Irene Burghardt

List of Publications by Year
in descending order

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113	5,038	109321	95266
papers	citations	35 h-index	68 g-index

116	116	116	3911
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ultrafast and efficient energy transfer in a one- and two-photon sensitized rhodamine-BODIPY dyad: a perspective for broadly absorbing photocages. Physical Chemistry Chemical Physics, 2022, 24, 1795-1802.	2.8	4
2	Dynamical approximations for composite quantum systems: assessment of error estimates for a separable ansatz. Journal of Physics A: Mathematical and Theoretical, 2022, 55, 224010.	2.1	2
3	Modelling ultrafast dynamics at a conical intersection with regularized diabatic states: An approach based on multiplicative neural networks. Chemical Physics, 2022, 560, 111542.	1.9	1
4	Quantum Dynamics with Electronic Friction. Physical Review Letters, 2022, 128, .	7.8	7
5	Quantum theory of electronic friction. Physical Review A, 2022, 105, .	2.5	4
6	Electronâ€“Hole Separation in Perylene Diimide Based Self-Assembled Nanostructures: Microelectrostatics Analysis and Kinetic Monte Carlo Simulations. Journal of Physical Chemistry C, 2022, 126, 9762-9776.	3.1	3
7	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
8	Quantum Dynamics of Exciton Transport and Dissociation in Multichromophoric Systems. Annual Review of Physical Chemistry, 2021, 72, 591-616.	10.8	31
9	Separation of scales: dynamical approximations for composite quantum systems*. Journal of Physics A: Mathematical and Theoretical, 2021, 54, 414002.	2.1	3
10	Excitons: Energetics and spatiotemporal dynamics. Journal of Chemical Physics, 2021, 155, 200401.	3.0	3
11	Quantum Dynamics of Electronâ€“Hole Separation in Stacked Perylene Diimide-Based Self-Assembled Nanostructures. Journal of Physical Chemistry C, 2021, 125, 25030-25043.	3.1	6
12	First-Principles Quantum and Quantum-Classical Simulations of Exciton Diffusion in Semiconducting Polymer Chains at Finite Temperature. Journal of Chemical Theory and Computation, 2020, 16, 5441-5455.	5.3	13
13	First-principles description of intra-chain exciton migration in an oligo(para-phenylene) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T 204119.	3.0	8
14	First-principles description of intra-chain exciton migration in an oligo(para-phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 Chemical Physics, 2020, 152, 204120.	3.0	21
15	Local-in-Time Error in Variational Quantum Dynamics. Physical Review Letters, 2020, 124, 150601.	7.8	19
16	Photochemical mechanism of DEACM uncaging: a combined time-resolved spectroscopic and computational study. Physical Chemistry Chemical Physics, 2020, 22, 13418-13430.	2.8	13
17	Quantum dynamical simulations of intra-chain exciton diffusion in an oligo (para-phenylene) Tj ETQq1 1 0.784314 rgBT /Overlo	3.0	19
18	Infrared pre-excitation grants isotopomer-specific photochemistry. EPJ Web of Conferences, 2019, 205, 03001.	0.3	0

