

# Uwe Manthe

## List of Publications by Year in descending order

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145  
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158  
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158  
docs citations

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times ranked

3016  
citing authors

#	ARTICLE	IF	CITATIONS
1	The multi-configurational time-dependent Hartree approach in optimized second quantization: Thermal ensembles and statistical sampling. <i>Chemical Physics</i> , 2022, 555, 111413.	0.9	2
2	First-Principles Theory for the Reaction of Chlorine with Methane. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2563-2566.	2.1	3
3	A non-hierarchical correlation discrete variable representation. <i>Journal of Chemical Physics</i> , 2022, 156, 134107.	1.2	5
4	Vibrational control of the reaction pathway in the $\text{H} + \text{CHD}_3 \rightarrow \text{H}_2 + \text{CD}_3$ reaction. <i>Science Advances</i> , 2022, 8, eabm9820.	4.7	6
5	Direct product-type grid representations for angular coordinates in extended space and their application in the MCTDH approach. <i>Journal of Chemical Physics</i> , 2021, 154, 104115.	1.2	2
6	Symmetries in the multi-configurational time-dependent Hartree wavefunction representation and propagation. <i>Journal of Chemical Physics</i> , 2021, 154, 194108.	1.2	7
7	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of $\text{OH}(A^2\Sigma^+)$ by $\text{H}_2$ . <i>Nature Chemistry</i> , 2021, 13, 909-915.	6.6	17
8	Non-adiabatic transitions in the reaction of fluorine with methane. <i>Journal of Chemical Physics</i> , 2020, 152, 231102.	1.2	8
9	Eight-Dimensional Wave Packet Dynamics Within the Quantum Transition-State Framework: State-to-State Reactive Scattering for $\text{H}_2 + \text{CH}_3 \rightarrow \text{H} + \text{CH}_4$ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 9400-9412.	1.1	4
10	The multi-configurational time-dependent Hartree approach in optimized second quantization: Imaginary time propagation and particle number conservation. <i>Journal of Chemical Physics</i> , 2020, 152, 034101.	1.2	12
11	Vibronically and spin-orbit coupled diabatic potentials for $\text{X}(2P) + \text{CH}_4 \rightarrow \text{HX} + \text{CH}_3$ reactions: Neural network potentials for $\text{X} = \text{Cl}$ . <i>Journal of Chemical Physics</i> , 2019, 150, 244115.	1.2	16
12	A Quasi-Classical Evaluation of the $\langle i \rangle$ -Shifting Approximation for the Reactive Cross Sections of $\text{F} + \text{CHD}_3$ and $\text{F} + \text{CH}_4$ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 7237-7245.	1.1	5
13	Counter-propagating wave packets in the quantum transition state approach to reactive scattering. <i>Journal of Chemical Physics</i> , 2019, 150, 184103.	1.2	6
14	Vibronically and spin-orbit coupled diabatic potentials for $\text{X}(P) + \text{CH}_4 \rightarrow \text{HX} + \text{CH}_3$ reactions: General theory and application for $\text{X}(P) = \text{F}(2P)$ . <i>Journal of Chemical Physics</i> , 2019, 150, 064102.	1.2	11
15	Long-Distance Rate Acceleration by Bulk Gold. <i>Angewandte Chemie</i> , 2019, 131, 6646-6650.	1.6	8
16	Long-Distance Rate Acceleration by Bulk Gold. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6574-6578.	7.2	25
17	Vibronic coupling in the $\text{F} \cdots \text{CH}_4$ prereactive complex. <i>Journal of Chemical Physics</i> , 2019, 151, 104106.	1.2	6
18	Coordinate systems and kinetic energy operators for multi-configurational time-dependent Hartree calculations studying reactions of methane. <i>Chemical Physics</i> , 2018, 509, 37-44.	0.9	7

