Nancy Makri

List of Publications by Year in Descending Order

104 papers	5,651 citations	40 h-index	74 g-index
109 ext. papers	6,057 ext. citations	4 avg, IF	6.51 L-index

#	Paper	IF	Citations
104	Intramolecular Vibrations in Excitation Energy Transfer: Insights from Real-Time Path Integral Calculations.. *Annual Review of Physical Chemistry*, **2022**,	15.7	5
103	Synthetic Control of Exciton Dynamics in Bioinspired Cofacial Porphyrin Dimers.. *Journal of the American Chemical Society*, **2022**,	16.4	3
102	Small Matrix Quantum-Classical Path Integral.. *Journal of Physical Chemistry Letters*, **2022**, 3492-3498	6.4	0
101	Small Matrix Path Integral for Driven Dissipative Dynamics. *Journal of Physical Chemistry A*, **2021**, 125, 10500-10506	2.8	2
100	Exciton–Vibration Dynamics in J-Aggregates of a Perylene Bisimide from Real-Time Path Integral Calculations. *Journal of Physical Chemistry C*, **2021**, 125, 201-210	3.8	8
99	Origin of vibrational features in the excitation energy transfer dynamics of perylene bisimide J-aggregates. *Journal of Chemical Physics*, **2021**, 154, 114301	3.9	5
98	Small Matrix Decomposition of Feynman Path Amplitudes. *Journal of Chemical Theory and Computation*, **2021**, 17, 3825-3829	6.4	2
97	Efficient matrix factorisation of the modular path integral for extended systems. *Molecular Physics*, **2021**, 119, e1797200	1.7	9
96	Small Matrix Path Integral with Extended Memory. *Journal of Chemical Theory and Computation*, **2021**, 17, 1-6	6.4	10
95	Density matrix and purity evolution in dissipative two-level systems: I. Theory and path integral results for tunneling dynamics. *Physical Chemistry Chemical Physics*, **2021**, 23, 5113-5124	3.6	0
94	Quantum-Classical Path Integral Simulation of Excess Proton Dynamics in a Water Dimer Embedded in the Gramicidin Channel. *Journal of Chemical Theory and Computation*, **2021**, 17, 627-638	6.4	1
93	Density matrix and purity evolution in dissipative two-level systems: II. Relaxation. *Physical Chemistry Chemical Physics*, **2021**, 23, 5125-5133	3.6	1
92	Small matrix modular path integral: iterative quantum dynamics in space and time. *Physical Chemistry Chemical Physics*, **2021**, 23, 12537-12540	3.6	5
91	Electronic-vibrational density evolution in a perylene bisimide dimer: mechanistic insights into excitation energy transfer. *Physical Chemistry Chemical Physics*, **2021**, 23, 15503-15514	3.6	3
90	Quantum-classical path integral evaluation of reaction rates with a near-equilibrium flux formulation. *International Journal of Quantum Chemistry*, **2021**, 121, qua26618	2.1	0
89	Time Evolution of Bath Properties in Spin-Boson Dynamics. *Journal of Physical Chemistry B*, **2021**, 125, 8137-8151	3.4	4
88	Quantum quench and coherent-incoherent dynamics of Ising chains interacting with dissipative baths.. *Journal of Chemical Physics*, **2021**, 155, 234705	3.9	0

