Maxim F Gelin

List of Publications by Year in Descending Order

87 papers	1,291 citations	20 h-index	31 g-index
91 ext. papers	1,558 ext. citations	4.2 avg, IF	5.26 L-index

#	Paper	IF	Citations
87	Ultrafast Internal Conversion Dynamics through the on-the-Fly Simulation of Transient Absorption Pump-Probe Spectra with Different Electronic Structure Methods.. *Journal of Physical Chemistry Letters*, **2022**, 13, 661-668	6.4	1
86	Dynamics of disordered Tavis-Cummings and Holstein-Tavis-Cummings models.. *Journal of Chemical Physics*, **2022**, 156, 024102	3.9	2
85	Ultrafast carrier dynamics at organic donor–acceptor interfaces: quantum-based assessment of the hopping model. *JPhys Materials*, **2022**, 5, 024001	4.2	1
84	Accurate Simulation of Spectroscopic Signatures of Cavity-Assisted, Conical-Intersection-Controlled Singlet Fission Processes.. *Journal of Physical Chemistry Letters*, **2022**, 4280-4288	6.4	1
83	Engineering Cavity Singlet Fission in Rubrene.. *Journal of Physical Chemistry Letters*, **2022**, 4090-4097	6.4	1
82	Ab Initio Quasiclassical Simulation of Femtosecond Time-Resolved Two-Dimensional Electronic Spectra of Pyrazine. *Journal of Physical Chemistry Letters*, **2021**, 12, 11736-11744	6.4	2
81	Toward efficient photochemistry from upper excited electronic states: Detection of long S lifetime of perylene. *Journal of Chemical Physics*, **2021**, 155, 191102	3.9	1
80	Ab Initio Surface-Hopping Simulation of Femtosecond Transient-Absorption Pump-Probe Signals of Nonadiabatic Excited-State Dynamics Using the Doorway-Window Representation. *Journal of Chemical Theory and Computation*, **2021**, 17, 2394-2408	6.4	7
79	Hierarchical Equations-of-Motion Method for Momentum System-Bath Coupling. *Journal of Physical Chemistry B*, **2021**, 125, 4863-4873	3.4	0
78	Finite temperature quantum dynamics of complex systems: Integrating thermo-field theories and tensor-train methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1539	7.9	13
77	Simulation of Time- and Frequency-Resolved Four-Wave-Mixing Signals at Finite Temperatures: A Thermo-Field Dynamics Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 4359-4373	6.4	7
76	Simulation of Nonlinear Femtosecond Signals at Finite Temperature via a Thermo Field Dynamics-Tensor Train Method: General Theory and Application to Time- and Frequency-Resolved Fluorescence of the Fenna-Matthews-Olson Complex. *Journal of Chemical Theory and Computation*, **2021**, 17, 4316-4331	6.4	11
75	A model for dynamical solvent control of molecular junction electronic properties. *Journal of Chemical Physics*, **2021**, 154, 044107	3.9	0
74	Efficient simulation of time- and frequency-resolved four-wave-mixing signals with a multiconfigurational Ehrenfest approach. *Journal of Chemical Physics*, **2021**, 154, 054105	3.9	7
73	First-passage time theory of activated rate chemical processes in electronic molecular junctions. *Journal of Chemical Physics*, **2021**, 154, 114108	3.9	1
72	Combined Surface-Hopping, Dyson Orbital, and B-Spline Approach for the Computation of Time-Resolved Photoelectron Spectroscopy Signals: The Internal Conversion in Pyrazine. *Journal of Chemical Theory and Computation*, **2021**, 17, 5098-5109	6.4	4
71	Theory helps experiment to reveal VOCs in human breath. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 258, 119785	4.4	6

