyl Bromides with Aliphatic Alcohols. ACS Catalysis, 2020, 10, 5990-6001.	5.5	30
18	Effect of spinâ€“orbit coupling on strong field ionization simulated with time-dependent configuration interaction. Journal of Chemical Physics, 2020, 153, 244109.	1.2	9

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19	Angular dependence of strong field ionization of N2 by time-dependent configuration interaction using density functional theory and the Tamm-Dancoff approximation. Journal of Chemical Physics, 2019, 151, .	1.2	15
20	Computational Study of the Oxidation of Guanine To Form 5-Carboxyamido-5-formamido-2-iminohydantoin (2Ih). Chemical Research in Toxicology, 2019, 32, 2295-2304.	1.7	6
21	Are BrÃ¸nsted Acids the True Promoter of Metal-Triflate-Catalyzed Glycosylations? A Mechanistic Probe into 1,2-cis-Aminoglycoside Formation by Nickel Triflate. ACS Catalysis, 2019, 9, 2110-2123.	5.5	35
22	Virtual Issue on Strong Field Chemistry. Journal of Physical Chemistry A, 2019, 123, 4095-4095.	1.1	0
23	Virtual Issue on Strong Field Chemistry. Journal of Physical Chemistry Letters, 2019, 10, 2393-2393.	2.1	2
24	Computational Study of the Formation of C8, C5, and C4 Guanine:Lysine Adducts via Oxidation of Guanine by Sulfate Radical Anion. Journal of Physical Chemistry A, 2019, 123, 5150-5163.	1.1	7
25	Phenanthrolineâ€Catalyzed Stereoretentive Glycosylations. Angewandte Chemie - International Edition, 2019, 58, 6957-6961.	7.2	38
26	Phenanthrolineâ€Catalyzed Stereoretentive Glycosylations. Angewandte Chemie, 2019, 131, 7031-7035.	1.6	5
27	Ab initio molecular dynamics study of the reactions of allene cation induced by intense 7 micron laser pulses. Molecular Physics, 2019, 117, 1088-1096.	0.8	1
28	Computational Study of the pH-Dependent Competition between Carbonate and Thymine Addition to the Guanine Radical. Chemical Research in Toxicology, 2019, 32, 195-210.	1.7	9
29	Controlling the strong field fragmentation of ClCHO + using two laser pulses â€“an ab initio molecular dynamics simulation. Journal of Computational Chemistry, 2019, 40, 200-205.	1.5	6
30	Angular Dependence of Strong Field Ionization of Haloacetylenes HCCX (X = F, Cl, Br, I), Using Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry C, 2018, 122, 13751-13757.	1.5	19
31	Photophysical characterization of a highly luminescent divalent-europium-containing azacryptate. Chemical Communications, 2018, 54, 4545-4548.	2.2	36
32	DFT Investigation of Ligand Photodissociation in [Ru^{II}(tpy)(bpy)(py)]²⁺ and [Ru^{II}(tpy)(Me₂bpy)(py)]²⁺ Complexes. Inorganic Chemistry, 2018, 57, 231-240.	1.9	35
33	Disentangling Strong-Field Multielectron Dynamics with Angular Streaking. Journal of Physical Chemistry Letters, 2018, 9, 2539-2545.	2.1	26
34	Luminescence differences between two complexes of divalent europium. Journal of Organometallic Chemistry, 2018, 857, 88-93.	0.8	25
35	Synthetic and Computational Study of Tin-Free Reductive Tandem Cyclizations of Neutral Aminyl Radicals. Organic Letters, 2018, 20, 6340-6344.	2.4	8
36	Immobilization of an Amphiphilic Molecular Cobalt Catalyst on Carbon Black for Ligand-Assisted Water Oxidation. Inorganic Chemistry, 2018, 57, 9748-9756.	1.9	18

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37	Angular Dependence of Ionization by Circularly Polarized Light Calculated with Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2017, 121, 1336-1343.	1.1	23
38	Computational Study of Oxidation of Guanine by Singlet Oxygen (¹Î”_g) and Formation of Guanine:Lysine Crossâ€Links. Chemistry - A European Journal, 2017, 23, 5804-5813.	1.7	34
39	Deactivation of a Cobalt Catalyst for Water Reduction through Valence Tautomerism. Chemistry - A European Journal, 2017, 23, 9266-9271.	1.7	14
40	Bimetallic Cooperativity in Proton Reduction with an Amidoâ€Bridged Cobalt Catalyst. Chemistry - A European Journal, 2017, 23, 9272-9279.	1.7	21