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19	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	1.6	1
20	Quantum dynamics of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 281-306.	1.6	0
21	Natural reaction channels in $\text{H}\hat{\text{A}}^+ \text{CHD}_3 \hat{\text{A}}^+ \text{H}_2 + \text{CD}_3$ . Faraday Discussions, 2018, 212, 217-235.	1.6	18
22	Optimized unoccupied single-particle functions in the (multi-layer) multi-configurational time-dependent Hartree approach. Chemical Physics, 2018, 515, 279-286.	0.9	9
23	Full-dimensional quantum dynamics calculations for $\text{H} + \text{CHD}_3 \hat{\text{A}}^+ \text{H}_2 + \text{CD}_3$ : The effect of multiple vibrational excitations. Journal of Chemical Physics, 2018, 148, 224303.	1.2	33
24	Fermi resonance controlled product branching in the $\text{H} + \text{HOD}$ reaction. Physical Chemistry Chemical Physics, 2018, 20, 17029-17037.	1.3	16
25	On the multi-layer multi-configurational time-dependent Hartree approach for bosons and fermions. Journal of Chemical Physics, 2017, 146, 064117.	1.2	32
26	Wavepacket dynamics and the multi-configurational time-dependent Hartree approach. Journal of Physics Condensed Matter, 2017, 29, 253001.	0.7	33
27	A transition-state based rotational sudden (TSRS) approximation for polyatomic reactive scattering. Journal of Chemical Physics, 2017, 147, 144104.	1.2	4
28	Non-adiabatic effects in $\text{F} + \text{CHD}_3$ reactive scattering. Journal of Chemical Physics, 2017, 146, 214117.	1.2	15
29	Neural network based coupled diabatic potential energy surfaces for reactive scattering. Journal of Chemical Physics, 2017, 147, 084105.	1.2	46
30	Quantum dynamics of $\text{H}_2$ in a carbon nanotube: Separation of time scales and resonance enhanced tunneling. Journal of Chemical Physics, 2017, 147, 084103.	1.2	6
31	$\text{H} + \text{CH}_4 \hat{\text{A}}^+ \text{H}_2 + \text{CH}_3$ initial state-selected reaction probabilities on different potential energy surfaces. Chemical Physics, 2017, 482, 106-112.	0.9	25
32	Communication: Reactivity borrowing in the mode selective chemistry of $\text{H} + \text{CHD}_3 \hat{\text{A}}^+ \text{H}_2 + \text{CD}_3$ . Journal of Chemical Physics, 2017, 147, 241104.	1.2	43
33	Wave packet dynamics in the optimal superadiabatic approximation. Journal of Chemical Physics, 2016, 144, 224109.	1.2	2
34	S-matrix decomposition, natural reaction channels, and the quantum transition state approach to reactive scattering. Journal of Chemical Physics, 2016, 144, 204119.	1.2	17
35	Communication: Mode specific quantum dynamics of the $\text{F} + \text{CHD}_3 \hat{\text{A}}^+ \text{HF} + \text{CD}_3$ reaction. Journal of Chemical Physics, 2016, 144, 171101.	1.2	47
36	Quasi-Bound States of the $\text{F}\hat{\text{A}}\text{-CH}_4$ Complex. Journal of Physical Chemistry A, 2016, 120, 3186-3195.	1.1	15