70	Spectral Fingerprint of Excited-State Energy Transfer in Dendrimers through Polarization-Sensitive Transient-Absorption Pump-Probe Signals: On-the-Fly Nonadiabatic Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2021**, 12, 9710-9719	6.4	2
69	Efficient quantum dynamics simulations of complex molecular systems: A unified treatment of dynamic and static disorder. *Journal of Chemical Physics*, **2021**, 155, 134102	3.9	3
68	Upper Excited State Photophysics of Malachite Green in Solution and Films. *Journal of Physical Chemistry B*, **2020**, 124, 4293-4302	3.4	4
67	Effects of high pulse intensity and chirp in two-dimensional electronic spectroscopy of an atomic vapor. *Optics Express*, **2020**, 28, 25806-25829	3.3	5
66	Quantum dynamics of vibrational energy flow in oscillator chains driven by anharmonic interactions. *New Journal of Physics*, **2020**, 22, 123002	2.9	5
65	Temperature effects on singlet fission dynamics mediated by a conical intersection. *Journal of Chemical Physics*, **2020**, 153, 194106	3.9	15
64	Multi-faceted spectroscopic mapping of ultrafast nonadiabatic dynamics near conical intersections: A computational study. *Journal of Chemical Physics*, **2020**, 153, 174111	3.9	18
63	Generalized Huang-Rhys factors for molecular aggregates. *Chemical Physics*, **2020**, 528, 110495	2.3	7
62	Mapping of Wave Packet Dynamics at Conical Intersections by Time- and Frequency-Resolved Fluorescence Spectroscopy: A Computational Study. *Journal of Physical Chemistry Letters*, **2019**, 10, 5873-5880	6.4	14
61	Monitoring of singlet fission via two-dimensional photon-echo and transient-absorption spectroscopy: Simulations by multiple Davydov trial states. *Journal of Chemical Physics*, **2019**, 151, 114102	3.9	12
60	Analysis of transient-absorption pump-probe signals of nonadiabatic dissipative systems: "Ideal" and "real" spectra. *Journal of Chemical Physics*, **2019**, 150, 204102	3.9	12
59	Origin of Unexpectedly Simple Oscillatory Responses in the Excited-State Dynamics of Disordered Molecular Aggregates. *Journal of Physical Chemistry Letters*, **2019**, 10, 2806-2810	6.4	15
58	Orientational relaxation of a quantum linear rotor in a dissipative environment: Simulations with the hierarchical equations-of-motion method. *Journal of Chemical Physics*, **2019**, 151, 034101	3.9	4
57	Dynamics of a one-dimensional Holstein polaron: The multiconfigurational Ehrenfest method. *Journal of Chemical Physics*, **2019**, 151, 244116	3.9	9
56	Multimode quantum dynamics with multiple Davydov D trial states: Application to a 24-dimensional conical intersection model. *Journal of Chemical Physics*, **2019**, 150, 024101	3.9	21
55	Simulation of Femtosecond Phase-Locked Double-Pump Signals of Individual Light-Harvesting Complexes LH2. *Journal of Physical Chemistry Letters*, **2018**, 9, 4488-4494	6.4	5
54	Pulse-shape effects in fifth-order multidimensional optical spectroscopy. *Chemical Physics*, **2018**, 515, 119-128	2.3	6
53	Dynamics of the spin-boson model: A comparison of the multiple Davydov D1,D1.5,D2 Ansätze. *Chemical Physics*, **2018**, 515, 108-118	2.3	11

