List of Publications by Year in descending order

183 papers	5,167 citations	87723 38 h-index	128067 60 g-index
188 all docs	188 docs citations	188 times ranked	2137 citing authors

#	Article	IF	Citations
1	Recalibration of a single-valued double many-body expansion potential energy surface for ground-state hydroperoxy and dynamics calculations for the oxygen atom + hydroxyl .fwdarw. oxygen + hydrogen atom reaction. The Journal of Physical Chemistry, 1990, 94, 8073-8080.	2.9	244
2	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
3	Extrapolating to the one-electron basis-set limit in electronic structure calculations. Journal of Chemical Physics, 2007, 126, 244105.	1.2	176
4	Intermolecular and Intramolecular Potentials: Topographical Aspects, Calculation, and Functional Representation via A Double Many-Body Expansion Method. Advances in Chemical Physics, 2007, , 255-338.	0.3	160
5	Basis-set extrapolation of the correlation energy. Journal of Chemical Physics, 2000, 113, 8880-8887.	1.2	151
6	Quasiclassical trajectory calculations of the thermal rate coefficients for the reactions H(D)+O2â†'OH(D)+O and O+OH(D)â†'O2+H(D) as a function of temperature. Journal of Chemical Physics, 1992, 96, 5137-5150.	1.2	125
7	Excitation function for H+O2 reaction: A study of zeroâ€point energy effects and rotational distributions in trajectory calculations. Journal of Chemical Physics, 1993, 99, 1076-1085.	1.2	120
8	Energy switching approach to potential surfaces: An accurate singleâ€valued function for the water molecule. Journal of Chemical Physics, 1996, 105, 3524-3531.	1.2	111
9	A realistic hydroperoxo(~X2A") potential energy surface from the double many-body expansion method. The Journal of Physical Chemistry, 1988, 92, 3732-3742.	2.9	83
10	A semiempirical method for correcting configuration interaction potential energy surfaces. Journal of Chemical Physics, 1989, 90, 4379-4391.	1.2	83
11	Four-atom bimolecular reactions with relevance in environmental chemistry: Theoretical work. International Reviews in Physical Chemistry, 2000, 19, 199-245.	0.9	82
12	Narrowing the error in electron correlation calculations by basis set re-hierarchization and use of the unified singlet and triplet electron-pair extrapolation scheme: Application to a test set of 106 systems. Journal of Chemical Physics, 2014, 141, 224113.	1.2	76
13	Accurate DMBE Potential Energy Surface For the N(2D) + H2(1Î£ g +) Reaction Using an Improved Switching Function Formalism. Theoretical Chemistry Accounts, 2006, 116, 404-419.	0.5	73
14	Extrapolation to the Complete Basis Set Limit without Counterpoise. The Pair Potential of Helium Revisited^{â€}. Journal of Physical Chemistry A, 2010, 114, 8505-8516.	1.1	69
15	Method for quasiclassical trajectory calculations on potential energy surfaces defined from gradients and Hessians, and model to constrain the energy in vibrational modes. Journal of Chemical Physics, 1994, 100, 1908-1920.	1.2	66
16	Single-Valued DMBE Potential Energy Surface for HSO:Â A Distributedn-Body Polynomial Approach. Journal of Physical Chemistry A, 2001, 105, 5923-5932.	1.1	64
17	Accurate ab initio potential energy curves for the classic Liâ€“F ionic-covalent interaction by extrapolation to the complete basis set limit and modeling of the radial nonadiabatic coupling. Journal of Chemical Physics, 2009, 131, 124128.	1.2	62
18	Extrapolation to the complete-basis-set limit and the implications of avoided crossings: The Xâ€‰Î£1g+, Bâ€‰Î”1g, and Bâ€²â€‰Î£1g+ states of C2. Journal of Chemical Physics, 2008, 129, 234103.	1.2	60

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19	Implications of the O + OH reaction in hydroxyl nightglow modeling. Atmospheric Chemistry and Physics, 2013, 13, 1-13.	1.9	60