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37	The multi-configurational time-dependent Hartree approach revisited. <i>Journal of Chemical Physics</i> , 2015, 142, 244109.	1.2	57
38	Full-dimensional and reduced-dimensional calculations of initial state-selected reaction probabilities studying the $H + CH_4 \hat{\rightarrow} H_2 + CH_3$ reaction on a neural network PES. <i>Journal of Chemical Physics</i> , 2015, 142, 064309.	1.2	68
39	Loss of Memory in $H + CH_4 \hat{\rightarrow} H_2 + CH_3$ State-to-State Reactive Scattering. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 338-342.	2.1	82
40	$CH_5^+$ : Symmetry and the Entangled Rovibrational Quantum States of a Fluxional Molecule. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4229-4232.	2.1	32
41	A Quasiclassical Study of the $F(^2P) + CHD_3 (\hat{v}_1 = 0, 1)$ Reactive System on an Accurate Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12209-12217.	1.1	27
42	Communication: Ro-vibrational control of chemical reactivity in $H+CH_4 \hat{\rightarrow} H_2+CH_3$ : Full-dimensional quantum dynamics calculations and a sudden model. <i>Journal of Chemical Physics</i> , 2014, 141, 051102.	1.2	84
43	Correlation functions for fully or partially state-resolved reactive scattering calculations. <i>Journal of Chemical Physics</i> , 2014, 140, 244113.	1.2	37
44	The role of the transition state in polyatomic reactions: Initial state-selected reaction probabilities of the $H + CH_4 \hat{\rightarrow} H_2 + CH_3$ reaction. <i>Journal of Chemical Physics</i> , 2014, 141, 174313.	1.2	58
45	Resonances in the Entrance Channel of the Elementary Chemical Reaction of Fluorine and Methane. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 1122-1126.	7.2	66
46	Coupled potential energy surface for the $F(2P) + CH_4 \hat{\rightarrow} HF + CH_3$ entrance channel and quantum dynamics of the $CH_4 \hat{\rightarrow} F + CH_3$ photodetachment. <i>Journal of Chemical Physics</i> , 2013, 139, 014309.	1.2	40
47	Iterative Diagonalization in the Multiconfigurational Time-Dependent Hartree Approach: Ro-vibrational Eigenstates. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7246-7255.	1.1	15
48	Fast Shepard interpolation on graphics processing units: Potential energy surfaces and dynamics for $H + CH_4 \hat{\rightarrow} H_2 + CH_3$ . <i>Journal of Chemical Physics</i> , 2013, 138, 164118.	1.2	50
49	Decoherence induced by conical intersections: Complexity constrained quantum dynamics of photoexcited pyrazine. <i>Journal of Chemical Physics</i> , 2012, 137, 22A509.	1.2	9
50	First principle nonlinear quantum dynamics using a correlation-based von Neumann entropy. <i>Journal of Chemical Physics</i> , 2012, 136, 204116.	1.2	10
51	A full-dimensional wave packet dynamics study of the photodetachment spectra of $FCH_4^+$ . <i>Journal of Chemical Physics</i> , 2012, 137, 044306.	1.2	19
52	A multi-configurational time-dependent Hartree approach to the eigenstates of multi-well systems. <i>Journal of Chemical Physics</i> , 2012, 136, 124119.	1.2	13
53	Iterative diagonalization in the state-averaged multi-configurational time-dependent Hartree approach: Excited state tunneling splittings in malonaldehyde. <i>Journal of Chemical Physics</i> , 2012, 136, 054105.	1.2	78
54	Vibrational Dynamics of the $CH_4 \hat{\rightarrow} F + CH_3$ Complex. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11249-11259.	1.1	26

