Uwe Manthe

List of Publications by Year
in descending order

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145	10,155	26567 56	33814 99
papers	citations	h-index	g-index

158	158	158	3016
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The multi-configurational time-dependent Hartree approach. Chemical Physics Letters, 1990, 165, 73-78.	1.2	1,678
2	Waveâ€packet dynamics within the multiconfiguration Hartree framework: General aspects and application to NOCl. Journal of Chemical Physics, 1992, 97, 3199-3213.	1.2	879
3	A multilayer multiconfigurational time-dependent Hartree approach for quantum dynamics on general potential energy surfaces. Journal of Chemical Physics, 2008, 128, 164116.	1.2	339
4	First-Principles Theory for the H + CH4 -> H2 + CH3 Reaction. Science, 2004, 306, 2227-2229.	6.0	238
5	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
6	Full dimensional quantum calculations of the CH[sub 4]+Hâ†'CH[sub 3]+H[sub 2] reaction rate. Journal of Chemical Physics, 2000, 113, 5115.	1.2	178
7	Dynamics on potential energy surfaces with a conical intersection: Adiabatic, intermediate, and diabatic behavior. Journal of Chemical Physics, 1990, 93, 1658-1669.	1.2	166
8	The cumulative reaction probability as eigenvalue problem. Journal of Chemical Physics, 1993, 99, 3411-3419.	1.2	165
9	Fullâ€dimensional quantum mechanical calculation of the rate constant for the H2+OHâ†'H2O+H reaction. Journal of Chemical Physics, 1993, 99, 10078-10081.	1.2	165
10	A timeâ€dependent discrete variable representation for (multiconfiguration) Hartree methods. Journal of Chemical Physics, 1996, 105, 6989-6994.	1.2	164
11	New method for calculating wave packet dynamics: Strongly coupled surfaces and the adiabatic basis. Journal of Chemical Physics, 1990, 93, 345-356.	1.2	163
12	Multiconfigurational timeâ€dependent Hartree study of complex dynamics: Photodissociation of NO2. Journal of Chemical Physics, 1992, 97, 9062-9071.	1.2	162
13	Timeâ€dependent photodissociation of methyl iodide with five active modes. Journal of Chemical Physics, 1994, 101, 5623-5646.	1.2	162
14	Quantum mechanical calculations of the rate constant for the H2+OHâ†'H+H2O reaction: Fullâ€dimensional results and comparison to reduced dimensionality models. Journal of Chemical Physics, 1994, 101, 4759-4768.	1.2	150
15	Accurate quantum calculations of thermal rate constants employing MCTDH: H2+OHâ†'H+H2O and D2+OHâ†'D+DOH. Journal of Chemical Physics, 1998, 108, 4828-4836.	1.2	140
16	Comparison of Quantum Dynamics and Quantum Transition State Theory Estimates of the H + CH₄ Reaction Rate. Journal of Physical Chemistry A, 2009, 113, 4468-4478.	1.1	140
17	Quantum Dynamics of the CH4+ H â†' CH3+ H2Reaction:Â Full-Dimensional and Reduced Dimensionality Rate Constant Calculationsâ€. Journal of Physical Chemistry A, 2001, 105, 2522-2529.	1.1	120
18	The ground state tunneling splitting of malonaldehyde: Accurate full dimensional quantum dynamics calculations. Journal of Chemical Physics, 2004, 121, 9207-9210.	1.2	116