20	Double many-body expansion potential energy surface for ground state HSO2. Physical Chemistry Chemical Physics, 2005, 7, 2305.	1.3	56
21	Double many-body expansion potential energy surface for ground-state HCN based on realistic long range forces and accurateab initiocalculations. Journal of Chemical Physics, 1997, 106, 9647-9658.	1.2	55
22	A detailed stateâ€toâ€state lowâ€energy dynamics study of the reaction O(3P)+OH(2Î)â†'O2(XÌƒâ€‰3Î£gâ^')+H(2S) using a quasiclassical trajectoryâ€"internalâ€energy quantumâ€mechanicalâ€threshold method. Journal of Chemical Physics, 1992, 97, 4050-4065.	1.2	52
23	Quasiclassical trajectory calculations of the thermal rate coefficient for the oxygen atom + hydroxyl .fwdarw. oxygen + hydrogen atom reaction on realistic double many-body expansion potential energy surfaces for ground-state hydroperoxy. The Journal of Physical Chemistry, 1988, 92, 4552-4555.	2.9	51
24	Accurate Double Many-Body Expansion Potential Energy Surface for N₃(⁴Aâ€²â€²) from Correlation Scaled ab Initio Energies with Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2009, 113, 14424-14430.	1.1	51
25	Unimolecular and Bimolecular Calculations for HN2. Journal of Physical Chemistry A, 2005, 109, 2356-2363.	1.1	50
26	Accurate ab initio double many-body expansion potential energy surface for ground-state H2S by extrapolation to the complete basis set limit. Journal of Chemical Physics, 2009, 130, 134317.	1.2	50
27	Energy switching approach to potential surfaces. II. Two-valued function for the water molecule. Journal of Chemical Physics, 1997, 107, 867-878.	1.2	49
28	Dynamics of H(D)+O3 reactions on a double many-body expansion potential-energy surface for ground state HO3. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2651-2656.	1.7	48
29	Semiclassical variational transition state calculations for the reactions of H and D with thermal and vibrationally excited H2. International Journal of Chemical Kinetics, 1986, 18, 1065-1077.	1.0	47
30	Nuclear dynamics in the vicinity of the crossing seam: Theory and application to vibrational spectrum of H3. Journal of Chemical Physics, 2000, 112, 2121-2127.	1.2	46
31	A realistic multi-sheeted potential energy surface for NO2(2Aâ€²) from the double many-body expansion method and a novel multiple energy-switching scheme. Journal of Chemical Physics, 2003, 119, 2596-2613.	1.2	46
32	Accurate ab initio potentials at low cost via correlation scaling and extrapolation: Application to CO(AÎ1). Journal of Chemical Physics, 2007, 127, 114316.	1.2	45
33	Ab Initio Treatment of Bond-Breaking Reactions: Accurate Course of HO₃ Dissociation and Revisit to Isomerization. Journal of Chemical Theory and Computation, 2012, 8, 428-441.	2.3	45
34	Repulsive double many-body expansion potential energy surface for the reactions N(4S)+ H2â‡Œ NH(X3Î£â€")+ H from accurate ab initio calculations. Physical Chemistry Chemical Physics, 2005, 7, 2867.	1.3	44
35	New Double Many-Body Expansion Potential Energy Surface for Ground-State HCN from a Multiproperty Fit to Accurate ab Initio Energies and Rovibrational Calculationsâ€. Journal of Physical Chemistry A, 2006, 110, 485-493.	1.1	43
36	Geometric phase effects on transition-state resonances and bound vibrational states of H3 via a time-dependent wavepacket method. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 819-824.	1.7	42

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37	Can extrapolation to the basis set limit be an alternative to the counterpoise correction? A study on the helium dimer. Theoretical Chemistry Accounts, 2008, 119, 511-521.	0.5	40
38	Generalized Uniform Singlet- and Triplet-Pair Extrapolation of the Correlation Energy to the One Electron Basis Set Limit. Journal of Physical Chemistry A, 2008, 112, 1841-1850.	1.1	40