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55	Thermal flux based analysis of state-to-state reaction probabilities. <i>Molecular Physics</i> , 2012, 110, 703-715.	0.8	39
56	State-to-state reaction probabilities within the quantum transition state framework. <i>Journal of Chemical Physics</i> , 2012, 136, 064117.	1.2	58
57	Reaction dynamics with the multi-layer multi-configurational time-dependent Hartree approach: H + CH <sub>4</sub> → H <sub>2</sub> + CH <sub>3</sub> rate constants for different potentials. <i>Journal of Chemical Physics</i> , 2012, 137, 244106.	1.2	68
58	Accurate calculations of reaction rates: predictive theory based on a rigorous quantum transition state concept. <i>Molecular Physics</i> , 2011, 109, 1415-1426.	0.8	51
59	Photodissociation of CH <sub>3</sub> I: A Full-Dimensional (9D) Quantum Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5992-6001.	1.1	34
60	Photodissociation of methyl iodide embedded in a host-guest complex: A full dimensional (189D) quantum dynamics study of CH <sub>3</sub> I@resorc[4]arene. <i>Journal of Chemical Physics</i> , 2011, 135, 184102.	1.2	50
61	Intramolecular proton transfer in malonaldehyde: Accurate multilayer multi-configurational time-dependent Hartree calculations. <i>Journal of Chemical Physics</i> , 2011, 134, 224305.	1.2	87
62	On direct product based discrete variable representations for angular coordinates and the treatment of singular terms in the kinetic energy operator. <i>Chemical Physics</i> , 2010, 374, 118-125.	0.9	25
63	Communications: A rigorous transition state based approach to state-specific reaction dynamics: Full-dimensional calculations for H+CH <sub>4</sub> → H <sub>2</sub> +CH <sub>3</sub> . <i>Journal of Chemical Physics</i> , 2010, 132, 191101.	1.2	77
64	Full-Dimensional Quantum Reaction Rate Calculations for H + CH <sub>4</sub> → H <sub>2</sub> + CH <sub>3</sub> on a Recent Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9617-9622.	1.1	50
65	A transition state view on reactive scattering: Initial state-selected reaction probabilities for the H+CH <sub>4</sub> → H <sub>2</sub> +CH <sub>3</sub> reaction studied in full dimensionality. <i>Journal of Chemical Physics</i> , 2010, 133, 174124.	1.2	83
66	Quantum dynamics of the H+CH <sub>4</sub> → H <sub>2</sub> +CH <sub>3</sub> reaction in curvilinear coordinates: Full-dimensional and reduced dimensional calculations of reaction rates. <i>Journal of Chemical Physics</i> , 2010, 132, 084103.	1.2	89
67	Multiconfigurational time-dependent Hartree calculations for tunneling splittings of vibrational states: Theoretical considerations and application to malonaldehyde. <i>Journal of Chemical Physics</i> , 2009, 131, 224109.	1.2	70
68	Layered discrete variable representations and their application within the multiconfigurational time-dependent Hartree approach. <i>Journal of Chemical Physics</i> , 2009, 130, 054109.	1.2	115
69	Comparison of Quantum Dynamics and Quantum Transition State Theory Estimates of the H + CH <sub>4</sub> Reaction Rate. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4468-4478.	1.1	140
70	Multi Dimensional Quantum Dynamics of Chemical Reaction Processes. , 2009, , 143-152.		0
71	Photoionization-induced dynamics of the ammonia cation studied by wave packet calculations using curvilinear coordinates. <i>Chemical Physics</i> , 2008, 347, 331-339.	0.9	27
72	A multilayer multiconfigurational time-dependent Hartree approach for quantum dynamics on general potential energy surfaces. <i>Journal of Chemical Physics</i> , 2008, 128, 164116.	1.2	339

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73	Calculating vibrational spectra using modified Shepard interpolated potential energy surfaces. Journal of Chemical Physics, 2008, 129, 024104.	1.2	11
74	The state averaged multiconfigurational time-dependent Hartree approach: Vibrational state and reaction rate calculations. Journal of Chemical Physics, 2008, 128, 064108.	1.2	94
75	The ground state tunneling splitting and the zero point energy of malonaldehyde: A quantum Monte Carlo determination. Journal of Chemical Physics, 2007, 126, 024308.	1.2	61
76	Thermal Rate Constants for Polyatomic Reactions: First Principles Quantum Theory. Zeitschrift Fur Physikalische Chemie, 2007, 221, 171-213.	1.4	41
77	Quantum dynamics of the CH3 fragment: A curvilinear coordinate system and kinetic energy operators. Journal of Chemical Physics, 2007, 127, 144302.	1.2	43
78	Accurate quantum calculations of the reaction rates for $\text{H}^+\text{D}+\text{CH}_4$ . Journal of Chemical Physics, 2007, 126, 084303.	1.2	61
79	Thermochemistry and Accurate Quantum Reaction Rate Calculations for $\text{H}_2/\text{HD}/\text{D}_2+\text{CH}_3$ . Journal of Physical Chemistry A, 2007, 111, 10331-10337.	1.1	45
80	Predicting Catalysis: Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
81	Photoionization-induced dynamics of ammonia: Ab initio potential energy surfaces and time-dependent wave packet calculations for the ammonia cation. Journal of Chemical Physics, 2006, 124, 214306.	1.2	77
82	Accurate potential energy surface and quantum reaction rate calculations for the $\text{H}+\text{CH}_4 \rightarrow \text{H}_2+\text{CH}_3$ reaction. Journal of Chemical Physics, 2006, 124, 164307.	1.2	101
83	On the integration of the multi-configurational time-dependent Hartree (MCTDH) equations of motion. Chemical Physics, 2006, 329, 168-178.	0.9	58
84	The effect of surface relaxation on the $\text{N}_2$ dissociation rate on stepped Ru: A transition state theory study. Journal of Chemical Physics, 2006, 124, 026102.	1.2	5
85	The reaction rate for dissociative adsorption of $\text{N}_2$ on stepped Ru(0001): Six-dimensional quantum calculations. Journal of Chemical Physics, 2005, 122, 234702.	1.2	48
86	Multidimensional time-dependent discrete variable representations in multiconfiguration Hartree calculations. Journal of Chemical Physics, 2005, 123, 064106.	1.2	61
87	Calculating initial-state-selected reaction probabilities from thermal flux eigenstates: A transition-state-based approach. Journal of Chemical Physics, 2005, 123, 204114.	1.2	36
88	Off-normal incidence dissociative sticking of $\text{H}_2$ on Cu(100) studied using six-dimensional quantum calculations. Journal of Chemical Physics, 2005, 123, 124706.	1.2	7
89	Multi Dimensional Quantum Dynamics. , 2005, , 225-236.		0
90	Degeneracy in discrete variable representations: General considerations and application to the multiconfigurational time-dependent Hartree approach. Journal of Chemical Physics, 2004, 121, 5623-5628.	1.2	16

