# Maxim F Gelin

List of Publications by Year
in descending order

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|---|---|---|---|
| 89 papers | 1,766 citations | 279701 23 h-index | 345118 36 g-index |
| 91 all docs | 91 docs citations | 91 times ranked | 938 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Efficient Calculation of Time- and Frequency-Resolved Four-Wave-Mixing Signals. Accounts of Chemical Research, 2009, 42, 1290-1298. | 7.6 | 87 |
| 2 | 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. | 1.2 | 85 |
| 3 | 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. | 1.2 | 80 |
| 4 | Quantum electron-vibrational dynamics at finite temperature: Thermo field dynamics approach. Journal of Chemical Physics, 2016, 145, 224101. | 1.2 | 58 |
| 5 | Thermodynamics of a subensemble of a canonical ensemble. Physical Review E, 2009, 79, 051121. | 0.8 | 54 |
| 6 | Simulation of Quantum Dynamics of Excitonic Systems at Finite Temperature: an efficient method based on Thermo Field Dynamics. Scientific Reports, 2017, 7, 9127. | 1.6 | 50 |
| 7 | Ultrafast Relaxation Dynamics in Zinc Tetraphenylporphyrin Surface-Mounted Metal Organic Framework. Journal of Physical Chemistry C, 2018, 122, 50-61. | 1.5 | 48 |
| 8 | Effects of intense femtosecond pumping on ultrafast electronic-vibrational dynamics in molecular systems with relaxation. Journal of Chemical Physics, 2008, 129, 214303. | 1.2 | 45 |
| 9 | Time- and frequency-resolved fluorescence spectra of nonadiabatic dissipative systems: What photons can tell us. Journal of Chemical Physics, 2005, 122, 134504. | 1.2 | 44 |
| 10 | Polaron dynamics in two-dimensional photon-echo spectroscopy of molecular rings. Journal of Chemical Physics, 2013, 139, 104103. | 1.2 | 42 |
| 11 | Dissipative dynamics at conical intersections: simulations with the hierarchy equations of motion method. Faraday Discussions, 2016, 194, 61-80. | 1.6 | 39 |
| 12 | Davydov Ansatz as an efficient tool for the simulation of nonlinear optical response of molecular aggregates. Journal of Chemical Physics, 2015, 142, 212448. | 1.2 | 37 |
| 13 | Finite temperature quantum dynamics of complex systems: Integrating <scp>thermoâ€field</scp> theories and <scp>tensorâ€train</scp> methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1539. | 6.2 | 35 |
| 14 | Signatures of conical intersections in two-dimensional electronic spectra. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124019. | 0.6 | 32 |
| 15 | Interference of Interchromophoric Energy-Transfer Pathways in Ï€-Conjugated Macrocycles. Journal of Physical Chemistry Letters, 2016, 7, 4936-4944. | 2.1 | 32 |
| 16 | Multimode quantum dynamics with multiple Davydov D2 trial states: Application to a 24-dimensional conical intersection model. Journal of Chemical Physics, 2019, 150, 024101. | 1.2 | 32 |
| 17 | Simulation of femtosecond two-dimensional electronic spectra of conical intersections. Journal of Chemical Physics, 2015, 143, 074308. | 1.2 | 29 |
| 18 | Multi-faceted spectroscopic mapping of ultrafast nonadiabatic dynamics near conical intersections: A computational study. Journal of Chemical Physics, 2020, 153, 174111. | 1.2 | 29 |

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|---|---|---|---|
| 19 | Manipulating electronic couplings and nonadiabatic nuclear dynamics with strong laser pulses. Journal of Chemical Physics, 2009, 131, 124505. | 1.2 | 27 |
| 20 | Simplified expressions that incorporate finite pulse effects into coherent two-dimensional optical spectra. Journal of Chemical Physics, 2017, 147, 144103. | 1.2 | 26 |
| 21 | Temperature effects on singlet fission dynamics mediated by a conical intersection. Journal of Chemical Physics, 2020, 153, 194106. | 1.2 | 25 |