41	A theoretical study of ascorbic acid oxidation andHOOË™/O₂Ë™^{â¯}radical scavenging. Organic and Biomolecular Chemistry, 2017, 15, 4417-4431.	1.5	108
42	A new electron-ion coincidence 3D momentum-imaging method and its application in probing strong field dynamics of 2-phenylethyl-N, N-dimethylamine. Journal of Chemical Physics, 2017, 147, 013920.	1.2	15
43	Improved pK_a Prediction of Substituted Alcohols, Phenols, and Hydroperoxides in Aqueous Medium Using Density Functional Theory and a Cluster-Continuum Solvation Model. Journal of Physical Chemistry A, 2017, 121, 4698-4706.	1.1	77
44	Attosecond Electron Correlation Dynamics in Double Ionization of Benzene Probed with Two-Electron Angular Streaking. Physical Review Letters, 2017, 119, 123201.	2.9	34
45	Angular Dependence of Strong Field Ionization of CH₃X (X = F, Cl, Br, or I) Using Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2017, 121, 5940-5946.	1.1	26
46	Frontispiece: Bimetallic Cooperativity in Proton Reduction with an Amidoâ€Bridged Cobalt Catalyst. Chemistry - A European Journal, 2017, 23, .	1.7	0
47	Ultrafast 25-fs relaxation in highly excited states of methyl azide mediated by strong nonadiabatic coupling. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E11072-E11081.	3.3	13
48	A pentadentate nitrogen-rich copper electrocatalyst for water reduction with pH-dependent molecular mechanisms. Dalton Transactions, 2017, 46, 16812-16820.	1.6	21
49	Electronic Modulation of the SOMOâ€“HOMO Energy Gap in Iron(III) Complexes towards Unimolecular Current Rectification. Chemistry - A European Journal, 2016, 22, 10786-10790.	1.7	13
50	Computational simulations of hydrogen circular migration in protonated acetylene induced by circularly polarized light. Journal of Chemical Physics, 2016, 145, 084309.	1.2	4
51	Path optimization by a variational reaction coordinate method. II. Improved computational efficiency through internal coordinates and surface interpolation. Journal of Chemical Physics, 2016, 144, 184101.	1.2	5
52	Angle-dependent strong-field ionization of triple bonded systems calculated by time-dependent configuration interaction with an absorbing potential. Canadian Journal of Chemistry, 2016, 94, 989-997.	0.6	8
53	Computational Study of the Radical Mediated Mechanism of the Formation of C8, C5, and C4 Guanine:Lysine Adducts in the Presence of the Benzophenone Photosensitizer. Chemical Research in Toxicology, 2016, 29, 1396-1409.	1.7	16
54	Are Very Small Emission Quantum Yields Characteristic of Pure Metal-to-Ligand Charge-Transfer Excited States of Ruthenium(II)-(Acceptor Ligand) Chromophores?. Inorganic Chemistry, 2016, 55, 7341-7355.	1.9	8

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55	Theoretical Calculation of pK_aâ€™s of Selenols in Aqueous Solution Using an Implicit Solvation Model and Explicit Water Molecules. Journal of Physical Chemistry A, 2016, 120, 8916-8922.	1.1	38
56	Efficient electro/photocatalytic water reduction using a [Ni^{II}(N₂Py₃)]²⁺ complex. Chemical Communications, 2016, 52, 13357-13360.	2.2	30
57	Density Functional Theory Calculation of pK_aâ€™s of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. Journal of Physical Chemistry A, 2016, 120, 5726-5735.	1.1	146
58	Controlling Chemical Reactions by Short, Intense Mid-Infrared Laser Pulses: Comparison of Linear and Circularly Polarized Light in Simulations of ClCHO⁺ Fragmentation. Journal of Physical Chemistry A, 2016, 120, 1120-1126.	1.1	6
59	Effects of Methyl Substitution in Ruthenium Tris(2-pyridylmethyl)amine Photocaging Groups for Nitriles. Inorganic Chemistry, 2016, 55, 6968-6979.	1.9	24
60	Selective Release of Aromatic Heterocycles from Ruthenium Tris(2-pyridylmethyl)amine with Visible Light. Inorganic Chemistry, 2016, 55, 10-12.	1.9	29
61	Investigation into 9(S)-HPODE-derived allene oxide to cyclopentenone cyclization mechanism via diradical oxyallyl intermediates. Organic and Biomolecular Chemistry, 2016, 14, 3544-3557.	1.5	10
