Irene Burghardt

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7050375/publications.pdf

Version: 2024-02-01

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	Direct observation of ultrafast collective motions in CO myoglobin upon ligand dissociation. Science, 2015, 350, 445-450.	12.6	344
2	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
3	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
4	Quantum dynamics simulations using Gaussian wavepackets: the vMCG method. International Reviews in Physical Chemistry, 2015, 34, 269-308.	2.3	243
5	Using the MCTDH wavepacket propagation method to describe multimode non-adiabatic dynamics. International Reviews in Physical Chemistry, 2008, 27, 569-606.	2.3	237
6	A novel algorithm for non-adiabatic direct dynamics using variational Gaussian wavepackets. Faraday Discussions, 2004, 127, 307.	3.2	210
7	Full quantum mechanical molecular dynamics using Gaussian wavepackets. Chemical Physics Letters, 2003, 368, 502-508.	2.6	170
8	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
9	Short-Time Dynamics Through Conical Intersections in Macrosystems. Physical Review Letters, 2005, 94, 113003.	7.8	140
10	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
11	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
12	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
13	Exciton Dissociation at Thiophene/Fullerene Interfaces: The Electronic Structures and Quantum Dynamics. Journal of Physical Chemistry C, 2011, 115, 10205-10210.	3.1	102
14	Communication: Universal Markovian reduction of Brownian particle dynamics. Journal of Chemical Physics, 2011, 134, 011101.	3.0	97
15	Phonon-Driven Ultrafast Exciton Dissociation at Donor-Acceptor Polymer Heterojunctions. Physical Review Letters, 2008, 100, 107402.	7.8	89
16	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
17	Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. Journal of Chemical Physics, 2012, 137, 22A540.	3.0	85
18	Short-time dynamics through conical intersections in macrosystems. I. Theory: Effective-mode formulation. Journal of Chemical Physics, 2006, 124, 144103.	3.0	79

#	Article	IF	Citations
19	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
20	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
21	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
22	Exciton dissociation at donor-acceptor polymer heterojunctions: Quantum nonadiabatic dynamics and effective-mode analysis. Journal of Chemical Physics, 2007, 126, 021103.	3.0	63
23	Reversible Photoswitching of RNA Hybridization at Room Temperature with an Azobenzene Câ€Nucleoside. Chemistry - A European Journal, 2015, 21, 2845-2854.	3.3	59
24	Hydrodynamic equations for mixed quantum states. II. Coupled electronic states. Journal of Chemical Physics, 2001, 115, 10312.	3.0	55
25	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
26	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
27	Quantum dynamics for dissipative systems: A hydrodynamic perspective. Journal of Chemical Physics, 2002, 117, 7409-7425.	3.0	50
28	Ultrafast carbon monoxide photolysis and heme spin-crossover in myoglobin via nonadiabatic quantum dynamics. Nature Communications, 2018, 9, 4502.	12.8	48
29	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
30	Gaussian-based multiconfiguration time-dependent Hartree: A two-layer approach. I. Theory. Journal of Chemical Physics, 2013, 138, 064106.	3.0	43
31	Short-time dynamics through conical intersections in macrosystems. II. Applications. Journal of Chemical Physics, 2006, 124, 144104.	3.0	40
32	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
33	Conformational Dynamics Guides Coherent Exciton Migration in Conjugated Polymer Materials: First-Principles Quantum Dynamical Study. Physical Review Letters, 2018, 120, 227401.	7.8	40
34	The multiconfiguration time-dependent Hartree method generalized to the propagation of density operators. Journal of Chemical Physics, 1999, 111, 8759-8772.	3.0	39
35	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
36	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

#	Article	IF	Citations
37	Coherent Charge Transfer Exciton Formation in Regioregular P3HT: A Quantum Dynamical Study. Journal of Physical Chemistry Letters, 2019, 10, 3326-3332.	4.6	35
38	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
39	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
40	Quantum Dynamics of Exciton Transport and Dissociation in Multichromophoric Systems. Annual Review of Physical Chemistry, 2021, 72, 591-616.	10.8	31
41	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
42	Azobenzene Photoisomerization-Induced Destabilization of B-DNA. Biophysical Journal, 2014, 107, 932-940.	0.5	30
43	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
44	An effective Hamiltonian for the short-time dynamics at a conical intersection. Molecular Physics, 2006, 104, 1081-1093.	1.7	29
45	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
46	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. Journal of Chemical Physics, 2017, 147, 164116.	3.0	29
47	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
48	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
49	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
50	Unraveling a Brownian particleâ€™s memory with effective mode chains. Physical Review E, 2011, 84, 030102.	2.1	27
51	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
52	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
53	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
54	First-principles quantum simulations of exciton diffusion on a minimal oligothiophene chain at finite temperature. Faraday Discussions, 2019, 221, 406-427.	3.2	26