87	Small Matrix Path Integral for System-Bath Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 4038-4049	6.4	23
86	All-Mode Quantum-Classical Path Integral Simulation of Bacteriochlorophyll Dimer Exciton-Vibration Dynamics. *Journal of Physical Chemistry B*, **2020**, 124, 5028-5038	3.4	14
85	Recovery of Purity in Dissipative Tunneling Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 8592-8596	6.4	3
84	Small matrix disentanglement of the path integral: Overcoming the exponential tensor scaling with memory length. *Journal of Chemical Physics*, **2020**, 152, 041104	3.9	29
83	Real-Time Path Integral Simulation of Exciton-Vibration Dynamics in Light-Harvesting Bacteriochlorophyll Aggregates. *Journal of Physical Chemistry Letters*, **2020**, 11, 8783-8789	6.4	16
82	Modular path integral for finite-temperature dynamics of extended systems with intramolecular vibrations. *Journal of Chemical Physics*, **2020**, 153, 044124	3.9	11
81	Modular path integral for discrete systems with non-diagonal couplings. *Journal of Chemical Physics* , **2019**, 151, 074110	3.9	14
80	Coherent State-Based Path Integral Methodology for Computing the Wigner Phase Space Distribution. *Journal of Physical Chemistry A*, **2019**, 123, 4284-4294	2.8	7
79	Quasiclassical Correlation Functions from the Wigner Density Using the Stability Matrix. *Journal of Chemical Information and Modeling*, **2019**, 59, 2165-2174	6.1	1
78	Quantum-classical path integral with a harmonic treatment of the back-reaction. *Journal of Chemical Physics*, **2019**, 150, 184102	3.9	6
77	Real-Time Path Integral Methods, Quantum Master Equations, and Classical vs Quantum Memory. *Journal of Physical Chemistry B*, **2019**, 123, 10470-10482	3.4	7
76	Modular path integral methodology for real-time quantum dynamics. *Journal of Chemical Physics*, **2018**, 149, 214108	3.9	27
75	Wigner Distribution by Adiabatic Switching in Normal Mode or Cartesian Coordinates and Molecular Applications. *Journal of Chemical Theory and Computation*, **2018**, 14, 5446-5458	6.4	12
74	Communication: Modular path integral: Quantum dynamics via sequential necklace linking. *Journal of Chemical Physics*, **2018**, 148, 101101	3.9	27
73	Iterative blip-summed path integral for quantum dynamics in strongly dissipative environments. *Journal of Chemical Physics*, **2017**, 146, 134101	3.9	29
72	Non-equilibrium reactive flux: A unified framework for slow and fast reaction kinetics. *Journal of Chemical Physics*, **2017**, 147, 152723	3.9	7
71	Direct determination of discrete harmonic bath parameters from molecular dynamics simulations. *Journal of Computational Chemistry*, **2017**, 38, 110-115	3.5	18
70	Direct Computation of Influence Functional Coefficients from Numerical Correlation Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 4169-77	6.4	16

69	Blip-summed quantum-classical path integral with cumulative quantum memory. *Faraday Discussions*, **2016**, 195, 81-92	3.6	12
68	Iterative quantum-classical path integral with dynamically consistent state hopping. *Journal of Chemical Physics*, **2016**, 144, 044108	3.9	31
67	On iterative path integral calculations for a system interacting with a shifted dissipative bath. *Journal of Chemical Physics*, **2015**, 143, 074112	3.9	11
66	Quantum-classical path integral: A rigorous approach to condensed phase dynamics. *International Journal of Quantum Chemistry*, **2015**, 115, 1209-1214	2.1	54
65	Wigner phase space distribution via classical adiabatic switching. *Journal of Chemical Physics*, **2015**, 143, 114114	3.9	17
64	Quantum-Classical Path Integral Simulation of Ferrocene-Ferrocenium Charge Transfer in Liquid Hexane. *Journal of Physical Chemistry Letters*, **2015**, 6, 4959-65	6.4	41
63	Exploiting classical decoherence in dissipative quantum dynamics: Memory, phonon emission, and the blip sum. *Chemical Physics Letters*, **2014**, 593, 93-103	2.5	32
62	Blip decomposition of the path integral: exponential acceleration of real-time calculations on quantum dissipative systems. *Journal of Chemical Physics*, **2014**, 141, 134117	3.9	40
61	Quantum-classical path integral with self-consistent solvent-driven reference propagators. *Journal of Physical Chemistry B*, **2013**, 117, 13357-66	3.4	25
60	Quantum-classical path integral. I. Classical memory and weak quantum nonlocality. *Journal of Chemical Physics*, **2012**, 137, 22A552	3.9	48
59	Quantum-classical path integral. II. Numerical methodology. *Journal of Chemical Physics*, **2012**, 137, 22A553	3.9	45
58	Path integral renormalization for quantum dissipative dynamics with multiple timescales. *Molecular Physics*, **2012**, 110, 1001-1007	1.7	21
57	Memory propagator matrix for long-time dissipative charge transfer dynamics. *Molecular Physics*, **2012**, 110, 1967-1975	1.7	36
56	Forward-backward semiclassical and quantum trajectory methods for time correlation functions. *Physical Chemistry Chemical Physics*, **2011**, 13, 14442-52	3.6	20
55	Information-Guided Noise Reduction in Forward-Backward Semiclassical Dynamics. *Journal of Chemical Theory and Computation*, **2011**, 7, 4-9	6.4	1
54	Multitime response functions and nonlinear spectra for model quantum dissipative systems. *Journal of Chemical Physics*, **2010**, 132, 134506	3.9	19
53	Low-temperature correlation functions via forward–backward quantum dynamics. *Chemical Physics*, **2010**, 370, 15-19	2.3	5
52	Forward–backward semiclassical dynamics with single-bead coherent state density. *Molecular Physics*, **2008**, 106, 443-453	1.7	12