62	Evaluation of the coordination preferences and catalytic pathways of heteroaxial cobalt oximes towards hydrogen generation. Chemical Science, 2016, 7, 3264-3278.	3.7	35
63	Exploration of some refinements to geometry optimization methods. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	15
64	Path optimization by a variational reaction coordinate method. I. Development of formalism and algorithms. Journal of Chemical Physics, 2015, 143, 244101.	1.2	12
65	Distinct Proton and Water Reduction Behavior with a Cobalt(III) Electrocatalyst Based on Pentadentate Oximes. Angewandte Chemie, 2015, 127, 7245-7249.	1.6	8
66	Distinct Proton and Water Reduction Behavior with a Cobalt(III) Electrocatalyst Based on Pentadentate Oximes. Angewandte Chemie - International Edition, 2015, 54, 7139-7143.	7.2	21
67	Angle-Dependent Ionization of Hydrides AH_n Calculated by Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2015, 119, 10212-10220.	1.1	30
68	Energy Dependence of the Ruthenium(II)-Bipyridine Metal-to-Ligand-Charge-Transfer Excited State Radiative Lifetimes: Effects of Ï€Ï€*(bipyridine) Mixing. Journal of Physical Chemistry B, 2015, 119, 7393-7406.	1.2	17
69	Angle-Dependent Ionization of Small Molecules by Time-Dependent Configuration Interaction and an Absorbing Potential. Journal of Physical Chemistry Letters, 2015, 6, 2140-2146.	2.1	56
70	Modulation of electronic and redox properties in phenolate-rich cobalt(iii) complexes and their implications for catalytic proton reduction. Dalton Transactions, 2015, 44, 3454-3466.	1.6	17
71	Using bonding to guide transition state optimization. Journal of Computational Chemistry, 2015, 36, 1157-1166.	1.5	17
72	Relativistic and Solvation Effects on the Stability of Gold(III) Halides in Aqueous Solution. Inorganic Chemistry, 2015, 54, 9869-9875.	1.9	14

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73	Selective Photodissociation of Acetonitrile Ligands in Ruthenium Polypyridyl Complexes Studied by Density Functional Theory. Inorganic Chemistry, 2015, 54, 8003-8011.	1.9	38
74	Metal-to-Ligand Charge-Transfer Emissions of Ruthenium(II) Pentaammine Complexes with Monodentate Aromatic Acceptor Ligands and Distortion Patterns of their Lowest Energy Triplet Excited States. Inorganic Chemistry, 2015, 54, 8495-8508.	1.9	15
75	Ligand Transformations and Efficient Proton/Water Reduction with Cobalt Catalysts Based on Pentadentate Pyridineâ€Rich Environments. Angewandte Chemie - International Edition, 2015, 54, 2105-2110.	7.2	61
76	Calculations of pK_aâ€™s and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation. Journal of Physical Chemistry A, 2015, 119, 5134-5144.	1.1	111
77	The Mechanisms of Rectification in Au|Molecule|Au Devices Based on Langmuirâ€“Blodgett Monolayers of Iron(III) and Copper(II) Surfactants. Angewandte Chemie - International Edition, 2014, 53, 14462-14467.	7.2	22
78	A density functional theory and spectroscopic study of intramolecular quenching of metal-to-ligand charge-transfer excited states in some mono-bipyridine ruthenium(II) complexes. Canadian Journal of Chemistry, 2014, 92, 996-1009.	0.6	9
79	Strong-field ionization rates of linear polyenes simulated with time-dependent configuration interaction with an absorbing potential. Journal of Chemical Physics, 2014, 141, 174104.	1.2	37
80	Strong field ionization rates simulated with time-dependent configuration interaction and an absorbing potential. Journal of Chemical Physics, 2014, 140, 174113.	1.2	89
81	Molecular Dynamics of Methylamine, Methanol, and Methyl Fluoride Cations in Intense 7 Micron Laser Fields. Journal of Physical Chemistry A, 2014, 118, 10067-10072.	1.1	4
82	Molecular Dynamics of Methanol Monocation (CH_3OH^+) in Strong Laser Fields. Journal of Physical Chemistry A, 2014, 118, 1769-1776.	1.1	11
83	Molecular dynamics of methanol cation (CH 3 OH +) in strong fields: Comparison of 800 nm and 7 Î¼m laser fields. Chemical Physics Letters, 2014, 610-611, 219-222.	1.2	5