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19	Vibronic coupling models for donor-acceptor aggregates using an effective-mode scheme: Application to mixed Frenkel and charge-transfer excitons in oligothiophene aggregates. Journal of Chemical Physics, 2019, 150, 244114.	3.0	26
20	Two-layer Gaussian-based MCTDH study of the S1 â†•S0 vibronic absorption spectrum of formaldehyde using multiplicative neural network potentials. Journal of Chemical Physics, 2019, 151, 064121.	3.0	10
21	Open system dynamics using Gaussian-based multiconfigurational time-dependent Hartree wavefunctions: Application to environment-modulated tunneling. Journal of Chemical Physics, 2019, 150, 224106.	3.0	8
22	Coherent Charge Transfer Exciton Formation in Regioregular P3HT: A Quantum Dynamical Study. Journal of Physical Chemistry Letters, 2019, 10, 3326-3332.	4.6	35
23	Quantum dynamics and spectroscopy of dihalogens in solid matrices. I. Efficient simulation of the photodynamics of the embedded I2Kr18 cluster using the G-MCTDH method. Journal of Chemical Physics, 2019, 150, 064111.	3.0	11
24	Quantum dynamics and spectroscopy of dihalogens in solid matrices. II. Theoretical aspects and G-MCTDH simulations of time-resolved coherent Raman spectra of SchrÃ¶dinger cat states of the embedded I2Kr18 cluster. Journal of Chemical Physics, 2019, 150, 064112.	3.0	10
25	Complex Formation of the Tetracyclineâ€Binding Aptamer Investigated by Specific Crossâ€Relaxation under DNP. Angewandte Chemie - International Edition, 2019, 58, 4863-4868.	13.8	27
26	First-principles quantum simulations of exciton diffusion on a minimal oligothiophene chain at finite temperature. Faraday Discussions, 2019, 221, 406-427.	3.2	26
27	Time-resolved spectra of I₂ in a krypton crystal by G-MCTDH simulations: nonadiabatic dynamics, dissipation and environment driven decoherence. Faraday Discussions, 2019, 221, 30-58.	3.2	8
28	Emerging opportunities and future directions: general discussion. Faraday Discussions, 2019, 221, 564-581.	3.2	5
29	Spectroscopic signatures of quantum effects: general discussion. Faraday Discussions, 2019, 221, 322-349.	3.2	2
30	Zero-point energy and tunnelling: general discussion. Faraday Discussions, 2019, 221, 478-500.	3.2	4
31	Quantum coherence in complex environments: general discussion. Faraday Discussions, 2019, 221, 168-201.	3.2	5
32	Creation and Detection of Molecular SchrÃ¶dinger Cat States: Iodine in Cryogenic Krypton Observed via Four-Wave-Mixing Optics. Springer Proceedings in Physics, 2019, , 91-112.	0.2	0
33	Sensitized Two-Photon Activation of Coumarin Photocages. Journal of Physical Chemistry Letters, 2018, 9, 1448-1453.	4.6	21
34	Ultrafast photochemistry of free-base porphyrin: a theoretical investigation of B â†' Q internal conversion mediated by dark states. Physical Chemistry Chemical Physics, 2018, 20, 12483-12492.	2.8	14
35	Impact of charge-transfer excitons in regioregular polythiophene on the charge separation at polythiophene-fullerene heterojunctions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 014003.	1.5	27
36	Azobenzene as a photoregulator covalently attached to RNA: a quantum mechanics/molecular mechanics-surface hopping dynamics study. Chemical Science, 2018, 9, 4671-4681.	7.4	20