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91	Photoinduced dynamics of ethene in the N, V, and Z valence states: A six-dimensional nonadiabatic quantum dynamics investigation. <i>Journal of Chemical Physics</i> , 2004, 120, 11000-11010.	1.2	60
92	First-Principles Theory for the H + CH <sub>4</sub> → H <sub>2</sub> + CH <sub>3</sub> Reaction. <i>Science</i> , 2004, 306, 2227-2229.	6.0	238
93	The effect of spin-orbit coupling on the thermal rate constant of the H <sub>2</sub> + Cl → H + HCl reaction. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5026-5030.	1.3	26
94	The ground state tunneling splitting of malonaldehyde: Accurate full dimensional quantum dynamics calculations. <i>Journal of Chemical Physics</i> , 2004, 121, 9207-9210.	1.2	116
95	Multiconfigurational time-dependent Hartree calculations for dissociative adsorption of H <sub>2</sub> on Cu(100). <i>Journal of Chemical Physics</i> , 2004, 121, 3829-3835.	1.2	23
96	The Sudden-Polarization Effect and its Role in the Ultrafast Photochemistry of Ethene. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3434-3436.	7.2	33
97	Photoinduced dynamics of the valence states of ethene: A six-dimensional potential-energy surface of three electronic states with several conical intersections. <i>Journal of Chemical Physics</i> , 2003, 119, 1397-1411.	1.2	65
98	A potential energy surface construction scheme for accurate reaction rate calculations: General approach and a test for the H+CH <sub>4</sub> →H <sub>2</sub> +CH <sub>3</sub> reaction. <i>Journal of Chemical Physics</i> , 2003, 119, 14-23.	1.2	61
99	Quantum mechanical calculation of the OH+HCl→H <sub>2</sub> O+Cl reaction rate: Full-dimensional accurate, centrifugal sudden, and J-shifting results. <i>Journal of Chemical Physics</i> , 2003, 118, 8261-8267.	1.2	62
100	Vibrational excitation in the transition state: The CH <sub>4</sub> +H→CH <sub>3</sub> +H <sub>2</sub> reaction rate constant in an extended temperature interval. <i>Journal of Chemical Physics</i> , 2002, 116, 2863-2869.	1.2	109
101	REACTION RATES: ACCURATE QUANTUM DYNAMICAL CALCULATIONS FOR POLYATOMIC SYSTEMS. <i>Journal of Theoretical and Computational Chemistry</i> , 2002, 01, 153-172.	1.8	39
102	Accurate quantum dynamics of a combustion reaction: Thermal rate constants of O(3P)+CH <sub>4</sub> (X <sup>1</sup> A <sub>1</sub> )→OH(X <sup>2</sup> Σ <sup>+</sup> ) + CH <sub>3</sub> (X <sup>2</sup> A <sub>2</sub> ← <sup>3</sup> ). <i>Journal of Chemical Physics</i> , 2002, 117, 4635-4638.	1.2	103
103	Quantum Dynamics of the CH <sub>4</sub> + H → CH <sub>3</sub> + H <sub>2</sub> Reaction: Full-Dimensional and Reduced Dimensionality Rate Constant Calculations. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2522-2529.	1.1	120
104	Partition functions for reaction rate calculations: statistical sampling and MCTDH propagation. <i>Chemical Physics Letters</i> , 2001, 349, 321-328.	1.2	43
105	The importance of an accurate CH <sub>4</sub> vibrational partition function in full dimensionality calculations of the H+CH <sub>4</sub> →H <sub>2</sub> +CH <sub>3</sub> reaction. <i>Journal of Chemical Physics</i> , 2001, 114, 9683-9684.	1.2	89
106	Full-dimensional quantum study of the vibrational predissociation of the I <sub>2</sub> ←Ne <sub>2</sub> cluster. <i>Journal of Chemical Physics</i> , 2001, 115, 5477-5484.	1.2	33
107	Quantum-classical Liouville description of multidimensional nonadiabatic molecular dynamics. <i>Journal of Chemical Physics</i> , 2001, 114, 2001-2012.	1.2	79
108	Reaction Rates. <i>Lecture Notes in Quantum Chemistry II</i> , 2001, , 167-193.	0.3	1