| 22 | Theory of femtosecond coherent double-pump single-molecule spectroscopy: Application to light harvesting complexes. Journal of Chemical Physics, 2015, 142, 164106. | 1.2 | 24 |
| 23 | Calculation of third-order signals via driven SchrÃ¶dinger equations: General results and application to electronic 2D photon echo spectroscopy. Chemical Physics, 2013, 422, 53-62. | 0.9 | 23 |
| 24 | Dynamics of disordered Tavisâ€“Cummings and Holsteinâ€“Tavisâ€“Cummings models. Journal of Chemical Physics, 2022, 156, 024102. | 1.2 | 23 |
| 25 | Time-resolved spontaneous emission beyond the doorwayâ€“window approximation. Chemical Physics, 2004, 301, 129-139. | 0.9 | 22 |
| 26 | Analysis of vibrational coherences in homodyne and two-dimensional heterodyne photon-echo spectra of Nile Blue. Chemical Physics, 2007, 341, 113-122. | 0.9 | 22 |
| 27 | Efficient calculation of the polarization induced by N coherent laser pulses. Journal of Chemical Physics, 2009, 131, 194103. | 1.2 | 22 |
| 28 | Strong and Long Makes Short: Strong-Pump Strong-Probe Spectroscopy. Journal of Physical Chemistry Letters, 2011, 2, 114-119. | 2.1 | 22 |
| 29 | Bath-induced correlations and relaxation of vibronic dimers. Journal of Chemical Physics, 2012, 136, 034507. | 1.2 | 22 |
| 30 | Strong-pump strong-probe spectroscopy: effects of higher excited electronic states. Physical Chemistry Chemical Physics, 2013, 15, 8119. | 1.3 | 22 |
| 31 | The hierarchy of Davydov's AnsÃtze and its applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, . | 6.2 | 22 |
| 32 | 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. | 2.1 | 21 |
| 33 | Exact quantum master equation for a molecular aggregate coupled to a harmonic bath. Physical Review E, 2011, 84, 041139. | 0.8 | 20 |
| 34 | 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. | 1.2 | 20 |
| 35 | 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 Fennaâ€“Matthewsâ€“Olson Complex. Journal of Chemical Theory and Computation, 2021, 17, 4316-4331. | 2.3 | 20 |
| 36 | Optical N-Wave-Mixing Spectroscopy with Strong and Temporally Well-Separated Pulses: The Doorwayâ^'Window Representation. Journal of Physical Chemistry B, 2011, 115, 5648-5658. | 1.2 | 19 |

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|---|---|---|---|
| 37 | Thermal SchrÃ¶dinger Equation: Efficient Tool for Simulation of Manyâ€Body Quantum Dynamics at Finite Temperature. Annalen Der Physik, 2017, 529, 1700200. | 0.9 | 19 |
| 38 | Analysis of transient-absorption pump-probe signals of nonadiabatic dissipative systems: â€œIdealâ€•and â€œrealâ€•spectra. Journal of Chemical Physics, 2019, 150, 204102. | 1.2 | 19 |
| 39 | Origin of Unexpectedly Simple Oscillatory Responses in the Excited-State Dynamics of Disordered Molecular Aggregates. Journal of Physical Chemistry Letters, 2019, 10, 2806-2810. | 2.1 | 19 |
| 40 | Dynamics of the spin-boson model: A comparison of the multiple Davydov <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si45.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">D</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:mo>,</mml:mo><mml:mi mathvariant="normal">D</mml:mi></mml:mrow><mml:mrow><mml:mn>1.5</mml:mn></mml:mrow></mml:msub><mml:mo>,</mml:mo><mml:mi mathvariant="normal">D</mml:mi></mml:mrow><mml:mi></mml:mi>. Chemical Physics, 2018, 515, 108-118. | 0.9 | 17 |
| 41 | Ab Initio Surface-Hopping Simulation of Femtosecond Transient-Absorption Pumpâ€“Probe Signals of Nonadiabatic Excited-State Dynamics Using the Doorwayâ€“Window Representation. Journal of Chemical Theory and Computation, 2021, 17, 2394-2408. | 2.3 | 16 |
| 42 | Resonant Femtosecond Stimulated Raman Spectra: Theory and Simulations. Journal of Physical Chemistry A, 2016, 120, 3286-3295. | 1.1 | 15 |
