Graham A Worth

List of Publications by Year
in descending order

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73 papers	3,048 citations	201674 27 h-index	155660 55 g-index
97 all docs	97 docs citations	97 times ranked	2232 citing authors

#	Article	IF	Citations
1	Mixed-quantum-classical or fully-quantized dynamics? A unified code to compare methods. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200386.	3.4	11
2	Improved algorithm for the direct dynamics variational multi-configurational Gaussian method. Journal of Chemical Physics, 2021, 154, 124127.	3.0	12
3	Control of nuclear dynamics in the benzene cation by electronic wavepacket composition. Communications Chemistry, 2021, 4, .	4.5	9
4	Multi-layer Gaussian-based multi-configuration time-dependent Hartree (ML-GMCTDH) simulations of ultrafast charge separation in a donorâ€“acceptor complex. Journal of Chemical Physics, 2021, 154, 144106.	3.0	10
5	Unlocking the Double Bond in Protonated Schiff Bases by Coherent Superposition of S₁ and S₂. Journal of Physical Chemistry Letters, 2021, 12, 5639-5643.	4.6	8
6	Threshold Photoelectron Spectrum of Cyclobutadiene: Comparison with Time-Dependent Wavepacket Simulations. Journal of Physical Chemistry Letters, 2021, 12, 6901-6906.	4.6	8
7	Quantum dynamics with ab initio potentials. Journal of Chemical Physics, 2021, 155, 080401.	3.0	2
8	Direct nonadiabatic quantum dynamics simulations of the photodissociation of phenol. Physical Chemistry Chemical Physics, 2021, 23, 23684-23695.	2.8	9
9	Micro-Solvated DMABN: Excited State Quantum Dynamics and Dual Fluorescence Spectra. Molecules, 2021, 26, 7247.	3.8	4
10	Quantics: A general purpose package for Quantum molecular dynamics simulations. Computer Physics Communications, 2020, 248, 107040.	7.5	46
11	The quantum-Ehrenfest method with the inclusion of an IR pulse: Application to electron dynamics of the allene radical cation. Journal of Chemical Physics, 2020, 153, 031102.	3.0	3
12	The role of vibronic coupling in the electronic spectroscopy of maleimide: a multi-mode and multi-state quantum dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 25272-25283.	2.8	12
13	Shining light on the electronic structure and relaxation dynamics of the isolated oxyluciferin anion. Physical Chemistry Chemical Physics, 2020, 22, 19022-19032.	2.8	5
14	How important is roaming in the photodegradation of nitrobenzene?. Physical Chemistry Chemical Physics, 2020, 22, 15945-15952.	2.8	12
15	On the Intrinsically Low Quantum Yields of Pyrimidine DNA Photodamages: Evaluating the Reactivity of the Corresponding Minimum Energy Crossing Points. Journal of Physical Chemistry Letters, 2020, 11, 4984-4989.	4.6	8
16	MR-MCTDH[n]: Flexible Configuration Spaces and Nonadiabatic Dynamics within the MCTDH[n] Framework. Journal of Chemical Theory and Computation, 2020, 16, 4087-4097.	5.3	10
17	Time-Resolved Photoelectron Spectroscopy Studies of Isoxazole and Oxazole. Journal of Physical Chemistry A, 2020, 124, 3984-3992.	2.5	10
18	Systematic and variational truncation of the configuration space in the multiconfiguration time-dependent Hartree method: The MCTDH[n] hierarchy. Journal of Chemical Physics, 2020, 152, 084101.	3.0	13