39	Are Vibrationally Excited Molecules a Clue for the â€œO3Deficit Problemâ€•and â€œHOxDilemmaâ€•in the Middle Atmosphere?. Journal of Physical Chemistry A, 2004, 108, 758-769.	1.1	39
40	Accurate Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State HN2. Journal of Physical Chemistry A, 2003, 107, 7923-7930.	1.1	38
41	Dynamics of X+CH4 (X=H,O,Cl) reactions: How reliable is transition state theory for fine-tuning potential energy surfaces?. Journal of Chemical Physics, 2006, 125, 064312.	1.2	38
42	Double many-body expansion potential energy surface for ground-state HO3. Molecular Physics, 1997, 91, 301-318.	0.8	37
43	On the stability of the elusive HO3 radical. Physical Chemistry Chemical Physics, 2011, 13, 15619.	1.3	37
44	A LEPS potential for H3 from force field data. Journal of Chemical Physics, 1979, 70, 3786-3795.	1.2	36
45	Threeâ€dimensional quantum mechanical rate constants for the reaction O+O3â†'2O2, employing a sixâ€dimensional potential energy surface. Journal of Chemical Physics, 1995, 102, 3474-3476.	1.2	36
46	Dynamics Study of the N(4S) + O2Reaction and Its Reverse. Journal of Physical Chemistry A, 2004, 108, 3556-3564.	1.1	36
47	Combined-hyperbolic-inverse-power-representation of potential energy surfaces: A preliminary assessment for H3 and HO2. Journal of Chemical Physics, 2013, 138, 054120.	1.2	36
48	Accurate combined-hyperbolic-inverse-power-representation of ab initio potential energy surface for the hydroperoxyl radical and dynamics study of $f O+OH$O+OH reaction. Journal of Chemical Physics, 2013, 138, 134117.	1.2	36
49	Is HO3 minimum cis or trans? An analytic full-dimensional ab initio isomerization path. Physical Chemistry Chemical Physics, 2011, 13, 9796.	1.3	35
50	A realistic double many-body expansion potential energy surface for from a multiproperty fit to accurate ab initio energies and vibrational levels. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 629-647.	2.0	34
51	Energy switching approach to potential surfaces. III. Three-valued function for the water molecule. Journal of Chemical Physics, 1998, 108, 7623-7630.	1.2	32
52	Accurate Double Many-Body Expansion Potential Energy Surface for Ground-State HS₂Based on ab Initio Data Extrapolated to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2011, 115, 5274-5283.	1.1	30
53	Accurate Potential Energy Surface for the 1²Aâ€² State of NH₂: Scaling of External Correlation Versus Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2010, 114, 9644-9654.	1.1	29
54	Trajectory Surface Hopping Study of the Li + Li2(X1Î£g+) Dissociation Reaction. Journal of Physical Chemistry A, 1998, 102, 6057-6062.	1.1	28

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55	MODELING AND INTERPOLATION OF GLOBAL MULTI-SHEETED POTENTIAL ENERGY SURFACES. Advanced Series in Physical Chemistry, 2004, , 205-270.	1.5	28
56	Quasiclassical Trajectory Study of Atom-Exchange and Vibrational Relaxation Processes in Collisions of Atomic and Molecular Nitrogen. Journal of Physical Chemistry A, 2010, 114, 6063-6070.	1.1	28
57	Extrapolation of Hartreeâ€“Fock and multiconfiguration self-consistent-field energies to the complete basis set limit. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	28
58	Single-Valued Double Many-Body Expansion Potential Energy Surface of Ground-State SO2. Journal of Physical Chemistry A, 2002, 106, 556-562.	1.1	27
59	Accurate ab initio based DMBE potential energy surface for the ground electronic state of N2H2. Journal of Chemical Physics, 2009, 131, 044309.	1.2	27
60	N(4Sâ€‰/2D)+N2: Accurate ab initio-based DMBE potential energy surfaces and surface-hopping dynamics. Journal of Chemical Physics, 2012, 137, 22A515.	1.2	27