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19	Layered discrete variable representations and their application within the multiconfigurational time-dependent Hartree approach. Journal of Chemical Physics, 2009, 130, 054109.	1.2	115
20	Vibrational excitation in the transition state: The CH4+Hâ†'CH3+H2 reaction rate constant in an extended temperature interval. Journal of Chemical Physics, 2002, 116, 2863-2869.	1.2	109
21	Accurate quantum dynamics of a combustion reaction: Thermal rate constants of O(3P)+CH4(Xâ€Š1A1)â†'OH(Xâ€Š2Î)+CH3(Xâ€Š2A2â€³). Journal of Chemical Physics, 2002, 117, 4635-4638.	1.2	103
22	Accurate potential energy surface and quantum reaction rate calculations for the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2006, 124, 164307.	1.2	101
23	A multi-configurational time-dependent Hartree approach to the direct calculation of thermal rate constants. Journal of Chemical Physics, 1997, 106, 2646-2653.	1.2	97
24	The state averaged multiconfigurational time-dependent Hartree approach: Vibrational state and reaction rate calculations. Journal of Chemical Physics, 2008, 128, 064108.	1.2	94
25	The importance of an accurate CH4 vibrational partition function in full dimensionality calculations of the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2001, 114, 9683-9684.	1.2	89
26	Quantum dynamics of the H+CH4â†'H2+CH3 reaction in curvilinear coordinates: Full-dimensional and reduced dimensional calculations of reaction rates. Journal of Chemical Physics, 2010, 132, 084103.	1.2	89
27	Intramolecular proton transfer in malonaldehyde: Accurate multilayer multi-configurational time-dependent Hartree calculations. Journal of Chemical Physics, 2011, 134, 224305.	1.2	87
28	Accurate reaction rate calculations including internal and rotational motion: A statistical multi-configurational time-dependent Hartree approach. Journal of Chemical Physics, 1999, 110, 88-96.	1.2	85
29	Communication: Ro-vibrational control of chemical reactivity in H+CH4â†' H2+CH3 : Full-dimensional quantum dynamics calculations and a sudden model. Journal of Chemical Physics, 2014, 141, 051102.	1.2	84
30	A transition state view on reactive scattering: Initial state-selected reaction probabilities for the H+CH4â†'H2+CH3 reaction studied in full dimensionality. Journal of Chemical Physics, 2010, 133, 174124.	1.2	83
31	Loss of Memory in H + CH₄ â†' H₂ + CH₃ State-to-State Reactive Scattering. Journal of Physical Chemistry Letters, 2015, 6, 338-342.	2.1	82
32	Rotational effects in the H2+OHâ†'H+H2O reaction rate: Full-dimensional close-coupling results. Journal of Chemical Physics, 2000, 113, 5725-5731.	1.2	81
33	Dissociation and predissociation on coupled electronic potential energy surfaces: A threeâ€dimensional wave packet dynamical study. Journal of Chemical Physics, 1991, 95, 1708-1720.	1.2	79
34	Quantum-classical Liouville description of multidimensional nonadiabatic molecular dynamics. Journal of Chemical Physics, 2001, 114, 2001-2012.	1.2	79
35	Iterative diagonalization in the state-averaged multi-configurational time-dependent Hartree approach: Excited state tunneling splittings in malonaldehyde. Journal of Chemical Physics, 2012, 136, 054105.	1.2	78
36	Photoionization-induced dynamics of ammonia:Ab initiopotential energy surfaces and time-dependent wave packet calculations for the ammonia cation. Journal of Chemical Physics, 2006, 124, 214306.	1.2	77

