

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	From six to eight \hat{I} -electron bare rings of group-XIV elements and beyond: can planarity be deciphered from the \hat{I} -quasi-molecules they embed?. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8488-8507.	1.3	5
2	Quasiclassical Trajectory Study of the Si + SH Reaction on an Accurate Double Many-Body Expansion Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3555-3568.	1.1	2
3	Post-complete-basis-set extrapolation of conventional and explicitly correlated coupled-cluster energies: can the convergence to the CBS limit be diagnosed?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8717-8730.	1.3	10
4	Canonical and explicitly-correlated coupled cluster correlation energies of sub-kJ mol ⁻¹ accuracy via cost-effective hybrid-post-CBS extrapolation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9571-9584.	1.3	12
5	Accurate DMBE potential-energy surface for CNO(2 <i>A</i>) and rate coefficients in C(3P)+NO collisions. <i>Journal of Chemical Physics</i> , 2021, 154, 034303.	1.2	3
6	Modelling adiabatic cusps in via 2 \hat{A} - 2 diabatic matrix. <i>Molecular Physics</i> , 2021, 119, e1904157.	0.8	5
7	SiS Formation in the Interstellar Medium through Si+SH Gas-phase Reactions. <i>Astrophysical Journal</i> , 2021, 920, 37.	1.6	10
8	Optimized Structural Data at the Complete Basis Set Limit via Successive Quadratic Minimizations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10657-10666.	1.1	5
9	Extrapolation in quantum chemistry: Insights on energetics and reaction dynamics. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2030001.	1.8	11
10	Accurate Potential Energy Surface for Quartet State HN ₂ and Interplay of N ₄ S + NHX ₃ versus H + N ₂ (<i>A</i>)X ₃ (<i>A</i>) Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 781-789.	1.1	5
11	Effect of initial vibrational excitation on the methane cation sub-femtosecond photodynamics. <i>Molecular Physics</i> , 2020, 118, e1752403.	0.8	0
12	Quasiclassical Study of the C(3P) + NO(X ₂) and O(3P) + CN(X ₂) Collisional Processes on an Accurate DMBE Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7195-7200.	1.1	7
13	Global Potential Energy Surface for HO ₂ Using the CHIPR Method. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1613-1621.	1.1	8
14	Accurate CHIPR Potential Energy Surface for the Lowest Triplet State of C ₃ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 8154-8169.	1.1	13
15	Optimal basis sets for CBS extrapolation of the correlation energy: oV _Z and oV _Z . <i>Journal of Chemical Physics</i> , 2019, 150, 154106.	1.2	2
16	CBS extrapolation of Hartree-Fock energy: Pople and Dunning basis sets hand-to-hand on the endeavour. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8022-8034.	1.3	15
17	A global CHIPR potential energy surface for ground-state C ₂ H and exploratory dynamics studies of reaction C ₂ + CH \hat{I} C ₃ + H. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24406-24418.	1.3	11
18	Difficulties and Virtues in Assessing the Potential Energy Surfaces of Carbon Clusters via DMBE Theory: Stationary Points of C ₁₀ (\hat{I} = 2e ⁻¹⁰) at the Focal Point. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3121-3130.	1.1	5

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19	Accurate Explicit-Correlation-MRCI-Based DMBE Potential-Energy Surface for Ground-State CNO. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4198-4207.	1.1	13
20	C_n ($n = 2-4$): current status. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2018, 376, 20170145.	1.6	21
21	Multiple conical intersections in small linear parameter Jahn-Teller systems: the DMBE potential energy surface of ground-state C_3 revisited. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10319-10331.	1.3	6
22	The O + NO(v) Vibrational Relaxation Processes Revisited. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5299-5310.	1.1	10
23	CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22084-22098.	1.3	25
24	The Jahn-Teller plus pseudo-Jahn-Teller vibronic problem in the C_3 radical and its topological implications. <i>Journal of Chemical Physics</i> , 2016, 144, 064309.	1.2	19
25	Extrapolation of Hartree-Fock and multiconfiguration self-consistent-field energies to the complete basis set limit. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	28
26	Structural evolution of the methane cation in subfemtosecond photodynamics. <i>Journal of Chemical Physics</i> , 2015, 143, 014304.	1.2	17
27	Application of the Unified Singlet and Triplet Electron-Pair Extrapolation Scheme with Basis Set Rehierarchization to Tensorial Properties. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1208-1217.	1.1	14