| 43 | Dynamics of a one-dimensional Holstein polaron: The multiconfigurational Ehrenfest method. Journal of Chemical Physics, 2019, 151, 244116. | 1.2 | 15 |
| 44 | 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. | 2.3 | 15 |
| 45 | Generalized Huang-Rhys factors for molecular aggregates. Chemical Physics, 2020, 528, 110495. | 0.9 | 14 |
| 46 | Domain of validity of the perturbative approach to femtosecond optical spectroscopy. Journal of Chemical Physics, 2013, 139, 224107. | 1.2 | 13 |
| 47 | The Generalized Coherent State ansatz: Application to quantum electron-vibrational dynamics. Chemical Physics, 2016, 481, 91-98. | 0.9 | 13 |
| 48 | Efficient orientational averaging of nonlinear optical signals in multi-chromophore systems. Journal of Chemical Physics, 2017, 147, 044114. | 1.2 | 13 |
| 49 | Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. I. Weak-field regime. Physical Chemistry Chemical Physics, 2017, 19, 32296-32306. | 1.3 | 13 |
| 50 | Theory helps experiment to reveal VOCs in human breath. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 258, 119785. | 2.0 | 13 |
| 51 | Effects of high pulse intensity and chirp in two-dimensional electronic spectroscopy of an atomic vapor. Optics Express, 2020, 28, 25806. | 1.7 | 13 |
| 52 | Ultrafast Internal Conversion Dynamics through the on-the-Fly Simulation of Transient Absorption Pumpâ€“Probe Spectra with Different Electronic Structure Methods. Journal of Physical Chemistry Letters, 2022, 13, 661-668. | 2.1 | 13 |
| 53 | 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. | 1.2 | 12 |
| 54 | Strong field effects in rotational femtosecond degenerate four-wave mixing. Journal of Chemical Physics, 2010, 132, 134301. | 1.2 | 12 |

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| 55 | Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. II. Strong-field regime. Physical Chemistry Chemical Physics, 2017, 19, 32307-32319. | 1.3 | 12 |
| 56 | Enhanced S<sub>2</sub> Fluorescence from a Free-Base Tetraphenylporphyrin Surface-Mounted Metal Organic Framework. Journal of Physical Chemistry C, 2018, 122, 23321-23328. | 1.5 | 12 |
| 57 | Efficient simulation of time- and frequency-resolved four-wave-mixing signals with a multiconfigurational Ehrenfest approach. Journal of Chemical Physics, 2021, 154, 054105. | 1.2 | 12 |
| 58 | Spectral Fingerprint of Excited-State Energy Transfer in Dendrimers through Polarization-Sensitive Transient-Absorption Pumpâ€“Probe Signals: On-the-Fly Nonadiabatic Dynamics Simulations. Journal of Physical Chemistry Letters, 2021, 12, 9710-9719. | 2.1 | 12 |
| 59 | Alternative view of two-dimensional spectroscopy. Journal of Chemical Physics, 2016, 144, 194104. | 1.2 | 11 |
| 60 | Nonperturbative response functions: A tool for the interpretation of four-wave-mixing signals beyond third order. Journal of Chemical Physics, 2017, 147, 234104. | 1.2 | 11 |
| 61 | First-passage time theory of activated rate chemical processes in electronic molecular junctions. Journal of Chemical Physics, 2021, 154, 114108. | 1.2 | 11 |
| 62 | 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. | 2.3 | 11 |
| 63 | Efficient quantum dynamics simulations of complex molecular systems: A unified treatment of dynamic and static disorder. Journal of Chemical Physics, 2021, 155, 134102. | 1.2 | 11 |
| 64 | Pump-probe spectroscopy with strong pulses as a tool to enhance weak electronic transitions. Physical Review A, 2013, 87, . | 1.0 | 10 |
| 65 | Simple Recipes for Separating Excited-State Absorption and Cascading Signals by Polarization-Sensitive Measurements. Journal of Physical Chemistry A, 2013, 117, 11509-11513. | 1.1 | 10 |