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37	Communications: A rigorous transition state based approach to state-specific reaction dynamics: Full-dimensional calculations for H+CH4â†'H2+CH3. Journal of Chemical Physics, 2010, 132, 191101.	1.2	77
38	Iterative diagonalization within the multi-configurational time-dependent Hartree approach: calculation of vibrationally excited states and reaction rates. Chemical Physics Letters, 1996, 252, 71-76.	1.2	75
39	Quantum-mechanical calculation of the thermal rate constant for the H2+Clâ†'H+HCl reaction. Chemical Physics Letters, 1999, 313, 647-654.	1.2	74
40	A new timeâ€dependent approach to the direct calculation of reaction rates. Journal of Chemical Physics, 1995, 102, 9205-9213.	1.2	72
41	Combined iterative diagonalization and statistical sampling in accurate reaction rate calculations: Rotational effects in O+HClâ†'OH+Cl. Journal of Chemical Physics, 2000, 112, 130-136.	1.2	72
42	Wavepacket dynamics in five dimensions. Photodissociation of methyl iodide. Chemical Physics Letters, 1993, 211, 7-14.	1.2	71
43	Multiconfigurational time-dependent Hartree calculations for tunneling splittings of vibrational states: Theoretical considerations and application to malonaldehyde. Journal of Chemical Physics, 2009, 131, 224109.	1.2	70
44	Reaction dynamics with the multi-layer multi-configurational time-dependent Hartree approach: H + CH4 â†' H2 + CH3 rate constants for different potentials. Journal of Chemical Physics, 2012, 137, 244106.	1.2	68
45	Full-dimensional and reduced-dimensional calculations of initial state-selected reaction probabilities studying the H + CH4 â†' H2 + CH3 reaction on a neural network PES. Journal of Chemical Physics, 2015, 142, 064309.	1.2	68
46	Resonances in the Entrance Channel of the Elementary Chemical Reaction of Fluorine and Methane. Angewandte Chemie - International Edition, 2014, 53, 1122-1126.	7.2	66
47	Photoinduced dynamics of the valence states of ethene: A six-dimensional potential-energy surface of three electronic states with several conical intersections. Journal of Chemical Physics, 2003, 119, 1397-1411.	1.2	65
48	Quantum mechanical calculation of the OH+HClâ†'H2O+Cl reaction rate: Full-dimensional accurate, centrifugal sudden, andJ-shifting results. Journal of Chemical Physics, 2003, 118, 8261-8267.	1.2	62
49	A potential energy surface construction scheme for accurate reaction rate calculations: General approach and a test for the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2003, 119, 14-23.	1.2	61
50	Multidimensional time-dependent discrete variable representations in multiconfiguration Hartree calculations. Journal of Chemical Physics, 2005, 123, 064106.	1.2	61
51	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
52	Accurate quantum calculations of the reaction rates for Hâ•D+CH4. Journal of Chemical Physics, 2007, 126, 084303.	1.2	61
53	Quantum calculations of thermal rate constants and reaction probabilities: H2+CNâ†'H+HCN. Chemical Physics Letters, 1998, 282, 442-449.	1.2	60
54	Photoinduced dynamics of ethene in the N, V, and Z valence states: A six-dimensional nonadiabatic quantum dynamics investigation. Journal of Chemical Physics, 2004, 120, 11000-11010.	1.2	60

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55	On the integration of the multi-configurational time-dependent Hartree (MCTDH) equations of motion. Chemical Physics, 2006, 329, 168-178.	0.9	58
56	State-to-state reaction probabilities within the quantum transition state framework. Journal of Chemical Physics, 2012, 136, 064117.	1.2	58
57	The role of the transition state in polyatomic reactions: Initial state-selected reaction probabilities of the H + CH4 â†' H2 + CH3 reaction. Journal of Chemical Physics, 2014, 141, 174313.	1.2	58
58	The multi-configurational time-dependent Hartree approach revisited. Journal of Chemical Physics, 2015, 142, 244109.	1.2	57
59	Accurate calculations of reaction rates: predictive theory based on a rigorous quantum transition state concept. Molecular Physics, 2011, 109, 1415-1426.	0.8	51
60	Full-Dimensional Quantum Reaction Rate Calculations for H + CH₄ â†' H₂ + CH₃ on a Recent Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 9617-9622.	1.1	50
61	Photodissociation of methyl iodide embedded in a host-guest complex: A full dimensional (189D) quantum dynamics study of CH3I@resorc[4]arene. Journal of Chemical Physics, 2011, 135, 184102.	1.2	50
62	Fast Shepard interpolation on graphics processing units: Potential energy surfaces and dynamics for H + CH4 â†' H2 + CH3. Journal of Chemical Physics, 2013, 138, 164118.	1.2	50
63	The reaction rate for dissociative adsorption of N2 on stepped Ru(0001): Six-dimensional quantum calculations. Journal of Chemical Physics, 2005, 122, 234702.	1.2	48
64	Communication: Mode specific quantum dynamics of the F + CHD3 â†' HF + CD3 reaction. Journal of Chemical Physics, 2016, 144, 171101.	1.2	47
65	Neural network based coupled diabatic potential energy surfaces for reactive scattering. Journal of Chemical Physics, 2017, 147, 084105.	1.2	46
66	Thermochemistry and Accurate Quantum Reaction Rate Calculations for H2/HD/D2+ CH3â€. Journal of Physical Chemistry A, 2007, 111, 10331-10337.	1.1	45
67	Partition functions for reaction rate calculations: statistical sampling and MCTDH propagation. Chemical Physics Letters, 2001, 349, 321-328.	1.2	43
68	Quantum dynamics of the CH3 fragment: A curvilinear coordinate system and kinetic energy operators. Journal of Chemical Physics, 2007, 127, 144302.	1.2	43
69	Communication: Reactivity borrowing in the mode selective chemistry of H + CHD3 â†' H2 + CD3. Journal of Chemical Physics, 2017, 147, 241104.	1.2	43
70	Thermal Rate Constants for Polyatomic Reactions: First Principles Quantum Theory. Zeitschrift Fur Physikalische Chemie, 2007, 221, 171-213.	1.4	41
71	Coupled potential energy surface for the F(2P) + CH4 â†' HF + CH3 entrance channel and quantum dynamics of the CH4â€‰Â·â€‰Fâ^' photodetachment. Journal of Chemical Physics, 2013, 139, 014309.	1.2	40
72	REACTION RATES: ACCURATE QUANTUM DYNAMICAL CALCULATIONS FOR POLYATOMIC SYSTEMS. Journal of Theoretical and Computational Chemistry, 2002, 01, 153-172.	1.8	39