51	Forward--backward semiclassical dynamics with information-guided noise reduction for a molecule in solution. *Journal of Physical Chemistry A*, **2007**, 111, 11320-7	2.8	16
50	Symmetries and detailed balance in forward–backward semiclassical dynamics. *Chemical Physics*, **2006**, 322, 23-29	2.3	25
49	Simulation of dynamical properties of normal and superfluid helium. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 4230-4	11.5	56
48	Quantum stochastic resonance in the strong-field limit. *Physical Review A*, **2004**, 70,	2.6	14
47	FORWARD-BACKWARD SEMICLASSICAL SIMULATION OF DYNAMICAL PROCESSES IN LIQUIDS. *Journal of Theoretical and Computational Chemistry*, **2004**, 03, 391-417	1.8	35
46	Information guided noise reduction for Monte Carlo integration of oscillatory functions. *Chemical Physics Letters*, **2004**, 400, 446-452	2.5	15
45	Phase Space Features and Statistical Aspects of Forward–Backward Semiclassical Dynamics. *Journal of Physical Chemistry B*, **2004**, 108, 6816-6825	3.4	38
44	Bohmian versus semiclassical description of interference phenomena. *Journal of Chemical Physics*, **2003**, 119, 60-67	3.9	32
43	Forward–Backward semiclassical dynamics for quantum fluids using pair propagators: Application to liquid para-hydrogen. *Journal of Chemical Physics*, **2003**, 119, 8592-8605	3.9	90
42	Forward–Backward semiclassical dynamics for condensed phase time correlation functions. *Journal of Chemical Physics*, **2003**, 119, 1634-1642	3.9	65
41	Iterative path integral formulation of equilibrium correlation functions for quantum dissipative systems. *Journal of Chemical Physics*, **2002**, 116, 507-514	3.9	53
40	Monte Carlo Evaluation of Forward–Backward Semiclassical Correlation Functions with a Quantized Coherent State Density. *Journal of Physical Chemistry B*, **2002**, 106, 8390-8398	3.4	35
39	Coherent state semiclassical initial value representation for the Boltzmann operator in thermal correlation functions. *Journal of Chemical Physics*, **2002**, 116, 9207-9212	3.9	51
38	Iterative path integral calculation of quantum correlation functions for dissipative systems. *Chemical Physics*, **2001**, 268, 1-10	2.3	41
37	Finite Temperature Correlation Functions via Forward–Backward Semiclassical Dynamics *Journal of Physical Chemistry A*, **2001**, 105, 2851-2857	2.8	43
36	Iterative evaluation of the path integral for a system coupled to an anharmonic bath. *Journal of Chemical Physics*, **1999**, 111, 6164-6167	3.9	50
35	Dissipative tunneling in a bath of two-level systems. *Physical Review B*, **1999**, 60, 972-978	3.3	34
34	The Linear Response Approximation and Its Lowest Order Corrections: An Influence Functional Approach. *Journal of Physical Chemistry B*, **1999**, 103, 2823-2829	3.4	157