61	Quasiclassical Trajectory Study of the Environmental Reaction O + HO2 â†' OH + O2. Journal of Physical Chemistry A, 1998, 102, 6935-6941.	1.1	26
62	Anatomy of the S(1D) + H2 reaction: the dynamics on two new potential energy surfaces from quantum dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 13645.	1.3	26
63	Ab Initio Based Double-Sheeted DMBE Potential Energy Surface for N₃(²Aâ€³) and Exploratory Dynamics Calculations. Journal of Physical Chemistry A, 2011, 115, 12390-12398.	1.1	26
64	On the role of dynamical barriers in barrierless reactions at low energies: S(1D) + H2. Journal of Chemical Physics, 2011, 135, 134313.	1.2	26
65	Potential Energy Surface for Ground-State H2S via Scaling of the External Correlation, Comparison with Extrapolation to Complete Basis Set Limit, and Use in Reaction Dynamics. Journal of Physical Chemistry A, 2009, 113, 9213-9219.	1.1	25
66	Quasiclassical Trajectory Study of the C(¹D) + H₂ Reaction and Isotopomeric Variants: Kinetic Isotope Effect and CD/CH Branching Ratio. Journal of Physical Chemistry A, 2011, 115, 7882-7890.	1.1	25
67	CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. Physical Chemistry Chemical Physics, 2018, 20, 22084-22098.	1.3	25
68	Recalibrated Double Many-Body Expansion Potential Energy Surface and Dynamics Calculations for HN2. Journal of Physical Chemistry A, 2007, 111, 1172-1178.	1.1	24
69	Accurate MRCI and CC Study of the Most Relevant Stationary Points and Other Topographical Attributes for the Ground-State C₂H₂ Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 13277-13287.	1.1	24
70	The Jahn-Teller effect in the triply degenerate electronic state of methane radical cation. Journal of Chemical Physics, 2011, 135, 174304.	1.2	24
71	A VTST Study of the H + O3and O + HO2Reactions Using a Six-dimensional DMBE Potential Energy Surface for Ground State HO3. Journal of Physical Chemistry A, 2002, 106, 4077-4083.	1.1	23
72	Accurateab initio-based molecular potentials: from extrapolation methods to global modelling. Physica Scripta, 2007, 76, C28-C35.	1.2	23

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73	Potential Energy Surfaces for the Low-Lying 2A'' States of HO2 via a Multivalued Double Many-Body Expansion: Modeling Basic Attributes. The Journal of Physical Chemistry, 1995, 99, 15846-15857.	2.9	22
74	Dynamics of the OH(v = 1,2,4) + O3 atmospheric reaction. Physical Chemistry Chemical Physics, 2001, 3, 1439-1445.	1.3	22
75	Ab-Initio-Based Global Double Many-Body Expansion Potential Energy Surface for the Electronic Ground State of the Ammonia Molecule. Journal of Physical Chemistry A, 2010, 114, 6669-6680.	1.1	22
76	Electronic Quenching of N(²D) by N₂: Theoretical Predictions, Comparison with Experimental Rate Constants, and Impact on Atmospheric Modeling. Journal of Physical Chemistry Letters, 2013, 4, 2292-2297.	2.1	22
77	Double Many-Body Expansion Potential Energy Surface for O4(3A), Dynamics of the O(3P) + O3(1A1) Reaction, and Second Virial Coefficients of Molecular Oxygen. , 1991, , 55-78.		22
78	Quantum Dynamical Rate Constant for the H + O3 Reaction Using a Six-Dimensional Double Many-Body Expansion Potential Energy Surface. Journal of Physical Chemistry A, 1997, 101, 8817-8821.	1.1	21
79	Accurate Double Many-Body Expansion Potential Energy Surface for the Lowest Singlet State of Methylene. Journal of Physical Chemistry A, 2009, 113, 4175-4183.	1.1	21
80	C _n (n =2â^'4): current status. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170145.	1.6	21
81	The double many-body expansion of potential energy surfaces from interacting2S atoms. International Journal of Quantum Chemistry, 1987, 32, 563-574.	1.0	20
82	Dynamics Study of the H + ArO2Multichannel Reaction. The Journal of Physical Chemistry, 1996, 100, 17513-17522.	2.9	20
