

# Jiri Vanicek

## List of Publications by Year in descending order

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72  
papers

2,359  
citations

218592

26  
h-index

233338

45  
g-index

77  
all docs

77  
docs citations

77  
times ranked

2766  
citing authors

#	ARTICLE	IF	CITATIONS
1	Efficient use of accessibility in microRNA target prediction. <i>Nucleic Acids Research</i> , 2011, 39, 19-29.	6.5	409
2	Suppression of immediate-early viral gene expression by herpesvirus-coded microRNAs: Implications for latency. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 5453-5458.	3.3	248
3	A KRAB/KAP1-miRNA Cascade Regulates Erythropoiesis Through Stage-Specific Control of Mitophagy. <i>Science</i> , 2013, 340, 350-353.	6.0	95
4	Self-Assembled Molecular Rafts at Liquid   Liquid Interfaces for Four-Electron Oxygen Reduction. <i>Journal of the American Chemical Society</i> , 2012, 134, 498-506.	6.6	87
5	Host MicroRNA Regulation of Human Cytomegalovirus Immediate Early Protein Translation Promotes Viral Latency. <i>Journal of Virology</i> , 2014, 88, 5524-5532.	1.5	84
6	Semiclassical evaluation of quantum fidelity. <i>Physical Review E</i> , 2003, 68, 056208.	0.8	75
7	Quantum-instanton evaluation of the kinetic isotope effects. <i>Journal of Chemical Physics</i> , 2005, 123, 054108.	1.2	66
8	Efficient estimators for quantum instanton evaluation of the kinetic isotope effects: Application to the intramolecular hydrogen transfer in pentadiene. <i>Journal of Chemical Physics</i> , 2007, 127, 114309.	1.2	60
9	Dephasing representation: Employing the shadowing theorem to calculate quantum correlation functions. <i>Physical Review E</i> , 2004, 70, 055201.	0.8	53
10	On-the-fly <i>ab initio</i> semiclassical dynamics: Identifying degrees of freedom essential for emission spectra of oligothiophenes. <i>Journal of Chemical Physics</i> , 2014, 140, 244114.	1.2	51
11	Dephasing representation of quantum fidelity for general pure and mixed states. <i>Physical Review E</i> , 2006, 73, 046204.	0.8	50
12	On-the-Fly <i>ab Initio</i> Semiclassical Dynamics of Floppy Molecules: Absorption and Photoelectron Spectra of Ammonia. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5685-5690.	1.1	45
13	Proton Transfer Studied Using a Combined <i>Ab Initio</i> Reactive Potential Energy Surface with Quantum Path Integral Methodology. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2566-2580.	2.3	44
14	Kinetic isotope effects and how to describe them. <i>Structural Dynamics</i> , 2017, 4, 061501.	0.9	37
15	On-the-Fly <i>Ab Initio</i> Semiclassical Evaluation of Absorption Spectra of Polyatomic Molecules beyond the Condon Approximation. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2367-2372.	2.1	36
16	Relation of exact Gaussian basis methods to the dephasing representation: Theory and application to time-resolved electronic spectra. <i>Journal of Chemical Physics</i> , 2013, 139, 034112.	1.2	35
17	Efficient on-the-fly <i>ab initio</i> semiclassical method for computing time-resolved nonadiabatic electronic spectra with surface hopping or Ehrenfest dynamics. <i>Journal of Chemical Physics</i> , 2014, 141, 134102.	1.2	35
18	Kinetic isotope effect in malonaldehyde determined from path integral Monte Carlo simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 204-211.	1.3	35