28	Modeling Cusps in Adiabatic Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1415-1421.	1.1	15
29	Subfemtosecond Quantum Nuclear Dynamics in Water Isotopomers. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4856-4863.	1.1	7
30	Sub-femtosecond quantum dynamics of the strong-field ionization of water to the X^2B_1 and A^2A_1 states of the cation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6545-6553.	1.3	8
31	Effect of Initial Vibrational-State Excitation on Subfemtosecond Photodynamics of Water. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12367-12375.	1.1	4
32	Accurate <i>ab initio</i> -based double many-body expansion potential energy surface for the adiabatic ground-state of the C_3 radical including combined Jahn-Teller plus pseudo-Jahn-Teller interactions. <i>Journal of Chemical Physics</i> , 2015, 143, 074302.	1.2	19
33	Dynamics of the O + ClO Reaction: Reactive and Vibrational Relaxation Processes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12120-12129.	1.1	1
34	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. <i>Journal of Chemical Physics</i> , 2014, 141, 224113.	1.2	76
35	Exploring the Utility of Many-Body Expansions: A Consistent Set of Accurate Potentials for the Lowest Quartet and Doublet States of the Azide Radical with Revisited Dynamics. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10127-10133.	1.1	6
36	Is HO_3^- multiple-minimum and floppy? Covalent to van der Waals isomerization and bond rupture of a peculiar anion. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16997-17007.	1.3	5

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37	On Extracting Subfemtosecond Data from Femtosecond Quantum Dynamics Calculations: The Methane Cation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3606-3616.	2.3	20
38	Electronic Quenching in $N_2^+ + N_2$ Collisions: A State-Specific Analysis via Surface Hopping Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1872-1877.	2.3	16
39	Single-Sheeted Double Many-Body Expansion Potential Energy Surface for Ground-State ClO_2 . <i>Journal of Physical Chemistry A</i> , 2014, 118, 4851-4862.	1.1	6
40	Roadmap to spline-fitting potentials in high dimensions. <i>Journal of Mathematical Chemistry</i> , 2013, 51, 1729-1746.	0.7	15
41	Silane Radical Cation: A Theoretical Account on the Jahn-Teller Effect at a Triple Degeneracy. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8794-8805.	1.1	3
42	Accurate Determination of the Reaction Course in $HY_2 \rightarrow Y + YH$ ($Y = O, S$): Detailed Analysis of the Covalent- to Hydrogen-Bonding Transition. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7393-7407.	1.1	16
43	Combined-hyperbolic-inverse-power-representation of potential energy surfaces: A preliminary assessment for H_3 and HO_2 . <i>Journal of Chemical Physics</i> , 2013, 138, 054120.	1.2	36
44	Accurate Study of the Two Lowest Singlet States of HN_3 : Stationary Structures and Energetics at the MRCI Complete Basis Set Limit. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4044-4050.	1.1	7
45	Electronic Quenching of N_2^+ by N_2 : Theoretical Predictions, Comparison with Experimental Rate Constants, and Impact on Atmospheric Modeling. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2292-2297.	2.1	22
46	Accurate combined-hyperbolic-inverse-power-representation of <i>ab initio</i> potential energy surface for the hydroperoxyl radical and dynamics study of $O + OH \rightarrow O_2 + H$ reaction. <i>Journal of Chemical Physics</i> , 2013, 138, 134117.	1.2	36
47	Manifestation of external field effect in time-resolved photo-dissociation dynamics of LiF. <i>Chinese Physics B</i> , 2013, 22, 073303.	0.7	2
48	Implications of the $O + OH$ reaction in hydroxyl nightglow modeling. <i>Atmospheric Chemistry and Physics</i> , 2013, 13, 1-13.	1.9	60
49	Quadratic coupling treatment of the Jahn-Teller effect in the triply-degenerate electronic state of CH_4^+ : Can one account for floppiness?. <i>Journal of Chemical Physics</i> , 2012, 137, 214320.	1.2	12
50	$N_2^+ + N_2$: Accurate <i>ab initio</i> -based DMBE potential energy surfaces and surface-hopping dynamics. <i>Journal of Chemical Physics</i> , 2012, 137, 22A515.	1.2	27
51	<i>Ab Initio</i> Treatment of Bond-Breaking Reactions: Accurate Course of HO_3 Dissociation and Revisit to Isomerization. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 428-441.	2.3	45
52	<i>Ab Initio</i> -Based Global Double Many-Body Expansion Potential Energy Surface for the First $2A_1^3$ Electronic State of NO_2 . <i>Journal of Physical Chemistry A</i> , 2012, 116, 3023-3034.	1.1	17
53	Dynamics study of a three-fold pseudo-Jahn-Teller system using the extended Longuet-Higgins formalism. <i>Journal of Chemical Sciences</i> , 2012, 124, 115-120.	0.7	0