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19	Electron transfer in photoexcited pyrrole dimers. Journal of Chemical Physics, 2019, 151, 164304.	3.0	2
20	Similar chemical structures, dissimilar triplet quantum yields: a CASPT2 model rationalizing the trend of triplet quantum yields in nitroaromatic systems. Physical Chemistry Chemical Physics, 2019, 21, 10514-10522.	2.8	10
21	Field modified spinâ€“orbit potential curves of IBr. Preliminary dynamical results. Physical Chemistry Chemical Physics, 2019, 21, 14429-14439.	2.8	4
22	Unravelling the Role of an Aqueous Environment on the Electronic Structure and Ionization of Phenol Using Photoelectron Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 678-682.	4.6	36
23	Using time-resolved photoelectron spectroscopy to unravel the electronic relaxation dynamics of photoexcited molecules. Chemical Society Reviews, 2018, 47, 309-321.	38.1	27
24	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	3.2	1
25	Quantum dynamics of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 281-306.	3.2	0
26	The Ehrenfest method with fully quantum nuclear motion (Qu-Eh): Application to charge migration in radical cations. Journal of Chemical Physics, 2018, 149, 094108.	3.0	30
27	Curve crossing in a manifold of coupled electronic states: direct quantum dynamics simulations of formamide. Faraday Discussions, 2018, 212, 191-215.	3.2	10
28	Multi-state non-adiabatic direct-dynamics on propagated diabatic potential energy surfaces. Chemical Physics Letters, 2017, 683, 606-612.	2.6	31
29	Non-radiative relaxation dynamics of pyrrole following excitation in the range 249.5â€“200 nm. Chemical Physics Letters, 2017, 683, 179-185.	2.6	19
30	Insights into the Complex Photophysics and Photochemistry of the Simplest Nitroaromatic Compound: A CASPT2//CASSCF Study on Nitrobenzene. Journal of Chemical Theory and Computation, 2017, 13, 2777-2788.	5.3	34
31	Modelling the vibrationally mediated photo-dissociation of acetylene. Physical Chemistry Chemical Physics, 2017, 19, 29483-29497.	2.8	3
32	Photoelectron spectroscopy of isolated luciferin and infraluciferin anions in vacuo: competing photodetachment, photofragmentation and internal conversion. Physical Chemistry Chemical Physics, 2017, 19, 22711-22720.	2.8	14
33	ortho and para chromophores of green fluorescent protein: controlling electron emission and internal conversion. Chemical Science, 2017, 8, 1621-1630.	7.4	24
34	Two-dimensional vibronic spectroscopy of molecular aggregates: Trimers, dimers, and monomers. Journal of Chemical Physics, 2016, 145, 084305.	3.0	6
35	Excited state non-adiabatic dynamics of N-methylpyrrole: A time-resolved photoelectron spectroscopy and quantum dynamics study. Journal of Chemical Physics, 2016, 144, 014309.	3.0	21
36	Identification of a new electron-transfer relaxation pathway in photoexcited pyrrole dimers. Nature Communications, 2016, 7, 11357.	12.8	15

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37	A complete description of tunnelling using direct quantum dynamics simulation: Salicylaldimine proton transfer. Journal of Chemical Physics, 2015, 143, 084121.	3.0	22
38	Excited state non-adiabatic dynamics of pyrrole: A time-resolved photoelectron spectroscopy and quantum dynamics study. Journal of Chemical Physics, 2015, 142, 074302.	3.0	59
39	A Practical Diabatisation Scheme for Use with the Direct-Dynamics Variational Multi-Configuration Gaussian Method. Journal of Physical Chemistry A, 2015, 119, 12457-12470.	2.5	54
40	Generating symmetry-adapted bases for non-Abelian point groups to be used in vibronic coupling Hamiltonians. Chemical Physics, 2015, 460, 125-134.	1.9	9
41	Cu+NO scattering quantum dynamics. International Journal of Mass Spectrometry, 2014, 365-366, 121-127.	1.5	1
42	The time-resolved photoelectron spectrum of toluene using a perturbation theory approach. Journal of Chemical Physics, 2014, 141, 244115.	3.0	7
43	Optimal control by computer. Annual Reports on the Progress of Chemistry Section C, 2013, 109, 113.	4.4	14
44	Towards converging non-adiabatic direct dynamics calculations using frozen-width variational Gaussian product basis functions. Journal of Chemical Physics, 2012, 137, 22A548.	3.0	50
45	Dynamic stark control: model studies based on the photodissociation of IBr. Faraday Discussions, 2011, 153, 275.	3.2	34
46	Excitedâ€state dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 460-475.	14.6	64
47	A full-dimensional coupled-surface study of the photodissociation dynamics of ammonia using the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2011, 135, 044311.	3.0	26
48	Converged quantum dynamics with modified Shepard interpolation and Gaussian wave packets. Chemical Physics Letters, 2010, 489, 242-247.	2.6	38
49	Controlling the mechanism of fulvene S1/S0 decay: switching off the stepwise population transfer. Physical Chemistry Chemical Physics, 2010, 12, 15725.	2.8	50
50	A Straightforward Method of Analysis for Direct Quantum Dynamics: Application to the Photochemistry of a Model Cyanine^{â€}. Journal of Physical Chemistry A, 2010, 114, 8713-8729.	2.5	44
51	Exploring the sloped-to-peaked S2/S1 seam of intersection of thymine with electronic structure and direct quantum dynamics calculations. Physical Chemistry Chemical Physics, 2010, 12, 4949.	2.8	83
52	Guiding the time-evolution of a molecule: optical control by computer. Physical Chemistry Chemical Physics, 2010, 12, 15570.	2.8	21
53	The molecular dissociation of formaldehyde at medium photoexcitation energies: A quantum chemistry and direct quantum dynamics study. Journal of Chemical Physics, 2009, 131, 144301.	3.0	41
54	A model Hamiltonian to simulate the complex photochemistry of benzene II. Journal of Chemical Physics, 2009, 131, 064303.	3.0	34