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19	Single-Hessian thawed Gaussian approximation. <i>Journal of Chemical Physics</i> , 2019, 150, 154117.	1.2	35
20	Path integral evaluation of equilibrium isotope effects. <i>Journal of Chemical Physics</i> , 2009, 131, 024111.	1.2	33
21	Searching the coding region for microRNA targets. <i>Rna</i> , 2013, 19, 467-474.	1.6	31
22	Nonadiabatic effects in electronic and nuclear dynamics. <i>Structural Dynamics</i> , 2017, 4, 061510.	0.9	31
23	Semiclassical Approach to Photophysics Beyond Kasha's Rule and Vibronic Spectroscopy Beyond the Condon Approximation. The Case of Azulene. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2617-2626.	2.3	29
24	Communications: Evaluation of the nonadiabaticity of quantum molecular dynamics with the dephasing representation of quantum fidelity. <i>Journal of Chemical Physics</i> , 2010, 132, 241101.	1.2	28
25	On-the-fly <i>ab initio</i> semiclassical evaluation of vibronic spectra at finite temperature. <i>Journal of Chemical Physics</i> , 2020, 153, 024105.	1.2	28
26	Time-Resolved Electronic Spectra with Efficient Quantum Dynamics Methods. <i>Chimia</i> , 2011, 65, 334.	0.3	27
27	On-the-fly <i>ab initio</i> semiclassical evaluation of time-resolved electronic spectra. <i>Journal of Chemical Physics</i> , 2018, 149, 244115.	1.2	27
28	On-the-fly <i>ab initio</i> semiclassical evaluation of third-order response functions for two-dimensional electronic spectroscopy. <i>Journal of Chemical Physics</i> , 2020, 153, 184110.	1.2	25
29	Direct evaluation of the temperature dependence of the rate constant based on the quantum instanton approximation. <i>Journal of Chemical Physics</i> , 2010, 132, 194106.	1.2	23
30	Measuring nonadiabaticity of molecular quantum dynamics with quantum fidelity and with its efficient semiclassical approximation. <i>Journal of Chemical Physics</i> , 2012, 136, 094106.	1.2	23
31	On-the-fly <i>ab initio</i> three thawed Gaussians approximation: A semiclassical approach to Herzberg-Teller spectra. <i>Chemical Physics</i> , 2018, 515, 152-163.	0.9	22
32	On-the-Fly <i>ab initio</i> Semiclassical Evaluation of Electronic Coherences in Polyatomic Molecules Reveals a Simple Mechanism of Decoherence. <i>Physical Review Letters</i> , 2020, 125, 083001.	2.9	21
33	Monte Carlo evaluation of the equilibrium isotope effects using the Takahashi-Imada factorization of the Feynman path integral. <i>Chemical Physics Letters</i> , 2013, 588, 11-16.	1.2	20
34	PACCMIT/PACCMIT-CDS: identifying microRNA targets in 3' UTRs and coding sequences. <i>Nucleic Acids Research</i> , 2015, 43, W474-W479.	6.5	20
35	Efficient geometric integrators for nonadiabatic quantum dynamics. II. The diabatic representation. <i>Journal of Chemical Physics</i> , 2019, 150, 204113.	1.2	20
36	Finite-Temperature, Anharmonicity, and Duschinsky Effects on the Two-Dimensional Electronic Spectra from <i>Ab Initio</i> Thermo-Field Gaussian Wavepacket Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2997-3005.	2.1	20

#	ARTICLE	IF	CITATIONS
37	Beating the Efficiency of Both Quantum and Classical Simulations with a Semiclassical Method. <i>Physical Review Letters</i> , 2011, 107, 214101.	2.9	18
38	Core-Valence Attosecond Transient Absorption Spectroscopy of Polyatomic Molecules. <i>Physical Review Letters</i> , 2021, 127, 123001.	2.9	18
39	Uniform semiclassical wave function for coherent two-dimensional electron flow. <i>Physical Review E</i> , 2003, 67, 016211.	0.8	17
40	Three applications of path integrals: equilibrium and kinetic isotope effects, and the temperature dependence of the rate constant of the [1,5] sigmatropic hydrogen shift in (Z)-1,3-pentadiene. <i>Journal of Molecular Modeling</i> , 2010, 16, 1779-1787.	0.8	17
41	Optimal Use of Conservation and Accessibility Filters in MicroRNA Target Prediction. <i>PLoS ONE</i> , 2012, 7, e32208.	1.1	17
42	Accelerating the calculation of time-resolved electronic spectra with the cellular dephasing representation. <i>Molecular Physics</i> , 2012, 110, 945-955.	0.8	17
43	Efficient evaluation of accuracy of molecular quantum dynamics using dephasing representation. <i>Journal of Chemical Physics</i> , 2009, 131, 041101.	1.2	16
44	Efficient evaluation of the accuracy of molecular quantum dynamics on an approximate analytical or interpolated ab initio potential energy surface. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2426-2435.	1.0	16
45	Analysis of the accessibility of CLIP bound sites reveals that nucleation of the miRNA:mRNA pairing occurs preferentially at the 3'-end of the seed match. <i>Rna</i> , 2012, 18, 1760-1770.	1.6	16
46	Improving the accuracy and efficiency of time-resolved electronic spectra calculations: Cellular dephasing representation with a prefactor. <i>Journal of Chemical Physics</i> , 2013, 139, 054109.	1.2	16
47	Efficient geometric integrators for nonadiabatic quantum dynamics. I. The adiabatic representation. <i>Journal of Chemical Physics</i> , 2019, 150, 204112.	1.2	16
48	Accelerating quantum instanton calculations of the kinetic isotope effects. <i>Journal of Chemical Physics</i> , 2015, 143, 194104.	1.2	15
49	Replacement manifolds: a method to uniformize semiclassical wave functions. <i>Physical Review E</i> , 2001, 64, 026215.	0.8	13
50	Evaluation of the importance of spin-orbit couplings in the nonadiabatic quantum dynamics with quantum fidelity and with its efficient on-the-fly ab initio semiclassical approximation. <i>Journal of Chemical Physics</i> , 2012, 137, 22A516.	1.2	13
51	Applicability of the Thawed Gaussian Wavepacket Dynamics to the Calculation of Vibronic Spectra of Molecules with Double-Well Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3065-3074.	2.3	13
52	Semiclassical analysis of the quantum instanton approximation. <i>Journal of Chemical Physics</i> , 2019, 151, 144111.	1.2	12
53	Ab Initio Semiclassical Evaluation of Vibrationally Resolved Electronic Spectra With Thawed Gaussians. , 2021, , 199-229.		10
54	Search for long-lasting electronic coherence using on-the-fly ab initio semiclassical dynamics. <i>Journal of Chemical Physics</i> , 2022, 156, 034104.	1.2	10