84	Molecular Dynamics in Strong Laser Fields: A New Algorithm for abÂInitio Classical Trajectories. Journal of Chemical Theory and Computation, 2013, 9, 3293-3298.	2.3	10
85	Bond-Selective Dissociation of Polyatomic Cations in Mid-Infrared Strong Fields. Journal of Physical Chemistry A, 2013, 117, 11202-11209.	1.1	13
86	Computational Prediction of One-Electron Reduction Potentials and Acid Dissociation Constants for Guanine Oxidation Intermediates and Products. Journal of Physical Chemistry B, 2013, 117, 9518-9531.	1.2	43
87	Can Metallapyrimidines Be Aromatic? A Computational Study into a New Class of Metallacycles. Journal of Chemical Theory and Computation, 2012, 8, 4950-4959.	2.3	20
88	Metallapyrimidines and Metallapyrimidiniums from Oxidative Addition of Pyrazolate Nâ€“N Bonds to Niobium(III), Niobium(IV), and Tantalum(IV) Metal Centers and Assessment of Their Aromatic Character. Organometallics, 2012, 31, 5971-5974.	1.1	18
89	A Reaction Accelerator: Mid-infrared Strong Field Dissociation Yields Mode-Selective Chemistry. Journal of Physical Chemistry Letters, 2012, 3, 2541-2547.	2.1	24
90	Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. Journal of Chemical Theory and Computation, 2012, 8, 5107-5123.	2.3	72

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91	Sequential Phenolate Oxidations in Octahedral Cobalt(III) Complexes with [N2O3] Ligands. European Journal of Inorganic Chemistry, 2012, 2012, 4622-4631.	1.0	15
92	Back Cover: Bioinspired Five-Coordinate Iron(III) Complexes for Stabilization of Phenoxyl Radicals (Angew. Chem. Int. Ed. 13/2012). Angewandte Chemie - International Edition, 2012, 51, 3276-3276.	7.2	0
93	Coordinate reduction for exploring chemical reaction paths. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
94	HCO+ dissociation in a strong laser field: An ab initio classical trajectory study. Chemical Physics Letters, 2012, 536, 14-18.	1.2	9
95	Ab initio classical trajectory calculations of 1,3-cyclobutanedione radical cation dissociation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	4
96	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields II: Comparison of DFT Functionals and EOM-CCSD. Journal of Physical Chemistry A, 2011, 115, 11832-11840.	1.1	42
97	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields: Comparison of RPA, CIS, CIS(D), and EOM-CCSD. Journal of Physical Chemistry A, 2011, 115, 4678-4690.	1.1	62
98	Geometry optimization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 790-809.	6.2	250
99	Steepest descent reaction path integration using a first-order predictorâ€“corrector method. Journal of Chemical Physics, 2010, 133, 224101.	1.2	63
100	A toolkit to assist ONIOM calculations. Journal of Computational Chemistry, 2010, 31, 2363-2369.	1.5	51
101	Common basis for the mechanism of metallo and non-metallo KDO8P synthases. Journal of Inorganic Biochemistry, 2010, 104, 1267-1275.	1.5	5
102	Matrix Metalloproteinase 2 (MMP2) Inhibition: DFT and QM/MM Studies of the Deprotonation-Initialized Ring-Opening Reaction of the Sulfoxide Analogue of SB-3CT. Journal of Physical Chemistry B, 2010, 114, 1030-1037.	1.2	20
103	Ab Initio Classical Trajectory Study of the Fragmentation of C3H4Dications on the Singlet and Triplet Surfaces. Journal of Physical Chemistry A, 2010, 114, 7653-7660.	1.1	13
104	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. Journal of Chemical Theory and Computation, 2010, 6, 2566-2580.	2.3	44
105	QM/MM Studies of the Matrix Metalloproteinase 2 (MMP2) Inhibition Mechanism of (S)-SB-3CT and its Oxirane Analogue. Journal of Chemical Theory and Computation, 2010, 6, 3580-3587.	2.3	23
106	Large Nonstatistical Branching Ratio in the Dissociation of Pentane-2,4-dione Radical Cation: An Ab Initio Direct Classical Trajectory Study. Journal of Physical Chemistry A, 2009, 113, 1453-1458.	1.1	8