| 66 | Ab Initio Quasiclassical Simulation of Femtosecond Time-Resolved Two-Dimensional Electronic Spectra of Pyrazine. Journal of Physical Chemistry Letters, 2021, 12, 11736-11744. | 2.1 | 9 |
| 67 | Accurate Simulation of Spectroscopic Signatures of Cavity-Assisted, Conical-Intersection-Controlled Singlet Fission Processes. Journal of Physical Chemistry Letters, 2022, 13, 4280-4288. | 2.1 | 9 |
| 68 | Simulation of Femtosecond Phase-Locked Double-Pump Signals of Individual Light-Harvesting Complexes LH2. Journal of Physical Chemistry Letters, 2018, 9, 4488-4494. | 2.1 | 8 |
| 69 | Pulse-shape effects in fifth-order multidimensional optical spectroscopy. Chemical Physics, 2018, 515, 119-128. | 0.9 | 8 |
| 70 | Vibronic coherences in light harvesting nanotubes: unravelling the role of dark states. Journal of Materials Chemistry C, 2022, 10, 7216-7226. | 2.7 | 8 |
| 71 | Resonant femtosecond stimulated Raman spectroscopy with an intense actinic pump pulse: Application to conical intersections. Journal of Chemical Physics, 2017, 146, 084105. | 1.2 | 7 |
| 72 | Quantum dynamics of vibrational energy flow in oscillator chains driven by anharmonic interactions. New Journal of Physics, 2020, 22, 123002. | 1.2 | 7 |

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|---|---|---|---|
| 73 | Engineering Cavity Singlet Fission in Rubrene. Journal of Physical Chemistry Letters, 2022, 13, 4090-4097. | 2.1 | 7 |
| 74 | Inertial effects in the Brownian dynamics with rigid constraints. Macromolecular Theory and Simulations, 1999, 8, 529-543. | 0.6 | 6 |
| 75 | Ultrafast carrier dynamics at organic donorâ€“acceptor interfacesâ€”a quantum-based assessment of the hopping model. JPhys Materials, 2022, 5, 024001. | 1.8 | 6 |
| 76 | Transient Phenomena in Time- and Frequency-Gated Spontaneous Emission. Journal of Physical Chemistry A, 2005, 109, 3587-3597. | 1.1 | 5 |
| 77 | Ring-puckering motion in cyclopentene studied by time-resolved rotational coherence spectroscopy and ab initio calculations. Physical Chemistry Chemical Physics, 2010, 12, 8190. | 1.3 | 5 |
| 78 | 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. | 1.2 | 5 |
| 79 | Upper Excited State Photophysics of Malachite Green in Solution and Films. Journal of Physical Chemistry B, 2020, 124, 4293-4302. | 1.2 | 5 |
| 80 | Microscopic derivation of the Keilsonâ€“Storer master equation. Chemical Physics, 2015, 462, 35-40. | 0.9 | 4 |
| 81 | Femtosecond stimulated Raman spectroscopy as a tool to detect molecular vibrations in ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 184307. | 1.2 | 4 |
| 82 | A model for dynamical solvent control of molecular junction electronic properties. Journal of Chemical Physics, 2021, 154, 044107. | 1.2 | 4 |
| 83 | Markovian master equation for a classical particle coupled with arbitrary strength to a harmonic bath. Journal of Chemical Physics, 2014, 141, 214109. | 1.2 | 3 |
| 84 | Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257. | 1.6 | 3 |
| 85 | Towards efficient photochemistry from upper excited electronic states: detection of long S2 lifetime of perylene. Journal of Chemical Physics, 2021, 155, 191102. | 1.2 | 3 |
| 86 | Hierarchical Equations-of-Motion Method for Momentum Systemâ€“Bath Coupling. Journal of Physical Chemistry B, 2021, 125, 4863-4873. | 1.2 | 2 |
| 87 | Calculation of semiclassical free energy differences along nonequilibrium classical trajectories. Journal of Chemical Physics, 2009, 131, 164510. | 1.2 | 0 |
| 88 | Photosynthetic light harvesting: Insights from multidisciplinary approaches. Chemical Physics, 2020, 533, 110746. | 0.9 | 0 |
| 89 | Beyond Third-Order Response: Strong-Pulse and N-Wave-Mixing Optical Spectroscopies. , 2011, , . | | 0 |