54	Toward the modeling of the $NO_2^+(\sigma^3)$ manifold. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3776-3785.	1.0	12

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55	Anatomy of the S(1D) + H ₂ reaction: the dynamics on two new potential energy surfaces from quantum dynamics calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13645.	1.3	26
56	Is HO ₃ minimum cis or trans? An analytic full-dimensional ab initio isomerization path. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9796.	1.3	35
57	Accurate Double Many-Body Expansion Potential Energy Surface for Ground-State HS ₂ Based on ab Initio Data Extrapolated to the Complete Basis Set Limit. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5274-5283.	1.1	30
58	Quasiclassical Trajectory Study of the C(¹ D) + H ₂ Reaction and Isotomeric Variants: Kinetic Isotope Effect and CD/CH Branching Ratio. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7882-7890.	1.1	25
59	Ab Initio Based Double-Sheeted DMBE Potential Energy Surface for N ₃ (² A _g) and Exploratory Dynamics Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12390-12398.	1.1	26
60	Generalized Born-Oppenheimer treatment of Jahn-Teller systems in Hilbert spaces of arbitrary dimension: theory and application to a three-state model potential. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 8131.	1.3	13
61	On the stability of the elusive HO ₃ radical. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15619.	1.3	37
62	The Jahn-Teller effect in the triply degenerate electronic state of methane radical cation. <i>Journal of Chemical Physics</i> , 2011, 135, 174304.	1.2	24
63	Helium-fullerene pair interactions: An ab initio study by perturbation theory and coupled cluster methods. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 416-429.	1.0	14
64	Quasiclassical trajectory study of the rotational distribution for the O+NO(<i>v</i> = 0) fundamental vibrational excitation. <i>International Journal of Chemical Kinetics</i> , 2011, 43, 345-352.	1.0	3
65	Quantum calculations for the S(1D)+H ₂ reaction employing the ground adiabatic electronic state. <i>Physica Scripta</i> , 2011, 84, 028102.	1.2	14
66	On the role of dynamical barriers in barrierless reactions at low energies: S(1D) + H ₂ . <i>Journal of Chemical Physics</i> , 2011, 135, 134313.	1.2	26
67	Spin-component-scaling second-order Møller-Plesset theory and its variants for economical correlation energies: Unified theoretical interpretation and use for quartet N ₃ . <i>Journal of Chemical Physics</i> , 2010, 133, 064104.	1.2	16
68	Extrapolation to the Complete Basis Set Limit without Counterpoise. The Pair Potential of Helium Revisited. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8505-8516.	1.1	69
69	Ab Initio Study of Hydrazinyl Radical: Toward a DMBE Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11663-11669.	1.1	3
70	Quasiclassical Trajectory Study of Atom-Exchange and Vibrational Relaxation Processes in Collisions of Atomic and Molecular Nitrogen. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6063-6070.	1.1	28
71	Accurate MRCI and CC Study of the Most Relevant Stationary Points and Other Topographical Attributes for the Ground-State C ₂ H ₂ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13277-13287.	1.1	24
72	Ab-Initio-Based Global Double Many-Body Expansion Potential Energy Surface for the Electronic Ground State of the Ammonia Molecule. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6669-6680.	1.1	22

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73	Accurate Potential Energy Surface for the $1^2\text{A}''$ State of NH_2 : Scaling of External Correlation Versus Extrapolation to the Complete Basis Set Limit. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9644-9654.	1.1	29
74	Ab initio Based DMBE Potential Energy Surface for the Ground Electronic State of the C_2H Molecule. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2655-2664.	1.1	7
75	Accurate Double Many-Body Expansion Potential Energy Surface for N_3 ($4^2\text{A}''$) from Correlation Scaled ab Initio Energies with Extrapolation to the Complete Basis Set Limit. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14424-14430.	1.1	51
76	DIABATIC ELECTRONIC MANIFOLD OF HN_2 ($2^2\text{A}''$) AND $\text{N} + \text{NH}$ REACTION DYNAMICS ON ITS LOWEST ADIABAT. <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 08, 849-859.	1.8	11
77	Accurate <i>ab initio</i> potential energy curves for the classic Li^+F ionic-covalent interaction by extrapolation to the complete basis set limit and modeling of the radial nonadiabatic coupling. <i>Journal of Chemical Physics</i> , 2009, 131, 124128.	1.2	62