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109	Rotational effects in the $\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$ reaction rate: Full-dimensional close-coupling results. <i>Journal of Chemical Physics</i> , 2000, 113, 5725-5731.	1.2	81
110	Combined iterative diagonalization and statistical sampling in accurate reaction rate calculations: Rotational effects in $\text{O} + \text{HCl} \rightarrow \text{OH} + \text{Cl}$ . <i>Journal of Chemical Physics</i> , 2000, 112, 130-136.	1.2	72
111	Full dimensional quantum calculations of the $\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2$ reaction rate. <i>Journal of Chemical Physics</i> , 2000, 113, 5115.	1.2	178
112	Direct Calculation of Reaction Rates. <i>Lecture Notes in Quantum Chemistry II</i> , 2000, , 130-149.	0.3	1
113	Accurate reaction rate calculations including internal and rotational motion: A statistical multi-configurational time-dependent Hartree approach. <i>Journal of Chemical Physics</i> , 1999, 110, 88-96.	1.2	85
114	Quantum-mechanical calculation of the thermal rate constant for the $\text{H}_2 + \text{Cl} \rightarrow \text{H} + \text{HCl}$ reaction. <i>Chemical Physics Letters</i> , 1999, 313, 647-654.	1.2	74
115	Quantum calculations of thermal rate constants and reaction probabilities: $\text{H}_2 + \text{CN} \rightarrow \text{H} + \text{HCN}$ . <i>Chemical Physics Letters</i> , 1998, 282, 442-449.	1.2	60
116	Variational wave packet method for dissipative photodesorption problems. <i>Chemical Physics Letters</i> , 1998, 288, 383-390.	1.2	17
117	A microscopic description of dissipation in systems with strong vibronic coupling: the S1 and S2 absorption spectra of pyrazine. <i>Chemical Physics Letters</i> , 1998, 295, 167-174.	1.2	15
118	An effective method for the quantum mechanical description of photoionization with ultrashort intense laser pulses. <i>Journal of Chemical Physics</i> , 1998, 109, 36-41.	1.2	29
119	Accurate quantum calculations of thermal rate constants employing MCTDH: $\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$ and $\text{D}_2 + \text{OH} \rightarrow \text{D} + \text{DOH}$ . <i>Journal of Chemical Physics</i> , 1998, 108, 4828-4836.	1.2	140
120	A multi-configurational time-dependent Hartree approach to the direct calculation of thermal rate constants. <i>Journal of Chemical Physics</i> , 1997, 106, 2646-2653.	1.2	97
121	A wave packet approach to the Liouville-von Neumann equation for dissipative systems. <i>Journal of Chemical Physics</i> , 1997, 106, 3017-3023.	1.2	22
122	The resonance Raman spectrum of $\text{CH}_3\text{I}$ : An application of the MCTDH approach. <i>Journal of Chemical Physics</i> , 1997, 107, 6584-6593.	1.2	25
123	A time-dependent discrete variable representation for (multiconfiguration) Hartree methods. <i>Journal of Chemical Physics</i> , 1996, 105, 6989-6994.	1.2	164
124	Improved L2-stabilization theory to compute resonances under multichannel conditions. <i>Chemical Physics Letters</i> , 1996, 249, 237-243.	1.2	12
125	Iterative diagonalization within the multi-configurational time-dependent Hartree approach: calculation of vibrationally excited states and reaction rates. <i>Chemical Physics Letters</i> , 1996, 252, 71-76.	1.2	75
126	Calculation of initial state-selected reaction probabilities by a minimal number of wavepackets. <i>Chemical Physics Letters</i> , 1995, 241, 497-501.	1.2	37