83	Dynamics Study of the OH + O2 Branching Atmospheric Reaction. 2. Influence of Reactants Internal Energy in HO2 and O3 Formation. Journal of Physical Chemistry A, 2001, 105, 4395-4402.	1.1	20
84	On Extracting Subfemtosecond Data from Femtosecond Quantum Dynamics Calculations: The Methane Cation. Journal of Chemical Theory and Computation, 2014, 10, 3606-3616.	2.3	20
85	Dynamics Study of the Reaction Ar + HCN â†' Ar + H + CN. Journal of Physical Chemistry A, 1998, 102, 6266-6273.	1.1	19
86	Steady-State Distributions of O2 and OH in the High Atmosphere and Implications in the Ozone Chemistry. Journal of Physical Chemistry A, 2003, 107, 3769-3777.	1.1	19
87	What are the Implications of Nonequilibrium in the O+OH and O+HO2 Reactions?. ChemPhysChem, 2005, 6, 453-465.	1.0	19
88	Accurate ab initio-based double many-body expansion potential energy surface for the adiabatic ground-state of the C3 radical including combined Jahn-Teller plus pseudo-Jahn-Teller interactions. Journal of Chemical Physics, 2015, 143, 074302.	1.2	19
89	The Jahn-Teller plus pseudo-Jahn-Teller vibronic problem in the C3 radical and its topological implications. Journal of Chemical Physics, 2016, 144, 064309.	1.2	19
90	On the variation of the electric quadrupole moment with internuclear distance and the atomâ€“diatom long-range electrostatic interaction energy. Physical Chemistry Chemical Physics, 2000, 2, 435-439.	1.3	18

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91	Vibrational spectrum of Li3 first-excited electronic doublet state: Geometric-phase effects and statistical analysis. International Journal of Quantum Chemistry, 1999, 75, 89-109.	1.0	17
92	Dynamics Study of the OH + O2Branching Atmospheric Reaction. 4. Influence of Vibrational Relaxation in Collisions Involving Highly Excited Species. Journal of Physical Chemistry A, 2002, 106, 5314-5322.	1.1	17
93	Dynamics of OHâ€‰+â€‰O2vibrational relaxation processes. Physical Chemistry Chemical Physics, 2002, 4, 4959-4969.	1.3	17
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95	Structural evolution of the methane cation in subfemtosecond photodynamics. Journal of Chemical Physics, 2015, 143, 014304.	1.2	17
96	Dynamics Study of the HO(vâ€˜=0) + O2(vâ€˜Ââ€˜) Branching Atmospheric Reaction. 1. Formation of Hydroperoxyl Radical. Journal of Physical Chemistry A, 1999, 103, 4815-4822.	1.1	16
97	Spin-component-scaling second-order MÃ¸llerâ€“Plesset theory and its variants for economical correlation energies: Unified theoretical interpretation and use for quartet N3. Journal of Chemical Physics, 2010, 133, 064104.	1.2	16
98	Accurate Determination of the Reaction Course in HY₂ â‡Œ Y + YH (Y = O, S): Detailed Analysis of the Covalent- to Hydrogen-Bonding Transition. Journal of Physical Chemistry A, 2013, 117, 7393-7407.	1.1	16
99	Electronic Quenching in N(²D) + N₂ Collisions: A State-Specific Analysis via Surface Hopping Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1872-1877.	2.3	16
100	Classical Trajectory Study of Mode Specificity and Rotational Effects in Unimolecular Dissociation of HO2. Journal of Physical Chemistry A, 1997, 101, 5168-5173.	1.1	15
101	Vibrational spectrum of ground state Li₃and statistical analysis of the energy levels. Molecular Physics, 1999, 96, 1193-1206.	0.8	15
102	Approximate Quantum Mechanical Cross Sections and Rate Constants for the H + O3 Atmospheric Reaction Using Novel Elastic Optimum Angle Adiabatic Approaches. Journal of Physical Chemistry A, 1999, 103, 1967-1971.	1.1	15
103	Reply to the â€˜Comment on â€œOn the high pressure rate constants for the H/Mu + O2 addition reactionsâ€™'' by L. B. Harding, J. Troe and V. G. Ushakov, Phys. Chem. Chem. Phys., 2001, 3, 2630. Physical Chemistry Chemical Physics, 2001, 3, 2632-2633.	1.3	15