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55	Path integral approach to the quantum fidelity amplitude. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150164.	1.6	9
56	Efficient Semiclassical Dynamics for Vibronic Spectroscopy beyond Harmonic, Condon, and Zero-Temperature Approximations. Chimia, 2021, 75, 261.	0.3	8
57	Several Semiclassical Approaches to Time-resolved Spectroscopy. Chimia, 2017, 71, 283.	0.3	7
58	A combined on-the-fly/interpolation procedure for evaluating energy values needed in molecular simulations. Journal of Chemical Physics, 2019, 151, 174116.	1.2	7
59	A time-reversible integrator for the time-dependent Schrödinger equation on an adaptive grid. Journal of Chemical Physics, 2019, 151, 234102.	1.2	7
60	How important are the residual nonadiabatic couplings for an accurate simulation of nonadiabatic quantum dynamics in a quasidiabatic representation?. Journal of Chemical Physics, 2021, 154, 124119.	1.2	6
61	Time-reversible and norm-conserving high-order integrators for the nonlinear time-dependent Schrödinger equation: Application to local control theory. Journal of Chemical Physics, 2021, 154, 154106.	1.2	5
62	High-order geometric integrators for representation-free Ehrenfest dynamics. Journal of Chemical Physics, 2021, 155, 124104.	1.2	5
63	Which form of the molecular Hamiltonian is the most suitable for simulating the nonadiabatic quantum dynamics at a conical intersection?. Journal of Chemical Physics, 2020, 153, 211101.	1.2	4
64	An implicit split-operator algorithm for the nonlinear time-dependent Schrödinger equation. Journal of Chemical Physics, 2021, 155, 204109.	1.2	4
65	Role of sampling in evaluating classical time autocorrelation functions. Journal of Chemical Physics, 2013, 139, 104105.	1.2	3
66	Accelerating equilibrium isotope effect calculations. I. Stochastic thermodynamic integration with respect to mass. Journal of Chemical Physics, 2017, 146, .	1.2	3
67	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. Structural Dynamics, 2017, 4, 061509.	0.9	3
68	Efficient sampling avoids the exponential wall in classical simulations of fidelity. Physical Review E, 2011, 84, 066205.	0.8	2
69	Beyond Transition State Theory: Accurate Description of Nuclear Quantum Effects on the Rate and Equilibrium Constants of Chemical Reactions Using Feynman Path Integrals. Chimia, 2011, 65, 715.	0.3	1
70	Imaginary-time nonuniform mesh method for solving the multidimensional Schrödinger equation: Fermionization and melting of quantum Lennard-Jones crystals. Physical Review A, 2013, 88, .	1.0	1
71	Predicting the Genes Regulated by MicroRNAs via Binding Sites in the 3' Untranslated and Coding Regions. Chimia, 2014, 68, 629.	0.3	1
72	Accelerating equilibrium isotope effect calculations. II. Stochastic implementation of direct estimators. Journal of Chemical Physics, 2019, 151, 134116.	1.2	1