33	Time-dependent quantum methods for large systems. *Annual Review of Physical Chemistry*, **1999**, 50, 167-91	15.7	199
32	Short-Range Coherence in the Energy Transfer of Photosynthetic Light-Harvesting Systems. *Journal of Physical Chemistry A*, **1999**, 103, 9417-9422	2.8	46
31	Influence functionals with semiclassical propagators in combined forwardBackward time. *Journal of Chemical Physics*, **1999**, 110, 1343-1353	3.9	158
30	ForwardBackward Semiclassical Dynamics with Linear Scaling. *Journal of Physical Chemistry A*, **1999**, 103, 9479-9486	2.8	92
29	ForwardBackward Semiclassical Dynamics without Prefactors. *Journal of Physical Chemistry A*, **1999**, 103, 7753-7756	2.8	135
28	Semiclassical influence functionals for quantum systems in anharmonic environments1Presented at the American Physical Society Meeting in Los Angeles, California, USA, March 19, 1998.1. *Chemical Physics Letters*, **1998**, 291, 101-109	2.5	172
27	Quantum Dissipative Dynamics: A Numerically Exact Methodology. *Journal of Physical Chemistry A*, **1998**, 102, 4414-4427	2.8	129
26	Dynamics of reduced density matrices: Classical memory versus quantum nonlocality. *Journal of Chemical Physics*, **1998**, 109, 2994-2998	3.9	20
25	Effects of periodic driving on asymmetric two-level systems coupled to dissipative environments. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1998**, 31, 209-226	1.3	16
24	Path integral study of hydrogen and deuterium diffusion in crystalline silicon. *Journal of Chemical Physics*, **1998**, 108, 6819-6828	3.9	19
23	Universal delocalization rate in driven dissipative two-level systems at high temperature. *Physical Review E*, **1997**, 55, 2475-2478	2.4	16
22	Stabilization of localized states in dissipative tunneling systems interacting with monochromatic fields. *Journal of Chemical Physics*, **1997**, 106, 2286-2297	3.9	37
21	Filtered propagator functional for iterative dynamics of quantum dissipative systems. *Computer Physics Communications*, **1997**, 99, 335-354	4.2	87
20	Tensor propagator with weight-selected paths for quantum dissipative dynamics with long-memory kernels. *Chemical Physics Letters*, **1996**, 249, 224-230	2.5	59
19	Tensor propagator for iterative quantum time evolution of reduced density matrices. I. Theory. *Journal of Chemical Physics*, **1995**, 102, 4600-4610	3.9	410
18	Tensor propagator for iterative quantum time evolution of reduced density matrices. II. Numerical methodology. *Journal of Chemical Physics*, **1995**, 102, 4611-4618	3.9	329
17	Control of dissipative tunneling dynamics by continuous wave electromagnetic fields: Localization and large-amplitude coherent motion. *Physical Review E*, **1995**, 52, 5863-5872	2.4	51
16	Time-dependent discrete variable representations for quantum wave packet propagation. *Journal of Chemical Physics*, **1995**, 102, 5616-5625	3.9	42

15	Numerical path integral techniques for long time dynamics of quantum dissipative systems. *Journal of Mathematical Physics*, **1995**, 36, 2430-2457	1.2	254
14	Stochastic resonance and nonlinear response in double-quantum-well structures. *Physical Review B*, **1995**, 52, R2257-R2260	3.3	51
13	Real time path integral methods for a system coupled to an anharmonic bath. *Journal of Chemical Physics*, **1994**, 101, 6708-6716	3.9	37
12	Path integrals for dissipative systems by tensor multiplication. Condensed phase quantum dynamics for arbitrarily long time. *Chemical Physics Letters*, **1994**, 221, 482-491	2.5	242
11	Quantum rates for a double well coupled to a dissipative bath: Accurate path integral results and comparison with approximate theories. *Journal of Chemical Physics*, **1994**, 101, 7500-7519	3.9	253
10	On smooth Feynman propagators for real time path integrals. *The Journal of Physical Chemistry*, **1993**, 97, 2417-2424		38
9	System-specific discrete variable representations for path integral calculations with quasi-adiabatic propagators. *Chemical Physics Letters*, **1993**, 210, 448-457	2.5	59
8	Improved Feynman propagators on a grid and non-adiabatic corrections within the path integral framework. *Chemical Physics Letters*, **1992**, 193, 435-445	2.5	139
7	Feynman path integration in quantum dynamics. *Computer Physics Communications*, **1991**, 63, 389-414	4.2	125
6	Exponential power series expansion for the quantum time evolution operator. *Journal of Chemical Physics*, **1989**, 90, 904-911	3.9	110
5	A semiclassical tunneling model for use in classical trajectory simulations. *Journal of Chemical Physics*, **1989**, 91, 4026-4036	3.9	186
4	Correct short time propagator for Feynman path integration by power series expansion in $\hbar$. *Chemical Physics Letters*, **1988**, 151, 1-8	2.5	57
3	Monte Carlo path integration for the real time propagator. *Journal of Chemical Physics*, **1988**, 89, 2170-2177	3.9	116
2	Time-dependent self-consistent field (TDSCF) approximation for a reaction coordinate coupled to a harmonic bath: Single and multiple configuration treatments. *Journal of Chemical Physics*, **1987**, 87, 5781-5787	3.9	232
1	Basis set methods for describing the quantum mechanics of a system interacting with a harmonic bath. *Journal of Chemical Physics*, **1987**, 86, 1451-1457	3.9	83