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73	Thermal flux based analysis of state-to-state reaction probabilities. Molecular Physics, 2012, 110, 703-715.	0.8	39
74	Calculation of initial state-selected reaction probabilities by a minimal number of wavepackets. Chemical Physics Letters, 1995, 241, 497-501.	1.2	37
75	Correlation functions for fully or partially state-resolved reactive scattering calculations. Journal of Chemical Physics, 2014, 140, 244113.	1.2	37
76	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
77	Photodissociation of CH₃I: A Full-Dimensional (9D) Quantum Dynamics Study. Journal of Physical Chemistry A, 2011, 115, 5992-6001.	1.1	34
78	Full-dimensional quantum study of the vibrational predissociation of the I2â‹¯Ne2 cluster. Journal of Chemical Physics, 2001, 115, 5477-5484.	1.2	33
79	The Sudden-Polarization Effect and its Role in the Ultrafast Photochemistry of Ethene. Angewandte Chemie - International Edition, 2003, 42, 3434-3436.	7.2	33
80	Wavepacket dynamics and the multi-configurational time-dependent Hartree approach. Journal of Physics Condensed Matter, 2017, 29, 253001.	0.7	33
81	Full-dimensional quantum dynamics calculations for H + CHD3 â†' H2 + CD3: The effect of multiple vibrational excitations. Journal of Chemical Physics, 2018, 148, 224303.	1.2	33
82	CH₅⁺: Symmetry and the Entangled Rovibrational Quantum States of a Fluxional Molecule. Journal of Physical Chemistry Letters, 2015, 6, 4229-4232.	2.1	32
83	On the multi-layer multi-configurational time-dependent Hartree approach for bosons and fermions. Journal of Chemical Physics, 2017, 146, 064117.	1.2	32
84	An effective method for the quantum mechanical description of photoionization with ultrashort intense laser pulses. Journal of Chemical Physics, 1998, 109, 36-41.	1.2	29
85	Three-dimensional wave-packet dynamics on vibronically coupled dissociative potential energy surfaces. Chemical Physics Letters, 1991, 178, 36-42.	1.2	28
86	Intersystem crossing dynamics in the spinâ€“crossover systems [M:Fe(pic)3]Cl2â‹…Sol (M=Mn or Zn,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.2	28
87	Comment on â€˜â€˜A multiconfiguration timeâ€dependent Hartree approximation based on natural singleâ€particle statesâ€™â€™ [J. Chem. Phys. 99,â€‰4055â€‰(1993)]. Journal of Chemical Physics, 1994, 101, 2652-2653.	1.2	27
88	Photoionization-induced dynamics of the ammonia cation studied by wave packet calculations using curvilinear coordinates. Chemical Physics, 2008, 347, 331-339.	0.9	27
89	A Quasiclassical Study of the F(²P) + CHD₃ (Î½₁ = 0,1) Reactive System on an Accurate Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 12209-12217.	1.1	27
90	The effect of spinâ€“orbit coupling on the thermal rate constant of the H2+ Cl â†' H + HCl reaction. Physical Chemistry Chemical Physics, 2004, 6, 5026-5030.	1.3	26