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37	Quantum dynamical studies of ultrafast charge separation in nanostructured organic polymer materials: Effects of vibronic interactions and molecular packing. International Journal of Quantum Chemistry, 2018, 118, e25502.	2.0	30
38	Controlling Photochemistry via Isotopomers and IR Pre-excitation. Journal of the American Chemical Society, 2018, 140, 926-931.	13.7	11
39	Gaussian-based multiconfiguration time-dependent Hartree: A two-layer approach. III. Application to nonadiabatic dynamics in a charge transfer complex. Journal of Chemical Physics, 2018, 149, 174102.	3.0	14
40	Ultrafast carbon monoxide photolysis and heme spin-crossover in myoglobin via nonadiabatic quantum dynamics. Nature Communications, 2018, 9, 4502.	12.8	48
41	Gaussian-based multiconfiguration time-dependent Hartree: A two-layer approach. II. Application to vibrational energy transport in a molecular chain. Journal of Chemical Physics, 2018, 149, 174101.	3.0	12
42	Multi-configurational Ehrenfest simulations of ultrafast nonadiabatic dynamics in a charge-transfer complex. Journal of Chemical Physics, 2018, 149, 244107.	3.0	17
43	Tangent space formulation of the Multi-Configuration Time-Dependent Hartree equations of motion: The projectorâ€“splitting algorithm revisited. Chemical Physics, 2018, 515, 252-261.	1.9	13
44	Conformational Dynamics Guides Coherent Exciton Migration in Conjugated Polymer Materials: First-Principles Quantum Dynamical Study. Physical Review Letters, 2018, 120, 227401.	7.8	40
45	The symmetrical quasi-classical approach to electronically nonadiabatic dynamics applied to ultrafast exciton migration processes in semiconducting polymers. Journal of Chemical Physics, 2018, 149, 044101.	3.0	31
46	Computation of the S₁ â†•S₀ Vibronic Absorption Spectrum of Formaldehyde by Variational Gaussian Wavepacket and Semiclassical IVR Methods. Journal of Chemical Theory and Computation, 2018, 14, 5310-5323.	5.3	28
47	A New Photocage Derived from Fluorene. Chemistry - A European Journal, 2018, 24, 13026-13035.	3.3	12
48	Implementation of a novel projector-splitting integrator for the multi-configurational time-dependent Hartree approach. Journal of Chemical Physics, 2017, 146, 174107.	3.0	29
49	Ultrafast exciton migration in an HJ-aggregate: Potential surfaces and quantum dynamics. Chemical Physics, 2017, 482, 16-26.	1.9	13
50	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. Journal of Chemical Physics, 2017, 147, 164116.	3.0	29
51	Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates. , 2017, , 407-436.		1
52	Controlling charge separation and recombination by chemical design in donorâ€“acceptor dyads. Physical Chemistry Chemical Physics, 2016, 18, 18536-18548.	2.8	16
53	Solvent Polarity Tunes the Barrier Height for Twisted Intramolecular Charge Transfer in N-Pyrrolobenzonitrile (PBN). Journal of Physical Chemistry A, 2016, 120, 14-27.	2.5	15
54	Molecular Packing Determines Charge Separation in a Liquid Crystalline Bisthiopheneâ€“Perylene Diimide Donorâ€“Acceptor Material. Journal of Physical Chemistry Letters, 2016, 7, 1327-1334.	4.6	28

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55	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>Stacking. Physical Review Letters, 2015, 115, 107401.	7.8	137
56	Vibrational coherence transfer in an electronically decoupled molecular dyad. Scientific Reports, 2015, 5, 9368.	3.3	14
57	Quantum dynamics of hydrogen atoms on graphene. II. Sticking. Journal of Chemical Physics, 2015, 143, 124704.	3.0	18
58	Quantum dynamics of hydrogen atoms on graphene. I. System-bath modeling. Journal of Chemical Physics, 2015, 143, 124703.	3.0	18
59	Ultrafast Spectroscopy of Hydroxyâ€Substituted Azobenzenes in Water. Chemistry - A European Journal, 2015, 21, 15720-15731.	3.3	17
60	Complex quantum systems. Annalen Der Physik, 2015, 527, A93-A94.	2.4	1
61	Reversible Photoswitching of RNA Hybridization at Room Temperature with an Azobenzene Câ€Nucleoside. Chemistry - A European Journal, 2015, 21, 2845-2854.	3.3	59
62	In Search of an Efficient Photoswitch for Functional RNA: Design Principles from a Microscopic Analysis of Azobenzene-linker-RNA Dynamics with Different Linkers. Journal of Physical Chemistry B, 2015, 119, 11275-11286.	2.6	17
63	Ultrafast coherent oscillations reveal a reactive mode in the ring-opening reaction of fulgides. Physical Chemistry Chemical Physics, 2015, 17, 14045-14053.	2.8	36
64	Concurrent Effects of Delocalization and Internal Conversion Tune Charge Separation at Regioregular Polythiopheneâ€“Fullerene Heterojunctions. Journal of Physical Chemistry Letters, 2015, 6, 1702-1708.	4.6	72
65	Vibrational relaxation and decoherence in structured environments: a numerical investigation. Annalen Der Physik, 2015, 527, 556-569.	2.4	10
66	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. Journal of Chemical Physics, 2015, 142, 184104.	3.0	40
67	Direct observation of ultrafast collective motions in CO myoglobin upon ligand dissociation. Science, 2015, 350, 445-450.	12.6	344
68	Quantum dynamics simulations using Gaussian wavepackets: the vMCG method. International Reviews in Physical Chemistry, 2015, 34, 269-308.	2.3	243
69	An analytic mapping of oligomer potential energy surfaces to an effective Frenkel model. Journal of Chemical Physics, 2014, 141, 014101.	3.0	21
70	Quantum dynamics of ultrafast exciton relaxation on a minimal lattice. Computational and Theoretical Chemistry, 2014, 1040-1041, 167-176.	2.5	16
71	Molecular Dynamics Study of the Controlled Destabilization of an RNA Hairpin Structure by a Covalently Attached Azobenzene Switch. Journal of Physical Chemistry B, 2014, 118, 8478-8488.	2.6	21
72	Azobenzene Photoisomerization-Induced Destabilization of B-DNA. Biophysical Journal, 2014, 107, 932-940.	0.5	30