52	Ultrafast Relaxation Dynamics in Zinc Tetraphenylporphyrin Surface-Mounted Metal Organic Framework. *Journal of Physical Chemistry C*, **2018**, 122, 50-61	3.8	38
51	Enhanced S2 Fluorescence from a Free-Base Tetraphenylporphyrin Surface-Mounted Metal Organic Framework. *Journal of Physical Chemistry C*, **2018**, 122, 23321-23328	3.8	7
50	Resonant femtosecond stimulated Raman spectroscopy with an intense actinic pump pulse: Application to conical intersections. *Journal of Chemical Physics*, **2017**, 146, 084105	3.9	5
49	Simplified expressions that incorporate finite pulse effects into coherent two-dimensional optical spectra. *Journal of Chemical Physics*, **2017**, 147, 144103	3.9	22
48	Thermal Schrödinger Equation: Efficient Tool for Simulation of Many-Body Quantum Dynamics at Finite Temperature. *Annalen Der Physik*, **2017**, 529, 1700200	2.6	13
47	Simulation of Quantum Dynamics of Excitonic Systems at Finite Temperature: an efficient method based on Thermo Field Dynamics. *Scientific Reports*, **2017**, 7, 9127	4.9	39
46	Efficient orientational averaging of nonlinear optical signals in multi-chromophore systems. *Journal of Chemical Physics*, **2017**, 147, 044114	3.9	9
45	Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. II. Strong-field regime. *Physical Chemistry Chemical Physics*, **2017**, 19, 32307-32319	3.6	9
44	Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. I. Weak-field regime. *Physical Chemistry Chemical Physics*, **2017**, 19, 32296-32306	3.6	9
43	Nonperturbative response functions: A tool for the interpretation of four-wave-mixing signals beyond third order. *Journal of Chemical Physics*, **2017**, 147, 234104	3.9	5
42	Interference of Interchromophoric Energy-Transfer Pathways in π-Conjugated Macrocycles. *Journal of Physical Chemistry Letters*, **2016**, 7, 4936-4944	6.4	26
41	Resonant Femtosecond Stimulated Raman Spectra: Theory and Simulations. *Journal of Physical Chemistry A*, **2016**, 120, 3286-95	2.8	12
40	Electronic and non-adiabatic dynamics: general discussion. *Faraday Discussions*, **2016**, 194, 209-257	3.6	3
39	Quantum electron-vibrational dynamics at finite temperature: Thermo field dynamics approach. *Journal of Chemical Physics*, **2016**, 145, 224101	3.9	46
38	Femtosecond stimulated Raman spectroscopy as a tool to detect molecular vibrations in ground and excited electronic states. *Journal of Chemical Physics*, **2016**, 144, 184307	3.9	3
37	Alternative view of two-dimensional spectroscopy. *Journal of Chemical Physics*, **2016**, 144, 194104	3.9	8
36	The Generalized Coherent State ansatz: Application to quantum electron-vibrational dynamics. *Chemical Physics*, **2016**, 481, 91-98	2.3	11
35	Dissipative dynamics at conical intersections: simulations with the hierarchy equations of motion method. *Faraday Discussions*, **2016**, 194, 61-80	3.6	31

34	Simulation of femtosecond two-dimensional electronic spectra of conical intersections. *Journal of Chemical Physics*, **2015**, 143, 074308	3.9	24
33	Davydov Ansatz as an efficient tool for the simulation of nonlinear optical response of molecular aggregates. *Journal of Chemical Physics*, **2015**, 142, 212448	3.9	31
32	Microscopic derivation of the Keilson-Storer master equation. *Chemical Physics*, **2015**, 462, 35-40	2.3	4
31	Theory of femtosecond coherent double-pump single-molecule spectroscopy: Application to light harvesting complexes. *Journal of Chemical Physics*, **2015**, 142, 164106	3.9	18
30	Markovian master equation for a classical particle coupled with arbitrary strength to a harmonic bath. *Journal of Chemical Physics*, **2014**, 141, 214109	3.9	3
29	Signatures of conical intersections in two-dimensional electronic spectra. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2014**, 47, 124019	1.3	26
28	Polaron dynamics in two-dimensional photon-echo spectroscopy of molecular rings. *Journal of Chemical Physics*, **2013**, 139, 104103	3.9	40
27	Strong-pump strong-probe spectroscopy: effects of higher excited electronic states. *Physical Chemistry Chemical Physics*, **2013**, 15, 8119-31	3.6	18
26	Calculation of third-order signals via driven Schrödinger equations: General results and application to electronic 2D photon echo spectroscopy. *Chemical Physics*, **2013**, 422, 53-62	2.3	21
25	Pump-probe spectroscopy with strong pulses as a tool to enhance weak electronic transitions. *Physical Review A*, **2013**, 87,	2.6	7
24	Simple recipes for separating excited-state absorption and cascading signals by polarization-sensitive measurements. *Journal of Physical Chemistry A*, **2013**, 117, 11509-13	2.8	7
23	Domain of validity of the perturbative approach to femtosecond optical spectroscopy. *Journal of Chemical Physics*, **2013**, 139, 224107	3.9	10
22	Bath-induced correlations and relaxation of vibronic dimers. *Journal of Chemical Physics*, **2012**, 136, 034507	3.9	22
21	Exact quantum master equation for a molecular aggregate coupled to a harmonic bath. *Physical Review E*, **2011**, 84, 041139	2.4	18
20	Efficient Methods for Computation of Ultrafast Time- and Frequency-Resolved Spectroscopic Signals **2011**, 445-473		1
19	Optical N-wave-mixing spectroscopy with strong and temporally well-separated pulses: the doorway-window representation. *Journal of Physical Chemistry B*, **2011**, 115, 5648-58	3.4	17
18	Strong and Long Makes Short: Strong-Pump Strong-Probe Spectroscopy. *Journal of Physical Chemistry Letters*, **2011**, 2, 114-9	6.4	18
17	Strong field effects in rotational femtosecond degenerate four-wave mixing. *Journal of Chemical Physics*, **2010**, 132, 134301	3.9	11

