Jiri Vanicek

List of Publications by Year
in descending order

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72	2,359	218592	233338
papers	citations	26	45
		h-index	g-index

77	77	77	2766
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Search for long-lasting electronic coherence using on-the-fly ab initio semiclassical dynamics. Journal of Chemical Physics, 2022, 156, 034104.	1.2	10
2	Applicability of the Thawed Gaussian Wavepacket Dynamics to the Calculation of Vibronic Spectra of Molecules with Double-Well Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2022, 18, 3065-3074.	2.3	13
3	Ab Initio Semiclassical Evaluation of Vibrationally Resolved Electronic Spectra With Thawed Gaussians. , 2021, , 199-229.		10
4	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
5	Finite-Temperature, Anharmonicity, and Duschinsky Effects on the Two-Dimensional Electronic Spectra from Ab Initio Thermo-Field Gaussian Wavepacket Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 2997-3005.	2.1	20
6	Efficient Semiclassical Dynamics for Vibronic Spectroscopy beyond Harmonic, Condon, and Zero-Temperature Approximations. Chimia, 2021, 75, 261.	0.3	8
7	Time-reversible and norm-conserving high-order integrators for the nonlinear time-dependent SchrÃ¶dinger equation: Application to local control theory. Journal of Chemical Physics, 2021, 154, 154106.	1.2	5
8	High-order geometric integrators for representation-free Ehrenfest dynamics. Journal of Chemical Physics, 2021, 155, 124104.	1.2	5
9	Core-Valence Attosecond Transient Absorption Spectroscopy of Polyatomic Molecules. Physical Review Letters, 2021, 127, 123001.	2.9	18
10	An implicit split-operator algorithm for the nonlinear time-dependent SchrÃ¶dinger equation. Journal of Chemical Physics, 2021, 155, 204109.	1.2	4
11	On-the-fly ab initio semiclassical evaluation of vibronic spectra at finite temperature. Journal of Chemical Physics, 2020, 153, 024105.	1.2	28
12	On-the-Fly abÂinitio Semiclassical Evaluation of Electronic Coherences in Polyatomic Molecules Reveals a Simple Mechanism of Decoherence. Physical Review Letters, 2020, 125, 083001.	2.9	21
13	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
14	Semiclassical Approach to Photophysics Beyond Kashaâ€™s Rule and Vibronic Spectroscopy Beyond the Condon Approximation. The Case of Azulene. Journal of Chemical Theory and Computation, 2020, 16, 2617-2626.	2.3	29
15	On-the-fly ab initio semiclassical evaluation of third-order response functions for two-dimensional electronic spectroscopy. Journal of Chemical Physics, 2020, 153, 184110.	1.2	25
16	Efficient geometric integrators for nonadiabatic quantum dynamics. I. The adiabatic representation. Journal of Chemical Physics, 2019, 150, 204112.	1.2	16
17	Efficient geometric integrators for nonadiabatic quantum dynamics. II. The diabatic representation. Journal of Chemical Physics, 2019, 150, 204113.	1.2	20
18	Accelerating equilibrium isotope effect calculations. II. Stochastic implementation of direct estimators. Journal of Chemical Physics, 2019, 151, 134116.	1.2	1

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19	Semiclassical analysis of the quantum instanton approximation. Journal of Chemical Physics, 2019, 151, 144111.	1.2	12
20	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
21	Single-Hessian thawed Gaussian approximation. Journal of Chemical Physics, 2019, 150, 154117.	1.2	35
22	A time-reversible integrator for the time-dependent SchrÃ¶dinger equation on an adaptive grid. Journal of Chemical Physics, 2019, 151, 234102.	1.2	7
23	On-the-Fly Ab Initio Semiclassical Evaluation of Absorption Spectra of Polyatomic Molecules beyond the Condon Approximation. Journal of Physical Chemistry Letters, 2018, 9, 2367-2372.	2.1	36
24	On-the-fly ab initio semiclassical evaluation of time-resolved electronic spectra. Journal of Chemical Physics, 2018, 149, 244115.	1.2	27
25	On-the-fly ab initio three thawed Gaussians approximation: A semiclassical approach to Herzberg-Teller spectra. Chemical Physics, 2018, 515, 152-163.	0.9	22
26	Accelerating equilibrium isotope effect calculations. I. Stochastic thermodynamic integration with respect to mass. Journal of Chemical Physics, 2017, 146, .	1.2	3
27	Kinetic isotope effects and how to describe them. Structural Dynamics, 2017, 4, 061501.	0.9	37
28	Nonadiabatic effects in electronic and nuclear dynamics. Structural Dynamics, 2017, 4, 061510.	0.9	31
29	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
30	Several Semiclassical Approaches to Time-resolved Spectroscopy. Chimia, 2017, 71, 283.	0.3	7
31	Path integral approach to the quantum fidelity amplitude. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150164.	1.6	9
32	Accelerating quantum instanton calculations of the kinetic isotope effects. Journal of Chemical Physics, 2015, 143, 194104.	1.2	15
33	PACCMIT/PACCMIT-CDS: identifying microRNA targets in 3â€² UTRs and coding sequences. Nucleic Acids Research, 2015, 43, W474-W479.	6.5	20
34	On-the-Fly ab Initio Semiclassical Dynamics of Floppy Molecules: Absorption and Photoelectron Spectra of Ammonia. Journal of Physical Chemistry A, 2015, 119, 5685-5690.	1.1	45
35	Efficient on-the-fly ab initio semiclassical method for computing time-resolved nonadiabatic electronic spectra with surface hopping or Ehrenfest dynamics. Journal of Chemical Physics, 2014, 141, 134102.	1.2	35
36	On-the-fly ab initio semiclassical dynamics: Identifying degrees of freedom essential for emission spectra of oligothiophenes. Journal of Chemical Physics, 2014, 140, 244114.	1.2	51