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73	Coherent exciton transport driven by torsional dynamics: a quantum dynamical study of phenylene-vinylene type conjugated systems. Faraday Discussions, 2013, 163, 205.	3.2	30
74	Potential Barrier and Excess Energy for Electronâ€“Hole Separation from the Charge-Transfer Exciton at Donorâ€“Acceptor Heterojunctions of Organic Solar Cells. Journal of Physical Chemistry C, 2013, 117, 15020-15025.	3.1	51
75	Ultrafast Charge Separation in Organic Photovoltaics Enhanced by Charge Delocalization and Vibronically Hot Exciton Dissociation. Journal of the American Chemical Society, 2013, 135, 16364-16367.	13.7	292
76	Gaussian-based multiconfiguration time-dependent Hartree: A two-layer approach. I. Theory. Journal of Chemical Physics, 2013, 138, 064106.	3.0	43
77	Electronically Excited States in Poly(p-phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level Ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 2181-2189.	2.5	65
78	Charge and energy transfer in a bithiophene perylenediimide based donorâ€“acceptorâ€“donor system for use in organic photovoltaics. Physical Chemistry Chemical Physics, 2013, 15, 11704.	2.8	20
79	Towards a variational formulation of mixed quantum-classical molecular dynamics. Molecular Physics, 2013, 111, 3618-3624.	1.7	25
80	Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. Journal of Chemical Physics, 2012, 137, 22A540.	3.0	85
81	Non-Markovian reduced dynamics based upon a hierarchical effective-mode representation. Journal of Chemical Physics, 2012, 137, 144107.	3.0	22
82	Hierarchical Effective-Mode Approach for Extended Molecular Systems. Progress in Theoretical Chemistry and Physics, 2012, , 269-283.	0.2	3
83	Conical Intersections Coupled to an Environment. Advanced Series in Physical Chemistry, 2011, , 301-346.	1.5	6
84	Coherent Excitation Transfer Driven by Torsional Dynamics: a Model Hamiltonian for PPV Type Systems. Zeitschrift Fur Physikalische Chemie, 2011, 225, 541-551.	2.8	22
85	Exciton Dissociation at Thiophene/Fullerene Interfaces: The Electronic Structures and Quantum Dynamics. Journal of Physical Chemistry C, 2011, 115, 10205-10210.	3.1	102
86	Communication: Universal Markovian reduction of Brownian particle dynamics. Journal of Chemical Physics, 2011, 134, 011101.	3.0	97
87	Unraveling a Brownian particleâ€™s memory with effective mode chains. Physical Review E, 2011, 84, 030102.	2.1	27
88	Effective spectral densities for system-environment dynamics at conical intersections: S2â€“S1 conical intersection in pyrazine. Chemical Physics, 2010, 377, 21-29.	1.9	33
89	Effective-mode representation of non-Markovian dynamics: A hierarchical approximation of the spectral density. I. Application to single surface dynamics. Journal of Chemical Physics, 2009, 131, 024109.	3.0	102
90	Effective-mode representation of non-Markovian dynamics: A hierarchical approximation of the spectral density. II. Application to environment-induced nonadiabatic dynamics. Journal of Chemical Physics, 2009, 131, 124108.	3.0	87