107	Mechanistic Aspects of the Formation of Guanidinohydantoin from Spiroiminodihydantoin under Acidic Conditions. Chemical Research in Toxicology, 2009, 22, 526-535.	1.7	27
108	Ab Initio Classical Trajectory Study of the Dissociation of Neutral and Positively Charged Methanimine (CH₂NHⁿ⁺ n = 0â“2). Journal of Physical Chemistry A, 2009, 113, 9958-9964.	1.1	22

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109	The Energy Landscape of 3-Deoxy-<scp>d</scp>-manno-octulosonate 8-Phosphate Synthase. Biochemistry, 2009, 48, 11706-11714.	1.2	13
110	Matrix Metalloproteinase 2 Inhibition: Combined Quantum Mechanics and Molecular Mechanics Studies of the Inhibition Mechanism of (4-Phenoxyphenylsulfonyl)methylthiirane and Its Oxirane Analogue. Biochemistry, 2009, 48, 9839-9847.	1.2	62
111	Distributed Gaussian Valence Bond Surface Derived from Ab Initio Calculations. Journal of Chemical Theory and Computation, 2009, 5, 949-961.	2.3	32
112	Calculation of pK_a Values of Nucleobases and the Guanine Oxidation Products Guanidinohydantoin and Spiroiminodihydantoin using Density Functional Theory and a Polarizable Continuum Model. Journal of Physical Chemistry B, 2008, 112, 16860-16873.	1.2	179
113	Dissociation of Acetone Radical Cation (CH3COCH3+Â· â†' CH3CO+ + CH3Â·): An Ab Initio Direct Classical Trajectory Study of the Energy Dependence of the Branching Ratio. Journal of Physical Chemistry A, 2008, 112, 13121-13127.	1.1	14
114	An Exploration of Mechanisms for the Transformation of 8-Oxoguanine to Guanidinohydantoin and Spiroiminodihydantoin by Density Functional Theory. Journal of the American Chemical Society, 2008, 130, 5245-5256.	6.6	85
115	Empirical valence bond models for reactive potential energy surfaces. II. Intramolecular proton transfer in pyridone and the Claisen reaction of allyl vinyl ether. Molecular Physics, 2007, 105, 2719-2729.	0.8	14
116	Electronic optical response of molecules in intense fields: Comparison of TD-HF, TD-CIS, and TD-CIS(D) approaches. Journal of Chemical Physics, 2007, 126, 244110.	1.2	96
117	Exploration of Mechanisms for the Transformation of 8-Hydroxy Guanine Radical to FAPyG by Density Functional Theory. Chemical Research in Toxicology, 2007, 20, 432-444.	1.7	46
118	Optimization of Equilibrium Geometries and Transition Structures. Advances in Chemical Physics, 2007, , 249-286.	0.3	124
119	AMBER Force Field Parameters for the Naturally Occurring Modified Nucleosides in RNA. Journal of Chemical Theory and Computation, 2007, 3, 1464-1475.	2.3	168
120	Protonated acetylene revisited. Theoretical Chemistry Accounts, 2007, 118, 75-80.	0.5	22
121	Structural, spectroscopic, and electrochemical behavior of trans-phenolato cobalt(iii) complexes of asymmetric NNâ€²O ligands as archetypes for metallomesogens. Dalton Transactions, 2006, , 2517-2525.	1.6	55
122	Molecular Orbital Studies of Zinc Oxide Chemical Vapor Deposition:â€‰ Gas-Phase Radical Reactions. Chemistry of Materials, 2006, 18, 1878-1884.	3.2	17
123	A Single Transition State Serves Two Mechanisms. The Branching Ratio for CH2Oâ€¢-+ CH3Cl on Improved Potential Energy Surfaces. Journal of Physical Chemistry A, 2006, 110, 2801-2806.	1.1	20
124	Empirical Valence-Bond Models for Reactive Potential Energy Surfaces Using Distributed Gaussians. Journal of Chemical Theory and Computation, 2006, 2, 905-911.	2.3	62
125	Optical Excitations in Carbon Architectures Based on Dodecadehydrotribenzo[18]annuleneâ€. Journal of Physical Chemistry A, 2006, 110, 1305-1318.	1.1	41
126	Electronic excitations in anti-aromatic dehydro[12]- and aromatic dehydro[18]annulenes: a time-dependent density functional theory study. Molecular Physics, 2006, 104, 933-941.	0.8	9

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127	Lysine carboxylation in proteins: OXA-10 Î²-lactamase. Proteins: Structure, Function and Bioinformatics, 2005, 61, 246-257.	1.5	41
128	Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces. , 2005, , 195-249.		266