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37	Host MicroRNA Regulation of Human Cytomegalovirus Immediate Early Protein Translation Promotes Viral Latency. Journal of Virology, 2014, 88, 5524-5532.	1.5	84
38	Kinetic isotope effect in malonaldehyde determined from path integral Monte Carlo simulations. Physical Chemistry Chemical Physics, 2014, 16, 204-211.	1.3	35
39	Predicting the Genes Regulated by MicroRNAs via Binding Sites in the 3' Untranslated and Coding Regions. Chimia, 2014, 68, 629.	0.3	1
40	Improving the accuracy and efficiency of time-resolved electronic spectra calculations: Cellular dephasing representation with a prefactor. Journal of Chemical Physics, 2013, 139, 054109.	1.2	16
41	Monte Carlo evaluation of the equilibrium isotope effects using the Takahashiâ€“Imada factorization of the Feynman path integral. Chemical Physics Letters, 2013, 588, 11-16.	1.2	20
42	A KRAB/KAP1-miRNA Cascade Regulates Erythropoiesis Through Stage-Specific Control of Mitophagy. Science, 2013, 340, 350-353.	6.0	95
43	Searching the coding region for microRNA targets. Rna, 2013, 19, 467-474.	1.6	31
44	Relation of exact Gaussian basis methods to the dephasing representation: Theory and application to time-resolved electronic spectra. Journal of Chemical Physics, 2013, 139, 034112.	1.2	35
45	Imaginary-time nonuniform mesh method for solving the multidimensional SchrÃ¶dinger equation: Fermionization and melting of quantum Lennard-Jones crystals. Physical Review A, 2013, 88, .	1.0	1
46	Role of sampling in evaluating classical time autocorrelation functions. Journal of Chemical Physics, 2013, 139, 104105.	1.2	3
47	Measuring nonadiabaticity of molecular quantum dynamics with quantum fidelity and with its efficient semiclassical approximation. Journal of Chemical Physics, 2012, 136, 094106.	1.2	23
48	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. Rna, 2012, 18, 1760-1770.	1.6	16
49	Evaluation of the importance of spin-orbit couplings in the nonadiabatic quantum dynamics with quantum fidelity and with its efficient â€œon-the-flyâ€•ab initio semiclassical approximation. Journal of Chemical Physics, 2012, 137, 22A516.	1.2	13
50	Self-Assembled Molecular Rafts at Liquid|Liquid Interfaces for Four-Electron Oxygen Reduction. Journal of the American Chemical Society, 2012, 134, 498-506.	6.6	87
51	Optimal Use of Conservation and Accessibility Filters in MicroRNA Target Prediction. PLoS ONE, 2012, 7, e32208.	1.1	17
52	Accelerating the calculation of time-resolved electronic spectra with the cellular dephasing representation. Molecular Physics, 2012, 110, 945-955.	0.8	17
53	Time-Resolved Electronic Spectra with Efficient Quantum Dynamics Methods. Chimia, 2011, 65, 334.	0.3	27
54	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

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55	Beating the Efficiency of Both Quantum and Classical Simulations with a Semiclassical Method. Physical Review Letters, 2011, 107, 214101.	2.9	18
56	Efficient sampling avoids the exponential wall in classical simulations of fidelity. Physical Review E, 2011, 84, 066205.	0.8	2
57	Efficient use of accessibility in microRNA target prediction. Nucleic Acids Research, 2011, 39, 19-29.	6.5	409
58	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. Journal of Molecular Modeling, 2010, 16, 1779-1787.	0.8	17
59	Efficient evaluation of the accuracy of molecular quantum dynamics on an approximate analytical or interpolated ab initio potential energy surface. International Journal of Quantum Chemistry, 2010, 110, 2426-2435.	1.0	16
60	Communications: Evaluation of the nondiabaticity of quantum molecular dynamics with the dephasing representation of quantum fidelity. Journal of Chemical Physics, 2010, 132, 241101.	1.2	28
61	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. Journal of Chemical Theory and Computation, 2010, 6, 2566-2580.	2.3	44
62	Direct evaluation of the temperature dependence of the rate constant based on the quantum instanton approximation. Journal of Chemical Physics, 2010, 132, 194106.	1.2	23
63	Efficient evaluation of accuracy of molecular quantum dynamics using dephasing representation. Journal of Chemical Physics, 2009, 131, 041101.	1.2	16
64	Path integral evaluation of equilibrium isotope effects. Journal of Chemical Physics, 2009, 131, 024111.	1.2	33
65	Suppression of immediate-early viral gene expression by herpesvirus-coded microRNAs: Implications for latency. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5453-5458.	3.3	248
66	Efficient estimators for quantum instanton evaluation of the kinetic isotope effects: Application to the intramolecular hydrogen transfer in pentadiene. Journal of Chemical Physics, 2007, 127, 114309.	1.2	60
67	Dephasing representation of quantum fidelity for general pure and mixed states. Physical Review E, 2006, 73, 046204.	0.8	50
68	Quantum-instanton evaluation of the kinetic isotope effects. Journal of Chemical Physics, 2005, 123, 054108.	1.2	66
69	Dephasing representation: Employing the shadowing theorem to calculate quantum correlation functions. Physical Review E, 2004, 70, 055201.	0.8	53
70	Semiclassical evaluation of quantum fidelity. Physical Review E, 2003, 68, 056208.	0.8	75
71	Uniform semiclassical wave function for coherent two-dimensional electron flow. Physical Review E, 2003, 67, 016211.	0.8	17
72	Replacement manifolds:â€ƒA method to uniformize semiclassical wave functions. Physical Review E, 2001, 64, 026215.	0.8	13