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127	A new time-dependent approach to the direct calculation of reaction rates. Journal of Chemical Physics, 1995, 102, 9205-9213.	1.2	72
128	Comment on "A multiconfiguration time-dependent Hartree approximation based on natural single-particle states" [J. Chem. Phys. 99, 4055 (1993)]. Journal of Chemical Physics, 1994, 101, 2652-2653.	1.2	27
129	Quantum mechanical calculations of the rate constant for the H <sub>2</sub> +OH <sup>+</sup> H+H <sub>2</sub> O reaction: Full-dimensional results and comparison to reduced dimensionality models. Journal of Chemical Physics, 1994, 101, 4759-4768.	1.2	150
130	Intersystem crossing dynamics in the spin-crossover systems [M:Fe(pic) <sub>3</sub> ]Cl <sub>2</sub> ·xH <sub>2</sub> O (M=Mn or Zn). J. Chem. Phys. 112, 1000 (2000).	1.2	28
131	Time-dependent photodissociation of methyl iodide with five active modes. Journal of Chemical Physics, 1994, 101, 5623-5646.	1.2	162
132	Wavepacket dynamics in five dimensions. Photodissociation of methyl iodide. Chemical Physics Letters, 1993, 211, 7-14.	1.2	71
133	The cumulative reaction probability as eigenvalue problem. Journal of Chemical Physics, 1993, 99, 3411-3419.	1.2	165
134	Full-dimensional quantum mechanical calculation of the rate constant for the H <sub>2</sub> +OH <sup>+</sup> H <sub>2</sub> O+H reaction. Journal of Chemical Physics, 1993, 99, 10078-10081.	1.2	165
135	Multiconfigurational time-dependent Hartree study of complex dynamics: Photodissociation of NO <sub>2</sub> . Journal of Chemical Physics, 1992, 97, 9062-9071.	1.2	162
136	Wavepacket dynamics within the multiconfiguration Hartree framework: General aspects and application to NOCl. Journal of Chemical Physics, 1992, 97, 3199-3213.	1.2	879
137	Femtosecond Wave-Packet Dynamics on Strongly Coupled Potential Energy Surfaces. NATO ASI Series Series B: Physics, 1992, , 83-95.	0.2	4
138	Approximate Methods for Time Evolution of Wave Packets. NATO ASI Series Series B: Physics, 1992, , 233-246.	0.2	0
139	Three-dimensional wave-packet dynamics on vibronically coupled dissociative potential energy surfaces. Chemical Physics Letters, 1991, 178, 36-42.	1.2	28
140	Dissociation and predissociation on coupled electronic potential energy surfaces: A three-dimensional wave packet dynamical study. Journal of Chemical Physics, 1991, 95, 1708-1720.	1.2	79
141	Advances in Mössbauer Emission Spectroscopy. Hyperfine Interactions, 1990, 53, 113-141.	0.2	21
142	The multi-configurational time-dependent Hartree approach. Chemical Physics Letters, 1990, 165, 73-78.	1.2	1,678
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