Ralph Welsch

List of Publications by Year
in descending order

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36	1,123	567144 15	395590 33
papers	citations	h-index	g-index

38	38	38	1170
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Initial state-selected scattering for the reactions H + CH4/CHD3 and F + CHD3 employing ring polymer molecular dynamics. Journal of Chemical Physics, 2022, 156, 044101.	1.2	6
2	Stateâ€selective cross sections from ring polymer molecular dynamics. International Journal of Quantum Chemistry, 2021, 121, e26447.	1.0	7
3	Ultrafast time-resolved x-ray absorption spectroscopy of ionized urea and its dimer through ab initio nonadiabatic dynamics. Structural Dynamics, 2021, 8, 034102.	0.9	3
4	Time-resolving the UV-initiated photodissociation dynamics of OCS. Faraday Discussions, 2021, 228, 413-431.	1.6	5
5	Observation of the fastest chemical processes in the radiolysis of water. Science, 2020, 367, 179-182.	6.0	149
6	Choice of the electronic basis for field-induced surface hopping. Physical Review A, 2020, 102, .	1.0	3
7	Calculations of quantum tunnelling rates for muonium reactions with methane, ethane and propane. Physical Chemistry Chemical Physics, 2020, 22, 16843-16854.	1.3	10
8	Field-enabled quantum interference in atomic Auger decay. Physical Review A, 2020, 102, .	1.0	0
9	Molecular electronic decoherence following attosecond photoionisation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 164006.	0.6	13
10	Nuclear quantum effects in state-selective scattering from ring polymer molecular dynamics. Journal of Chemical Physics, 2020, 152, 194113.	1.2	12
11	Hole dynamics in a photovoltaic donor-acceptor couple revealed by simulated time-resolved X-ray absorption spectroscopy. Structural Dynamics, 2019, 6, 044102.	0.9	13
12	Kinetic isotope effects in the water forming reaction H2/D2 + OH from rigorous close-coupling quantum dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 17054-17062.	1.3	3
13	Probing photodissociation dynamics using ring polymer molecular dynamics. Journal of Chemical Physics, 2019, 150, 114105.	1.2	6
14	Simulated XUV photoelectron spectra of THz-pumped liquid water. Journal of Chemical Physics, 2019, 150, 044505.	1.2	2
15	Challenges in XUV Photochemistry Simulations: A Case Study on Ultrafast Fragmentation Dynamics of the Benzene Radical Cation. Journal of Physical Chemistry A, 2018, 122, 1004-1010.	1.1	10
16	Control of Nuclear Dynamics through Conical Intersections and Electronic Coherences. Physical Review Letters, 2018, 120, 123001.	2.9	49
17	Infrared-laser-pulse-enhanced ultrafast fragmentation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:mo> following Auger decay: Mixed quantum-classical simulations. Physical Review A, 2018, 98, .	1.0	9
18	Prospects of Using High-Intensity THz Pulses To Induce Ultrafast Temperature-Jumps in Liquid Water. Journal of Physical Chemistry A, 2018, 122, 5211-5222.	1.1	14

#	Article	IF	Citations
19	Molecular polarizability anisotropy of liquid water revealed by terahertz-induced transient orientation. Nature Communications, 2018, 9, 2142.	5.8	63
20	Rigorous close-coupling quantum dynamics calculation of thermal rate constants for the water formation reaction of H2 + OH on a high-level PES. Journal of Chemical Physics, 2018, 148, 204304.	1.2	11
21	Lowâ€Temperature Thermal Rate Constants for the Water Formation Reaction H₂+OH from Rigorous Quantum Dynamics Calculations. Angewandte Chemie, 2018, 130, 13334-13337.	1.6	2
22	Lowâ€Temperature Thermal Rate Constants for the Water Formation Reaction H₂+OH from Rigorous Quantum Dynamics Calculations. Angewandte Chemie - International Edition, 2018, 57, 13150-13153.	7.2	5
23	2D THz-THz-Raman Photon-Echo Spectroscopy of Molecular Vibrations in Liquid Bromoform. Journal of Physical Chemistry Letters, 2017, 8, 4640-4644.	2.1	39
24	Non-equilibrium dynamics from RPMD and CMD. Journal of Chemical Physics, 2016, 145, 204118.	1.2	48
25	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	1.6	2
26	Molecular Seesaw: How Increased Hydrogen Bonding Can Hinder Excited-State Proton Transfer. Journal of Physical Chemistry Letters, 2016, 7, 3616-3620.	2.1	14
27	Coherent two-dimensional terahertz-terahertz-Raman spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 6857-6861.	3.3	80
28	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
29	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
30	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
31	Correlation functions for fully or partially state-resolved reactive scattering calculations. Journal of Chemical Physics, 2014, 140, 244113.	1.2	37
32	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
33	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
34	Thermal flux based analysis of state-to-state reaction probabilities. Molecular Physics, 2012, 110, 703-715.	0.8	39
35	State-to-state reaction probabilities within the quantum transition state framework. Journal of Chemical Physics, 2012, 136, 064117.	1.2	58
36	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