#	Article	IF	Citations
55	Towards a variational formulation of mixed quantum-classical molecular dynamics. Molecular Physics, 2013, 111, 3618-3624.	1.7	25
56	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
57	Non-Markovian reduced dynamics based upon a hierarchical effective-mode representation. Journal of Chemical Physics, 2012, 137, 144107.	3.0	22
58	An analytic mapping of oligomer potential energy surfaces to an effective Frenkel model. Journal of Chemical Physics, 2014, 141, 014101.	3.0	21
59	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
60	Sensitized Two-Photon Activation of Coumarin Photocages. Journal of Physical Chemistry Letters, 2018, 9, 1448-1453.	4.6	21
61	First-principles description of intra-chain exciton migration in an oligo(para-phenylene) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf Chemical Physics, 2020, 152, 204120.	3.0	21
62	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
63	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
64	Local-in-Time Error in Variational Quantum Dynamics. Physical Review Letters, 2020, 124, 150601.	7.8	19
65	Quantum dynamical simulations of intra-chain exciton diffusion in an oligo (para-phenylene) Tj ETQq1 1 0.784314 rgBT /Overlock	3.0	19
66	Quantum dynamics of hydrogen atoms on graphene. II. Sticking. Journal of Chemical Physics, 2015, 143, 124704.	3.0	18
67	Quantum dynamics of hydrogen atoms on graphene. I. System-bath modeling. Journal of Chemical Physics, 2015, 143, 124703.	3.0	18
68	Ultrafast Spectroscopy of Hydroxyâ€Substituted Azobenzenes in Water. Chemistry - A European Journal, 2015, 21, 15720-15731.	3.3	17
69	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
70	Multi-configurational Ehrenfest simulations of ultrafast nonadiabatic dynamics in a charge-transfer complex. Journal of Chemical Physics, 2018, 149, 244107.	3.0	17
71	Quantum dynamics of ultrafast exciton relaxation on a minimal lattice. Computational and Theoretical Chemistry, 2014, 1040-1041, 167-176.	2.5	16
72	Controlling charge separation and recombination by chemical design in donorâ€“acceptor dyads. Physical Chemistry Chemical Physics, 2016, 18, 18536-18548.	2.8	16

#	Article	IF	Citations
73	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
74	Time-Frequency and Coordinate-Momentum Wigner Wavepackets in Nonlinear Spectroscopy. Advances in Chemical Physics, 2007, , 345-372.	0.3	15
75	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
76	Vibrational coherence transfer in an electronically decoupled molecular dyad. Scientific Reports, 2015, 5, 9368.	3.3	14
77	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
78	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
79	Ultrafast exciton migration in an HJ-aggregate: Potential surfaces and quantum dynamics. Chemical Physics, 2017, 482, 16-26.	1.9	13
80	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
81	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
82	Photochemical mechanism of DEACM uncaging: a combined time-resolved spectroscopic and computational study. Physical Chemistry Chemical Physics, 2020, 22, 13418-13430.	2.8	13
83	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
84	A New Photocage Derived from Fluorene. Chemistry - A European Journal, 2018, 24, 13026-13035.	3.3	12
85	Controlling Photochemistry via Isotopomers and IR Pre-excitation. Journal of the American Chemical Society, 2018, 140, 926-931.	13.7	11
86	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
87	Vibrational relaxation and decoherence in structured environments: a numerical investigation. Annalen Der Physik, 2015, 527, 556-569.	2.4	10
88	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
89	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
90	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

#	Article	IF	Citations
91	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
92	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
93	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
94	Quantum Dynamics with Electronic Friction. Physical Review Letters, 2022, 128, .	7.8	7
95	Conical Intersections Coupled to an Environment. Advanced Series in Physical Chemistry, 2011, , 301-346.	1.5	6
96	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
97	Emerging opportunities and future directions: general discussion. Faraday Discussions, 2019, 221, 564-581.	3.2	5
98	Quantum coherence in complex environments: general discussion. Faraday Discussions, 2019, 221, 168-201.	3.2	5
99	Zero-point energy and tunnelling: general discussion. Faraday Discussions, 2019, 221, 478-500.	3.2	4
100	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
101	Quantum theory of electronic friction. Physical Review A, 2022, 105, .	2.5	4
102	Separation of scales: dynamical approximations for composite quantum systems*. Journal of Physics A: Mathematical and Theoretical, 2021, 54, 414002.	2.1	3
103	Hierarchical Effective-Mode Approach for Extended Molecular Systems. Progress in Theoretical Chemistry and Physics, 2012, , 269-283.	0.2	3
104	Excitons: Energetics and spatiotemporal dynamics. Journal of Chemical Physics, 2021, 155, 200401.	3.0	3
105	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
106	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
107	Spectroscopic signatures of quantum effects: general discussion. Faraday Discussions, 2019, 221, 322-349.	3.2	2
108	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

#	Article	IF	Citations
109	Complex quantum systems. Annalen Der Physik, 2015, 527, A93-A94.	2.4	1
110	Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates. , 2017, , 407-436.		1
111	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
112	Infrared pre-excitation grants isotopomer-specific photochemistry. EPJ Web of Conferences, 2019, 205, 03001.	0.3	0
113	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