104	Extrapolating to the One-Electron Basis Set Limit in Polarizability Calculations. Journal of Physical Chemistry A, 2008, 112, 10413-10419.	1.1	15
105	MÃ¸llerâ€“Plesset perturbation energies and distances for HeC₂₀ extrapolated to the complete basis set limit. Journal of Computational Chemistry, 2009, 30, 379-388.	1.5	15
106	Roadmap to spline-fitting potentials in high dimensions. Journal of Mathematical Chemistry, 2013, 51, 1729-1746.	0.7	15
107	Modeling Cusps in Adiabatic Potential Energy Surfaces. Journal of Physical Chemistry A, 2015, 119, 1415-1421.	1.1	15
108	CBS extrapolation of Hartreeâ€“Fock energy: Pople and Dunning basis sets hand-to-hand on the endeavour. Physical Chemistry Chemical Physics, 2019, 21, 8022-8034.	1.3	15

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109	Heliumâ€fullerene pair interactions: An ab initio study by perturbation theory and coupled cluster methods. International Journal of Quantum Chemistry, 2011, 111, 416-429.	1.0	14
110	Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. Physica Scripta, 2011, 84, 028102.	1.2	14
111	Application of the Unified Singlet and Triplet Electron-Pair Extrapolation Scheme with Basis Set Rehierarchization to Tensorial Properties. Journal of Physical Chemistry A, 2015, 119, 1208-1217.	1.1	14
112	Virial theorem decomposition as a tool for comparing and improving potential-energy surfaces: ground-state Li3. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1381.	1.7	13
113	Dynamics Study of the Reaction S + O2 â† SO + O and Its Reverse on a Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State SO2. Journal of Physical Chemistry A, 2003, 107, 5369-5374.	1.1	13
114	Generalized Bornâ€“Oppenheimer treatment of Jahnâ€“Teller systems in Hilbert spaces of arbitrary dimension: theory and application to a three-state model potential. Physical Chemistry Chemical Physics, 2011, 13, 8131.	1.3	13
115	Accurate Explicit-Correlation-MRCI-Based DMBE Potential-Energy Surface for Ground-State CNO. Journal of Physical Chemistry A, 2018, 122, 4198-4207.	1.1	13
116	Accurate CHIPR Potential Energy Surface for the Lowest Triplet State of C₃. Journal of Physical Chemistry A, 2019, 123, 8154-8169.	1.1	13
117	A Theoretical Study of Rate Coefficients for the O + NO Vibrational Relaxation. Journal of Physical Chemistry A, 2008, 112, 960-965.	1.1	12
118	Toward the modeling of the NO₂(²A^{â€³}) manifold. International Journal of Quantum Chemistry, 2011, 111, 3776-3785.	1.0	12
119	Quadratic coupling treatment of the Jahn-Teller effect in the triply-degenerate electronic state of $f CH_4^+$CH4+: Can one account for floppiness?. Journal of Chemical Physics, 2012, 137, 214320.	1.2	12
120	Canonical and explicitly-correlated coupled cluster correlation energies of sub-kJ mol^{â^'1} accuracy via cost-effective hybrid-post-CBS extrapolation. Physical Chemistry Chemical Physics, 2021, 23, 9571-9584.	1.3	12
121	Exponentiating trajectories on a realistic potential energy surface for sodium trimer. The Journal of Physical Chemistry, 1992, 96, 5704-5709.	2.9	11
122	Monte Carlo Simulation Approach to Internal Partition Functions for van der Waals Molecules. Journal of Physical Chemistry A, 1999, 103, 8303-8308.	1.1	11
123	DYNAMICS OF O + O3 REACTION ON A NEW POTENTIAL ENERGY SURFACE FOR GROUND-TRIPLET TETRAOXYGEN: SPECTATOR BOND MECHANISM REVISITED. Journal of Theoretical and Computational Chemistry, 2002, 01, 31-43.	1.8	11
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125	DIABATIC ELECTRONIC MANIFOLD OF HN₂(²Aâ€²) AND N + NH REACTION DYNAMICS ON ITS LOWEST ADIABAT. Journal of Theoretical and Computational Chemistry, 2009, 08, 849-859.	1.8	11
126	A global CHIPR potential energy surface for ground-state C₃H and exploratory dynamics studies of reaction C₂+ CH â† C₃+ H. Physical Chemistry Chemical Physics, 2019, 21, 24406-24418.	1.3	11