78	Møller-Plesset perturbation energies and distances for HeC_{20} extrapolated to the complete basis set limit. <i>Journal of Computational Chemistry</i> , 2009, 30, 379-388.	1.5	15
79	Theoretical study of the $\text{O} + \text{HSO}$ reaction. <i>International Journal of Chemical Kinetics</i> , 2009, 41, 455-462.	1.0	4
80	Potential Energy Surface for Ground-State H_2S via Scaling of the External Correlation, Comparison with Extrapolation to Complete Basis Set Limit, and Use in Reaction Dynamics. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9213-9219.	1.1	25
81	Accurate <i>ab initio</i> based DMBE potential energy surface for the ground electronic state of N_2H_2 . <i>Journal of Chemical Physics</i> , 2009, 131, 044309.	1.2	27
82	Accurate <i>ab initio</i> double many-body expansion potential energy surface for ground-state H_2S by extrapolation to the complete basis set limit. <i>Journal of Chemical Physics</i> , 2009, 130, 134317.	1.2	50
83	Accurate Double Many-Body Expansion Potential Energy Surface for the Lowest Singlet State of Methylene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4175-4183.	1.1	21
84	Can extrapolation to the basis set limit be an alternative to the counterpoise correction? A study on the helium dimer. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 511-521.	0.5	40
85	Dynamics and kinetics of the $\text{S} + \text{HO}_2$ reaction: A theoretical study. <i>International Journal of Chemical Kinetics</i> , 2008, 40, 533-540.	1.0	7
86	Extrapolation to the complete-basis-set limit and the implications of avoided crossings: The X^1g^+ , B^1g_2 , and B^2g^+ states of C_2 . <i>Journal of Chemical Physics</i> , 2008, 129, 234103.	1.2	60
87	A Theoretical Study of Rate Coefficients for the $\text{O} + \text{NO}$ Vibrational Relaxation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 960-965.	1.1	12
88	Extrapolating to the One-Electron Basis Set Limit in Polarizability Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10413-10419.	1.1	15
89	Generalized Uniform Singlet- and Triplet-Pair Extrapolation of the Correlation Energy to the One Electron Basis Set Limit. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1841-1850.	1.1	40
90	Energy-switching potential energy surface for the water molecule revisited: A highly accurate singled-sheeted form. <i>Journal of Chemical Physics</i> , 2008, 129, 044302.	1.2	11

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91	Intermolecular and Intramolecular Potentials: Topographical Aspects, Calculation, and Functional Representation via A Double Many-Body Expansion Method. <i>Advances in Chemical Physics</i> , 2007, , 255-338.	0.3	160
92	Accurate <i>ab initio</i> potentials at low cost via correlation scaling and extrapolation: Application to CO(A Σ 1). <i>Journal of Chemical Physics</i> , 2007, 127, 114316.	1.2	45
93	Accurate <i>ab initio</i> -based molecular potentials: from extrapolation methods to global modelling. <i>Physica Scripta</i> , 2007, 76, C28-C35.	1.2	23
94	Recalibrated Double Many-Body Expansion Potential Energy Surface and Dynamics Calculations for HN ₂ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 1172-1178.	1.1	24
95	Extrapolating to the one-electron basis-set limit in electronic structure calculations. <i>Journal of Chemical Physics</i> , 2007, 126, 244105.	1.2	176
96	Kinetics and dynamics of O + OCIO reaction in a modified many-body expansion potential energy surface for ClO ₃ . <i>International Journal of Chemical Kinetics</i> , 2007, 39, 422-430.	1.0	0
97	Predicting Catalysis: A Understanding Ammonia Synthesis from First-Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17719-17735.	1.2	192
98	Dynamics of X+CH ₄ (X=H,O,Cl) reactions: How reliable is transition state theory for fine-tuning potential energy surfaces?. <i>Journal of Chemical Physics</i> , 2006, 125, 064312.	1.2	38
99	New Double Many-Body Expansion Potential Energy Surface for Ground-State HCN from a Multiproperty Fit to Accurate <i>ab Initio</i> Energies and Rovibrational Calculations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 485-493.	1.1	43
100	Accurate DMBE Potential Energy Surface For the N(2D) + H ₂ (1 Σ g ⁺) Reaction Using an Improved Switching Function Formalism. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 404-419.	0.5	73
101	What are the Implications of Nonequilibrium in the O+OH and O+HO ₂ Reactions?. <i>ChemPhysChem</i> , 2005, 6, 453-465.	1.0	19
102	Double many-body expansion potential energy surface for ground state HSO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2305.	1.3	56