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91	Vibrational Dynamics of the CH4Â·Fâ€“Complex. Journal of Physical Chemistry A, 2012, 116, 11249-11259.	1.1	26
92	The resonance Raman spectrum of CH3I: An application of the MCTDH approach. Journal of Chemical Physics, 1997, 107, 6584-6593.	1.2	25
93	On direct product based discrete variable representations for angular coordinates and the treatment of singular terms in the kinetic energy operator. Chemical Physics, 2010, 374, 118-125.	0.9	25
94	H+CH4â†' H2+ CH3 initial state-selected reaction probabilities on different potential energy surfaces. Chemical Physics, 2017, 482, 106-112.	0.9	25
95	Longâ€Distance Rate Acceleration by Bulk Gold. Angewandte Chemie - International Edition, 2019, 58, 6574-6578.	7.2	25
96	Multiconfigurational time-dependent Hartree calculations for dissociative adsorption of H2 on Cu(100). Journal of Chemical Physics, 2004, 121, 3829-3835.	1.2	23
97	A wave packet approach to the Liouvilleâ€“von Neumann equation for dissipative systems. Journal of Chemical Physics, 1997, 106, 3017-3023.	1.2	22
98	Advances in MÃ¶ssbauer Emission Spectroscopy. Hyperfine Interactions, 1990, 53, 113-141.	0.2	21
99	A full-dimensional wave packet dynamics study of the photodetachment spectra of FCH 4â^'. Journal of Chemical Physics, 2012, 137, 044306.	1.2	19
100	Natural reaction channels in HÂ+ CHD₃ â†' H₂ + CD₃. Faraday Discussions, 2018, 212, 217-235.	1.6	18
101	Variational wave packet method for dissipative photodesorption problems. Chemical Physics Letters, 1998, 288, 383-390.	1.2	17
102	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
103	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of OH(A2Î£+) by H2. Nature Chemistry, 2021, 13, 909-915.	6.6	17
104	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
105	Fermi resonance controlled product branching in the H + HOD reaction. Physical Chemistry Chemical Physics, 2018, 20, 17029-17037.	1.3	16
106	Vibronically and spin-orbit coupled diabatic potentials for X(2P) + CH4 â†' HX + CH3 reactions: Neural network potentials for X = Cl. Journal of Chemical Physics, 2019, 150, 244115.	1.2	16
107	A microscopic description of dissipation in systems with strong vibronic coupling: the S1 and S2 absorption spectra of pyrazine. Chemical Physics Letters, 1998, 295, 167-174.	1.2	15
108	Iterative Diagonalization in the Multiconfigurational Time-Dependent Hartree Approach: Ro-vibrational Eigenstates. Journal of Physical Chemistry A, 2013, 117, 7246-7255.	1.1	15

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109	Quasi-Bound States of the FÂ·CH4 Complex. Journal of Physical Chemistry A, 2016, 120, 3186-3195.	1.1	15
110	Non-adiabatic effects in F + CHD3 reactive scattering. Journal of Chemical Physics, 2017, 146, 214117.	1.2	15
111	A multi-configurational time-dependent Hartree approach to the eigenstates of multi-well systems. Journal of Chemical Physics, 2012, 136, 124119.	1.2	13
112	Improved L2-stabilization theory to compute resonances under multichannel conditions. Chemical Physics Letters, 1996, 249, 237-243.	1.2	12
113	The multi-configurational time-dependent Hartree approach in optimized second quantization: Imaginary time propagation and particle number conservation. Journal of Chemical Physics, 2020, 152, 034101.	1.2	12
114	Calculating vibrational spectra using modified Shepard interpolated potential energy surfaces. Journal of Chemical Physics, 2008, 129, 024104.	1.2	11
115	Vibronically and spin-orbit coupled diabatic potentials for X(P) + CH4 â†' HX + CH3 reactions: General theory and application for X(P) = F(2P). Journal of Chemical Physics, 2019, 150, 064102.	1.2	11
116	First principle nonlinear quantum dynamics using a correlation-based von Neumann entropy. Journal of Chemical Physics, 2012, 136, 204116.	1.2	10
117	Decoherence induced by conical intersections: Complexity constrained quantum dynamics of photoexcited pyrazine. Journal of Chemical Physics, 2012, 137, 22A509.	1.2	9
118	Optimized unoccupied single-particle functions in the (multi-layer) multi-configurational time-dependent Hartree approach. Chemical Physics, 2018, 515, 279-286.	0.9	9
119	Longâ€Distance Rate Acceleration by Bulk Gold. Angewandte Chemie, 2019, 131, 6646-6650.	1.6	8
120	Non-adiabatic transitions in the reaction of fluorine with methane. Journal of Chemical Physics, 2020, 152, 231102.	1.2	8
121	Off-normal incidence dissociative sticking of H2 on Cu(100) studied using six-dimensional quantum calculations. Journal of Chemical Physics, 2005, 123, 124706.	1.2	7
122	Coordinate systems and kinetic energy operators for multi-configurational time-dependent Hartree calculations studying reactions of methane. Chemical Physics, 2018, 509, 37-44.	0.9	7
123	Symmetries in the multi-configurational time-dependent Hartree wavefunction representation and propagation. Journal of Chemical Physics, 2021, 154, 194108.	1.2	7
124	Quantum dynamics of H2 in a carbon nanotube: Separation of time scales and resonance enhanced tunneling. Journal of Chemical Physics, 2017, 147, 084103.	1.2	6
125	Counter-propagating wave packets in the quantum transition state approach to reactive scattering. Journal of Chemical Physics, 2019, 150, 184103.	1.2	6
126	Vibronic coupling in the FÂ·CH4 prereactive complex. Journal of Chemical Physics, 2019, 151, 104106.	1.2	6