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127	Extrapolation in quantum chemistry: Insights on energetics and reaction dynamics. Journal of Theoretical and Computational Chemistry, 2020, 19, 2030001.	1.8	11
128	Dynamics Study of the OH + O2 Branching Atmospheric Reaction. 3. Dissociation in Collisions of Vibrationally Excited Reactants. Journal of Physical Chemistry A, 2001, 105, 7435-7440.	1.1	10
129	The O + NO(v) Vibrational Relaxation Processes Revisited. Journal of Physical Chemistry A, 2018, 122, 5299-5310.	1.1	10
130	Post-complete-basis-set extrapolation of conventional and explicitly correlated coupled-cluster energies: can the convergence to the CBS limit be diagnosed?. Physical Chemistry Chemical Physics, 2021, 23, 8717-8730.	1.3	10
131	SiS Formation in the Interstellar Medium through Si+SH Gas-phase Reactions. Astrophysical Journal, 2021, 920, 37.	1.6	10
132	Quantum Dynamical Rate Constant for the H + O3Reaction Using a Six-Dimensional Double Many-Body Expansion Potential Energy Surface Revisited. Journal of Physical Chemistry A, 1998, 102, 8909-8912.	1.1	9
133	MRCI Calculation, Scaling of the External Correlation, and Modeling of Potential Energy Curves for HCl and OCl. Journal of Physical Chemistry A, 2000, 104, 6241-6246.	1.1	9
134	Dynamics of the Li + Li2Reaction:Â Coexistence of Statistical and Direct Attributes. The Journal of Physical Chemistry, 1996, 100, 7480-7487.	2.9	8
135	Coupled ab initio potential energy surfaces for the two lowest ²Aâ€² electronic states of the C₂H molecule. Molecular Physics, 2000, 98, 1925-1938.	0.8	8
136	Vibrational Calculations for the HD2First-Excited Electronic State Using a Coordinate-Transformation Techniqueâ€. Journal of Physical Chemistry A, 2001, 105, 2246-2250.	1.1	8
137	Reply to the Comment on â€œAre Vibrationally Excited Molecules a Clue for the O3Deficit Problem and HOxDilemma in the Middle Atmosphere?â€• Journal of Physical Chemistry A, 2005, 109, 2700-2702.	1.1	8
138	Sub-femtosecond quantum dynamics of the strong-field ionization of water to the Xì*f*²B₁ and Ã*f*²A₁ states of the cation. Physical Chemistry Chemical Physics, 2015, 17, 6545-6553.	1.3	8
139	Global Potential Energy Surface for HO₂⁺ Using the CHIPR Method. Journal of Physical Chemistry A, 2019, 123, 1613-1621.	1.1	8
140	On the Rate Constant for the Association Reaction H + CN + Ar â†' HCN + Ar. Journal of Physical Chemistry A, 1999, 103, 6366-6372.	1.1	7
141	Dynamics and kinetics of the S + HO₂ reaction: A theoretical study. International Journal of Chemical Kinetics, 2008, 40, 533-540.	1.0	7
142	Ab initio Based DMBE Potential Energy Surface for the Ground Electronic State of the C₂H Molecule. Journal of Physical Chemistry A, 2010, 114, 2655-2664.	1.1	7
143	Accurate Study of the Two Lowest Singlet States of HN₃: Stationary Structures and Energetics at the MRCI Complete Basis Set Limit. Journal of Physical Chemistry A, 2013, 117, 4044-4050.	1.1	7
144	Subfemtosecond Quantum Nuclear Dynamics in Water Isotopomers. Journal of Physical Chemistry A, 2015, 119, 4856-4863.	1.1	7

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145	Quasiclassical Study of the C(³P) + NO(X²Î) and O(³P) + CN(X²Î£⁺) Collisional Processes on an Accurate DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 7195-7200.	1.1	7
146	Geometric phase effect in isotopomers of X3 systems: Use of a split basis technique for the cone states of HD2. International Journal of Quantum Chemistry, 2000, 80, 454-460.	1.0	6
147	Isotope effect on unimolecular dissociation of MuO2: a classical trajectory study. Physical Chemistry Chemical Physics, 2000, 2, 3583-3589.	1.3	6
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