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91	Ab Initio Study of Excitation Energy Transfer between Quantum Dots and Dye Molecules. Journal of Physical Chemistry C, 2009, 113, 7548-7552.	3.1	28
92	Using the MCTDH wavepacket propagation method to describe multimode non-adiabatic dynamics. International Reviews in Physical Chemistry, 2008, 27, 569-606.	2.3	237
93	Multimode quantum dynamics using Gaussian wavepackets: The Gaussian-based multiconfiguration time-dependent Hartree (G-MCTDH) method applied to the absorption spectrum of pyrazine. Journal of Chemical Physics, 2008, 129, 174104.	3.0	159
94	Phonon-Driven Exciton Dissociation at Donorâ^'Acceptor Polymer Heterojunctions:â€‰ Direct versus Bridge-Mediated Vibronic Coupling Pathways. Journal of Physical Chemistry B, 2008, 112, 495-506.	2.6	39
95	Phonon-Driven Ultrafast Exciton Dissociation at Donor-Acceptor Polymer Heterojunctions. Physical Review Letters, 2008, 100, 107402.	7.8	89
96	Gaussian-based techniques for quantum propagation from the time-dependent variational principle: Formulation in terms of trajectories of coupled classical and quantum variables. Journal of Chemical Physics, 2008, 129, 084104.	3.0	67
97	Exciton dissociation at donor-acceptor polymer heterojunctions: Quantum nonadiabatic dynamics and effective-mode analysis. Journal of Chemical Physics, 2007, 126, 021103.	3.0	63
98	A Hybrid Hydrodynamicâ^'Liouvillian Approach to Mixed Quantumâ^'Classical Dynamics:Â Application to Tunneling in a Double Wellâ€. Journal of Physical Chemistry A, 2007, 111, 10269-10283.	2.5	15
99	Nonadiabatic quantum dynamics based on a hierarchical electron-phonon model: Exciton dissociation in semiconducting polymers. Journal of Chemical Physics, 2007, 127, 034706.	3.0	52
100	Time-Frequency and Coordinate-Momentum Wigner Wavepackets in Nonlinear Spectroscopy. Advances in Chemical Physics, 2007, , 345-372.	0.3	15
101	An effective Hamiltonian for the short-time dynamics at a conical intersection. Molecular Physics, 2006, 104, 1081-1093.	1.7	29
102	Short-time dynamics through conical intersections in macrosystems. II. Applications. Journal of Chemical Physics, 2006, 124, 144104.	3.0	40
103	Short-time dynamics through conical intersections in macrosystems. I. Theory: Effective-mode formulation. Journal of Chemical Physics, 2006, 124, 144103.	3.0	79
104	Short-Time Dynamics Through Conical Intersections in Macrosystems. Physical Review Letters, 2005, 94, 113003.	7.8	140
105	On the dynamics of coupled Bohmian and phase-space variables: A new hybrid quantum-classical approach. Journal of Chemical Physics, 2004, 120, 3055-3058.	3.0	45
106	A novel algorithm for non-adiabatic direct dynamics using variational Gaussian wavepackets. Faraday Discussions, 2004, 127, 307.	3.2	210
107	Full quantum mechanical molecular dynamics using Gaussian wavepackets. Chemical Physics Letters, 2003, 368, 502-508.	2.6	170
108	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

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109	Quantum dynamics for dissipative systems: A hydrodynamic perspective. Journal of Chemical Physics, 2002, 117, 7409-7425.	3.0	50
110	Hydrodynamic equations for mixed quantum states. II. Coupled electronic states. Journal of Chemical Physics, 2001, 115, 10312.	3.0	55
111	The multiconfiguration time-dependent Hartree method generalized to the propagation of density operators. Journal of Chemical Physics, 1999, 111, 8759-8772.	3.0	39
112	Approaches to the approximate treatment of complex molecular systems by the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 1999, 111, 2927-2939.	3.0	243
113	Signatures of coherent vibronic exciton dynamics and conformational control in the two-dimensional electronic spectroscopy of conjugated polymers. Faraday Discussions, 0, 237, 148-167.	3.2	3