16	Ring-puckering motion in cyclopentene studied by time-resolved rotational coherence spectroscopy and ab initio calculations. *Physical Chemistry Chemical Physics*, **2010**, 12, 8190-200	3.6	3
15	Thermodynamics of a subensemble of a canonical ensemble. *Physical Review E*, **2009**, 79, 051121	2.4	45
14	Efficient calculation of the polarization induced by N coherent laser pulses. *Journal of Chemical Physics*, **2009**, 131, 194103	3.9	20
13	Manipulating electronic couplings and nonadiabatic nuclear dynamics with strong laser pulses. *Journal of Chemical Physics*, **2009**, 131, 124505	3.9	23
12	Calculation of semiclassical free energy differences along nonequilibrium classical trajectories. *Journal of Chemical Physics*, **2009**, 131, 164510	3.9	
11	Efficient calculation of time- and frequency-resolved four-wave-mixing signals. *Accounts of Chemical Research*, **2009**, 42, 1290-8	24.3	76
10	Effects of intense femtosecond pumping on ultrafast electronic-vibrational dynamics in molecular systems with relaxation. *Journal of Chemical Physics*, **2008**, 129, 214303	3.9	43
9	Analysis of vibrational coherences in homodyne and two-dimensional heterodyne photon-echo spectra of Nile Blue. *Chemical Physics*, **2007**, 341, 113-122	2.3	20
8	Analysis of cross peaks in two-dimensional electronic photon-echo spectroscopy for simple models with vibrations and dissipation. *Journal of Chemical Physics*, **2007**, 126, 074314	3.9	79
7	Transient phenomena in time- and frequency-gated spontaneous emission. *Journal of Physical Chemistry A*, **2005**, 109, 3587-97	2.8	3
6	Efficient method for the calculation of time- and frequency-resolved four-wave mixing signals and its application to photon-echo spectroscopy. *Journal of Chemical Physics*, **2005**, 123, 164112	3.9	73
5	Time- and frequency-resolved fluorescence spectra of nonadiabatic dissipative systems: what photons can tell us. *Journal of Chemical Physics*, **2005**, 122, 134504	3.9	39
4	Time-resolved spontaneous emission beyond the doorway□window approximation. *Chemical Physics*, **2004**, 301, 129-139	2.3	20
3	Time domain fingerprints of a □perpendicular□rotational Raman band: formic acid studied by femtosecond degenerate four-wave mixing. *Journal of Raman Spectroscopy*, **2003**, 34, 1045-1050	2.3	11
2	Inertial effects in the Brownian dynamics with rigid constraints. *Macromolecular Theory and Simulations*, **1999**, 8, 529-543	1.5	5
1	The hierarchy of Davydov's Ans□ze and its applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	5