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55	Controlling S₁/S₀ Decay and the Balance between Photochemistry and Photostability in Benzene: A Direct Quantum Dynamics Study. Journal of Physical Chemistry A, 2008, 112, 13017-13027.	2.5	60
56	Automatic generation of active coordinates for quantum dynamics calculations: Application to the dynamics of benzene photochemistry. Journal of Chemical Physics, 2008, 128, 124307.	3.0	39
57	Direct quantum dynamics using variational multi-configuration Gaussian wavepackets. Chemical Physics Letters, 2006, 432, 604-609.	2.6	52
58	Wavepacket dynamics study of Cr(CO)5 after formation by photodissociation: relaxation through an (Eâ€‰âŠ•â€‰A)â€‰âŠ—â€‰e Jahnâ€“Teller conical intersection. Molecular Physics, 2006, 104, 1095-1105.	1.7	52
59	Conical intersections: A perspective on the computation of spectroscopic Jahnâ€“Teller parameters and the degenerate â€˜intersection spaceâ€™. Physical Chemistry Chemical Physics, 2005, 7, 2100.	2.8	67
60	Allene and pentatetraene cations as models for intramolecular charge transfer: Vibronic coupling Hamiltonian and conical intersections. Journal of Chemical Physics, 2005, 122, 144320.	3.0	22
61	Ultrafast Photoinitiated Long-Range Electron Transfer in Cyclophane-Bridged Zincporphyrinâ€'Quinone Complexes via Conical Intersections. Journal of Physical Chemistry B, 2004, 108, 19049-19055.	2.6	24
62	BEYOND BORN-OPPENHEIMER: Molecular Dynamics Through a Conical Intersection. Annual Review of Physical Chemistry, 2004, 55, 127-158.	10.8	694
63	Quantum molecular dynamics: propagating wavepackets and density operators using the multiconfiguration time-dependent Hartree method. Theoretical Chemistry Accounts, 2003, 109, 251-267.	1.4	500
64	Full quantum mechanical molecular dynamics using Gaussian wavepackets. Chemical Physics Letters, 2003, 368, 502-508.	2.6	170
65	Multiconfigurational system-bath dynamics using Gaussian wave packets: Energy relaxation and decoherence induced by a finite-dimensional bath. Journal of Chemical Physics, 2003, 119, 5364-5378.	3.0	126
66	Nonadiabatic Dynamics:Â A Comparison of Surface Hopping Direct Dynamics with Quantum Wavepacket Calculations. Journal of Physical Chemistry A, 2003, 107, 621-631.	2.5	76
67	Direct Dynamics with Quantum Nuclei. , 0, , 111-129.		1
68	Shared Memory Parallelization of the Multiconfiguration Time-Dependent Hartree Method. , 0, , 149-160.		0
69	Analysis of the Propagated Wavepacket. , 0, , 41-55.		0
70	The Road to MCTDH. , 0, , 9-15.		1
71	Multidimensional Non-Adiabatic Dynamics. , 0, , 209-230.		0
72	Iterative Diagonalization of Operators. , 0, , 69-71.		0

#	Article	IF	Citations
73	How electronic superpositions drive nuclear motion following the creation of a localized hole in the glycine radical cation. Journal of Chemical Physics, 0, , .	3.0	3