129	X-ray Crystal Structure of the Acylated Î²-Lactam Sensor Domain of BlaR1 fromStaphylococcus aureusand the Mechanism of Receptor Activation for Signal Transduction. Journal of the American Chemical Society, 2004, 126, 13945-13947.	6.6	51
130	Fragmentation Pathways in a Series of CH3COX Molecules in the Strong Field Regimeâ€. Journal of Physical Chemistry A, 2004, 108, 3162-3165.	1.1	17
131	Dissociation of acetone radical cation (CH3COCH3+Ë™ â†' CH3CO++CH3Ë™): An ab initio direct classical trajectory study. Physical Chemistry Chemical Physics, 2004, 6, 5166-5171.	1.3	21
132	Ab Initio Classical Trajectory Calculations of Acetylene Dication Dissociation. Journal of Physical Chemistry A, 2004, 108, 468-472.	1.1	10
133	Combined Experimental and Computational Investigation of the Mechanism of Nickel-Catalyzed Three-Component Addition Processes. Organometallics, 2004, 23, 4636-4646.	1.1	106
134	Single Transition State Serves Two Mechanisms. Ab Initio Classical Trajectory Calculations of the Substitutionâ^'Electron Transfer Branching Ratio in CH2Oâ€¢+ CH3Cl. Journal of Physical Chemistry A, 2004, 108, 8526-8532.	1.1	29
135	Accurate reaction paths using a Hessian based predictorâ€“corrector integrator. Journal of Chemical Physics, 2004, 120, 9918-9924.	1.2	796
136	Sequential nonadiabatic excitation of large molecules and ions driven by strong laser fields. Physical Review A, 2004, 69, .	1.0	92
137	Hybrid Ab-Initio/Empirical Molecular Dynamics:â€‰ Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. Journal of Physical Chemistry B, 2004, 108, 4210-4220.	1.2	131
138	Geometry optimization with QM/MM, ONIOM, and other combined methods. I. Microiterations and constraints. Journal of Computational Chemistry, 2003, 24, 760-769.	1.5	560
139	Exploring potential energy surfaces for chemical reactions: An overview of some practical methods. Journal of Computational Chemistry, 2003, 24, 1514-1527.	1.5	311
140	Geometry optimization methods for modeling large molecules. Computational and Theoretical Chemistry, 2003, 666-667, 31-39.	1.5	24
141	Synthesis, Structure, and Properties of Magnesocene Amine Adducts. Structural Distortions Arising from Nâ^'HÂ·Â·Â·C5H5-Hydrogen Bonding and Molecular Orbital Calculations Thereof. Organometallics, 2003, 22, 4060-4069.	1.1	22
142	Density matrix search using direct inversion in the iterative subspace as a linear scaling alternative to diagonalization in electronic structure calculations. Journal of Chemical Physics, 2003, 119, 7651-7658.	1.2	52
143	Nonadiabatic dynamics of polyatomic molecules and ions in strong laser fields. Physical Review A, 2003, 68, .	1.0	74
144	Unimolecular Dissociation of Formyl Halides HXCO â†' CO + HX (X= F, Cl):â€‰ An Ab Initio Direct Classical Trajectory Study. Journal of Physical Chemistry A, 2002, 106, 11623-11629.	1.1	19

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145	Methods for optimizing large molecules. Part III. An improved algorithm for geometry optimization using direct inversion in the iterative subspace (GDIIS). Physical Chemistry Chemical Physics, 2002, 4, 11-15.	1.3	114
146	Ab initio molecular dynamics: Propagating the density matrix with gaussian orbitals. IV. Formal analysis of the deviations from born-oppenheimer dynamics. Israel Journal of Chemistry, 2002, 42, 191-202.	1.0	71
147	Effects of the Protein Environment on the Structure and Energetics of Active Sites of Metalloenzymes. ONIOM Study of Methane Monooxygenase and Ribonucleotide Reductase. Journal of the American Chemical Society, 2002, 124, 192-193.	6.6	124
148	An ab initio direct classical trajectory study of s-tetrazine photodissociation. Physical Chemistry Chemical Physics, 2002, 4, 2554-2559.	1.3	8
149	Molecular Orbital Study of the First Excited State of the OLED Material Tris(8-hydroxyquinoline)aluminum(III). Chemistry of Materials, 2001, 13, 2632-2640.	3.2	221
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