103	Repulsive double many-body expansion potential energy surface for the reactions N(4S) + H ₂ \rightarrow NH(X Σ ⁺) + H from accurate <i>ab initio</i> calculations. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2867.	1.3	44
104	Reply to the Comment on "Are Vibrationally Excited Molecules a Clue for the O ₃ Deficit Problem and HO _x Dilemma in the Middle Atmosphere?". <i>Journal of Physical Chemistry A</i> , 2005, 109, 2700-2702.	1.1	8
105	Unimolecular and Bimolecular Calculations for HN ₂ . <i>Journal of Physical Chemistry A</i> , 2005, 109, 2356-2363.	1.1	50
106	MODELING AND INTERPOLATION OF GLOBAL MULTI-SHEETED POTENTIAL ENERGY SURFACES. <i>Advanced Series in Physical Chemistry</i> , 2004, , 205-270.	1.5	28
107	Geometric phase effect at N-fold electronic degeneracies in Jahn-Teller systems. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 385-392.	1.0	5
108	Dynamics study of ClO + O ₂ collisions and their role in the chemistry of stratospheric ozone. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2179-2184.	1.3	5

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109	Dynamics Study of the N(4S) + O ₂ Reaction and Its Reverse. Journal of Physical Chemistry A, 2004, 108, 3556-3564.	1.1	36
110	Are Vibrationally Excited Molecules a Clue for the "O ₃ Deficit Problem" and "HO _x Dilemma" in the Middle Atmosphere?. Journal of Physical Chemistry A, 2004, 108, 758-769.	1.1	39
111	Nascent versus "Steady-State" Rovibrational Distributions in the Products of the O(3P) + O ₃ (λ f 1A) Reaction. Journal of Physical Chemistry A, 2003, 107, 10926-10932.	1.1	2
112	Accurate Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State HN ₂ . Journal of Physical Chemistry A, 2003, 107, 7923-7930.	1.1	38
113	Steady-State Distributions of O ₂ and OH in the High Atmosphere and Implications in the Ozone Chemistry. Journal of Physical Chemistry A, 2003, 107, 3769-3777.	1.1	19
114	Dynamics Study of the Reaction S + O ₂ \rightarrow SO + O and Its Reverse on a Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State SO ₂ . Journal of Physical Chemistry A, 2003, 107, 5369-5374.	1.1	13
115	A realistic multi-sheeted potential energy surface for NO ₂ (2A \hat{e}) 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
116	Permutational Symmetry and the Role of Nuclear Spin in the Vibrational Spectra of Molecules in Doubly Degenerate Electronic States: The Trimers of 2 S Atoms. Advances in Chemical Physics, 2003, , 659-741.	0.3	3
117	On the Geometric Phase Effect in Jahn-Teller Systems. , 2003, , 707-766.		0
118	Li + Li ₂ Dissociation Reaction Using the Self-Consistent Potential and Trajectory Surface Hopping Methods. Journal of Physical Chemistry A, 2002, 106, 3673-3680.	1.1	1
119	Single-Valued Double Many-Body Expansion Potential Energy Surface of Ground-State SO ₂ . Journal of Physical Chemistry A, 2002, 106, 556-562.	1.1	27
120	Dynamics Study of the OH + O ₂ Branching 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
121	DYNAMICS OF O + O ₃ 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
122	Dynamics of OH + O ₂ vibrational relaxation processes. Physical Chemistry Chemical Physics, 2002, 4, 4959-4969.	1.3	17
123	Dynamics Study of the O ₂ + HO ₂ Atmospheric Reaction with Both Reactants Highly Vibrationally Excited. Journal of Physical Chemistry A, 2002, 106, 11911-11916.	1.1	6
124	A VTST Study of the H + O ₃ and O + HO ₂ Reactions Using a Six-dimensional DMBE Potential Energy Surface for Ground State HO ₃ . Journal of Physical Chemistry A, 2002, 106, 4077-4083.	1.1	23
125	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
126	Dynamics of the OH(v = 1,2,4) + O ₃ atmospheric reaction. Physical Chemistry Chemical Physics, 2001, 3, 1439-1445.	1.3	22

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127	Single-Valued DMBE Potential Energy Surface for HSO: A Distributedn-Body Polynomial Approach. Journal of Physical Chemistry A, 2001, 105, 5923-5932.	1.1	64
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	Vibrational Calculations for the HD2First-Excited Electronic State Using a Coordinate-Transformation Technique. Journal of Physical Chemistry A, 2001, 105, 2246-2250.	1.1	8
130	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
131	Nuclear dynamics in the vicinity of a crossing seam: Vibrational spectrum of HD2 revisited. International Journal of Quantum Chemistry, 2001, 83, 279-285.	1.0	3
132	Reply to the "Comment on "On the high pressure rate constants for the H/Mu + O2 addition reactions" 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
133	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
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135	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
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