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127	Vibrational control of the reaction pathway in the H + CHD ₃ â†' H ₂ + CD ₃ reaction. Science Advances, 2022, 8, eabm9820.	4.7	6
128	The effect of surface relaxation on the N2 dissociation rate on stepped Ru: A transition state theory study. Journal of Chemical Physics, 2006, 124, 026102.	1.2	5
129	A Quasi-Classical Evaluation of the J-Shifting Approximation for the Reactive Cross Sections of F + CHD₃ and F + CH₄. Journal of Physical Chemistry A, 2019, 123, 7237-7245.	1.1	5
130	A non-hierarchical correlation discrete variable representation. Journal of Chemical Physics, 2022, 156, 134107.	1.2	5
131	A transition-state based rotational sudden (TSRS) approximation for polyatomic reactive scattering. Journal of Chemical Physics, 2017, 147, 144104.	1.2	4
132	Eight-Dimensional Wave Packet Dynamics Within the Quantum Transition-State Framework: State-to-State Reactive Scattering for H₂ + CH₃ â‡† H + CH₄. Journal of Physical Chemistry A, 2020, 124, 9400-9412.	1.1	4
133	Femtosecond Wave-Packet Dynamics on Strongly Coupled Potential Energy Surfaces. NATO ASI Series Series B: Physics, 1992, , 83-95.	0.2	4
134	First-Principles Theory for the Reaction of Chlorine with Methane. Journal of Physical Chemistry Letters, 2022, 13, 2563-2566.	2.1	3
135	Wave packet dynamics in the optimal superadiabatic approximation. Journal of Chemical Physics, 2016, 144, 224109.	1.2	2
136	Direct product-type grid representations for angular coordinates in extended space and their application in the MCTDH approach. Journal of Chemical Physics, 2021, 154, 104115.	1.2	2
137	The multi-configurational time-dependent Hartree approach in optimized second quantization: Thermal ensembles and statistical sampling. Chemical Physics, 2022, 555, 111413.	0.9	2
138	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	1.6	1
139	Reaction Rates. Lecture Notes in Quantum Chemistry II, 2001, , 167-193.	0.3	1
140	Direct Calculation of Reaction Rates. Lecture Notes in Quantum Chemistry II, 2000, , 130-149.	0.3	1
141	Iterative Diagonalization of Operators. , 0, , 69-71.		0
142	Quantum dynamics of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 281-306.	1.6	0
143	Approximate Methods for Time Evolution of Wave Packets. NATO ASI Series Series B: Physics, 1992, , 233-246.	0.2	0
144	Multi Dimensional Quantum Dynamics. , 2005, , 225-236.		0

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145	Multi Dimensional Quantum Dynamics ofÂChemical Reaction Processes. , 2009, , 143-152.		0